Quantum Mechanics II

33-756

Nathaniel D. Hoffman

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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

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

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

$$O[f] = 0$$

where

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t'}\frac{\mathrm{d}t'}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t'}$$

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

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

so we can conclude that $f(t+a)$ must also be a solution. Therefore, if $Ae^{\imath t}$ is a solution, so is $Ae^{\imath a}e^{\imath t}$, 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

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

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

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 $e^{\imath\lambda}|\psi\rangle$.

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: $(\mathbb{Z}, +)$ ◇

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

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

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

$$U = e^{\imath X}$$

since $U^\dagger = e^{-\imath X^\dagger} = e^{-\imath X}$, 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:

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

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

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

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

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

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

Since these are elements of a group,

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

◇

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:

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

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

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

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

For Abelian groups,

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

or

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

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:

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

We can determine this element using the commutator:

$$\left[Y^a, Y^b\right] = \imath f^{abc}Y^c \qquad \text{(Lie Algebra)}$$

The value of $\vec{\lambda}_3$ only depends on the commutator of the $\vec{\mathbf{Y}}$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:

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

By this definition,

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

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 $\vec{\mathbf{L}}$ 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 $e^{\imath\vec{\lambda}\vec{\mathbf{L}}}$ so $\vec{\mathbf{L}}$ and $\vec{\lambda}$ must have the same dimensionality.

The Lie Algebra of SO(3) is

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

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 $g_1, g_2 \in \mathrm{SU}(2)$, we should find that $g_1 g_2 = g_3 \in \mathrm{SU}(2)$:

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

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

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

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

$$\det\left(e^{\imath\vec{\lambda}\cdot\vec{\mathbf{T}}}\right) = 1$$

In general,

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

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,

$$e^{\mathrm{Tr}\ln e^{\imath\vec{\lambda}\cdot\vec{\mathbf{T}}}} = e^{\mathrm{Tr}\left[\imath\vec{\lambda}\cdot\vec{\mathbf{T}}\right]} = 1$$

so

$$\mathrm{Tr}\left[\vec{\mathbf{T}}\right] = 0$$

We now know that $\vec{\mathbf{T}}$ 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 ($Tr(T) = 0$). There are many (infinite) choices of generators. Let's choose the Pauli matrices:

$$T_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$T_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}$$

$$T_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

From this choice, we can see that $[T_a, T_b] = \imath\epsilon_{abc}T_c$, 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

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

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

$$[X_i, X_j] = \imath f_{ijk} X_k$$

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 $\hat{\mathbf{O}}$ acting on an eigenstate:

$$\hat{\mathbf{O}}\left|\psi\right\rangle = \lambda\psi$$

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

$$\hat{\mathbf{O}} \to U\hat{\mathbf{O}}U^\dagger = \hat{\mathbf{O}}$$

Recall $U^\dagger U = 1$:

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

Multiply both sides by U:

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

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

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

so we find that $U\left|\psi\right\rangle$ 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 $\vec{\mathbf{x}} \to \vec{\mathbf{x}}'$. There is an action

$$S = \int \mathrm{d}t\, L(x, \dot{x})$$

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

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

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

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

Therefore, to minimize δS, we require

$$\frac{\delta L}{\delta x} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta L}{\delta \dot{x}}$$

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\delta L}{\delta \dot{x}}\delta x\right] = 0 \qquad \text{(Noether's Theorem)}$$

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, $\vec{\mathbf{x}} \to \vec{\mathbf{x}} + \vec{\epsilon}$ so $\delta\vec{\mathbf{x}} = \vec{\epsilon}$. 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), $\frac{\delta L}{\delta \dot{x}} = \vec{\mathbf{p}}$ is conserved (momentum conservation). ◇

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

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

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

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

so

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

so

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

so

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

so the generators are anti-symmetric.

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

so

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

Our conservation law is now

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

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.

$$(\vec{\mathbf{L}}) = (L)^a_{ij}$$

Recall the Lie algebra of the rotation group:

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

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

$$\imath L^a_{ij} = \epsilon^a_{ij}$$

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

$$\imath^2\epsilon^a_{ij}\epsilon^b_{jk} - \imath^2\epsilon^b_{ij}\epsilon^a_{jk} = \imath^2\epsilon^{abc}\epsilon^b_{ik}$$

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

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

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

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

so $A = 1$:

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

◇

Lecture 4: Conserved Charge of Rotational Invariance

Wednesday, January 22, 2020

Recall Noether's theorem from the previous lecture:

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

If the action is rotationally invariant,

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

where

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

In the previous lecture, we found that

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

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

$$e^{\imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta} \to 1 + \imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta + \mathcal{O}\left(\theta^2\right)$$

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

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

If our Lagrangian has the form

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

we find that Noether's theorem gives us

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

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

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

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:

$$\imath\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle$$

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:

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

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

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

We could equivalently define

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

such that

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

where

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

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

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

so

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

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

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

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

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

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

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

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

or

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

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

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

or

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

so

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

so

$$\delta x_a = \left[(x_a(\imath L_b)/\hbar) - (\imath L_b X_a)/\hbar\right] \hat{\mathbf{n}}_b \theta$$

We define the angular momentum operator as

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

We can also write this in index notation:

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

Let's now apply this to our δx_a formula:

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

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

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

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

$$[x_a, \imath x_c p_d] = \imath[x_a, x_c]p_d + x_c \imath[x_a, p_d]$$

since

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

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

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

Finally

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

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, $H \to U^\dagger H U$. We can write this as

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

As a consequence, if $\left[H, \vec{\mathbf{X}}\right] = 0$, 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 $x \to x + \delta v t$, so

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

The action is still invariant, since

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

Total derivatives have no effect on the equations of motion, since they don't change the Euler-Lagrange equations. A symmetry which takes $L \to L + \frac{\mathrm{d}}{\mathrm{d}t} f(x, \dot{x}, t)$ 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 $\vec{\mathbf{X}}$, then $\left[H, \vec{\mathbf{X}}\right] = 0$ implies

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

so if $\vec{\mathbf{X}}\left|\lambda\right\rangle \neq \left|\lambda\right\rangle$, 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

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

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 ($L^2 = \{f(x) \mid \int |f(x)|^2 \,\mathrm{d}x < \infty\}$). In other words, we can write

$$\vec{\mathbf{L}} = \imath\vec{\mathbf{r}} \times \vec{\mathbf{p}}$$

but we can also write

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

such that

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

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

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

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

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

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

Or you could just say $\vec{\mathbf{J}}^2$ 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 $\vec{\mathbf{J}}^2$ are the total angular momentum:

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

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

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

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

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

such that

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

$$J_zJ_\pm\left|a, b\right\rangle = (b \pm \hbar)J_\pm\left|a, b\right\rangle$$

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

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

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

$$J_\pm = J_x \pm \imath J_y$$

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 $J^2 - J_z^2 = J_x^2 + J_y^2$:

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

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

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

Since $\langle\psi|OO^\dagger|\psi\rangle \geq 0$ (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 $J_+ |b_{\max}\rangle = J_- |b_{\min}\rangle = 0$.

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

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:

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

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 SU(2), whereas integer $b_{\max}$ give representations of SO(3). $d = 2$ are not "faithful" (one-to-one) representations of SO(3), but they are faithful representations of 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:

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

so

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

0.4.2 Representations of Rotation Matrices

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

We can write the general matrix elements as

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

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

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

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

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

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:

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

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

We also showed that

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

so

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

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

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

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:

$$D^{(j)}_{m'm}(\alpha, \beta, \gamma) = \langle m'| e^{-\imath\alpha J_z/\hbar} e^{-\imath\beta J_y/\hbar} e^{-\imath\gamma J_z/\hbar} |m\rangle = e^{-\imath(\alpha m' + \gamma m)} \underbrace{\langle m'| e^{-\imath\beta J_y/\hbar} |m\rangle}_{d^j_{m'm}(\beta)}$$

0.5 Orbital Angular Momentum

Let's now look at the observable $\vec{\mathbf{L}}$. We can carry some similar terms over from the discussion of $\vec{\mathbf{J}}$. 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

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

Therefore

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

The solutions to this differential equation are the spherical harmonics:

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

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

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

We can write

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

and

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

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

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

Note

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

Therefore

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

We already know the φ-dependence:

Aside

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

$$L_z Y^l_m = \hbar m Y^l_m = -\imath\hbar \frac{\partial}{\partial \varphi} Y^l_m \implies Y^l_m \sim e^{\imath m \varphi} F(\theta)$$

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

$$Y^l_0(0,0) = \sqrt{\frac{2l+1}{4\pi}}$$

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

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

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

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

Galilean Boosts

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

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

so

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

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

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

Noether's theorem tells us that

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

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

so the conserved quantity(s) are

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

so we can define

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

as the conserved constant of motion. Since $\vec{\mathbf{p}}$ is conserved, we can say that if $p_i = 0$, then $m_1 \vec{\mathbf{r}}_1 + m_2 \vec{\mathbf{r}}_2$ 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, $\vec{\mathbf{K}}$ should generate boosts.

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

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

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

Recall that the infinitesimal transformation is

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

so technically we should be computing

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

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

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

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

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

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

$$\sum_{i=1}^{2} \frac{1}{m_i\dot{\vec{\mathbf{r}}}_1^2} = \frac{1}{2}M\dot{\vec{\mathbf{r}}}_{\text{com}}^2 + \frac{1}{2}\mu\dot{\vec{\mathbf{r}}}^2$$

where

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

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

$$H = \frac{\vec{\mathbf{p}}_{\text{com}}^2}{\cancel{2M}}^{0} + \frac{\vec{\mathbf{p}}^2}{2\mu} - V(\vec{\mathbf{r}})$$

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

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

Note

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

However, $\vec{\mathbf{L}}$ does commute with the Hamiltonian, so we expect a $(2l+1)$ degeneracy for $\vec{\mathbf{L}}^2 = \hbar^2 l(l+1)$. 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.

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

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,

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

If we operate this on energy eigenstates, the $\vec{\mathbf{L}}$ 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:

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

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 $\vec{\mathbf{L}}$ ($\vec{\mathbf{A}}\cdot\vec{\mathbf{L}} = 0$). Additionally,

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

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

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

and define

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

then

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

so

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

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

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

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 $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$. There is a $2l+1$ degeneracy from each $\mathrm{SU}(2)$ 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

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

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, $\vec{\mathbf{T}}$ and $\vec{\mathbf{S}}$ and found they both have $\mathrm{SU}(2)$ symmetry, so the symmetry group is $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$. We would now expect the degeneracy to be $(2t+1)(2s+1)$, but we can show that $\vec{\mathbf{T}}^2 = \vec{\mathbf{S}}^2$ 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

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

since

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

where

$$\tilde{\vec{\mathbf{A}}} = \sqrt{\frac{-m}{2E}}\vec{\mathbf{A}}$$

$$\vec{\mathbf{A}}^2 = e^4 + \frac{2H}{m}(\vec{\mathbf{L}}^2 + \hbar^2)$$

The first equation can then be shown by expanding

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

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

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

or

$$\frac{me^4}{2E} = (4t(t+1)+1)\hbar^2$$
$$\implies E = \frac{me^4}{2\hbar^2 n^2} \qquad n^2 = (2t+1)^2$$

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

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

Using the ansatz wave function, we know that

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

Recall that

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

but

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

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:

$$HR_{kl} = ER_{kl}$$

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 $\rho = \frac{r}{a_0}$

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

or

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

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 $\rho \to \infty$,

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

so

$$U \overbrace{\sim}^{\rho\to\infty} e^{-\lambda_{kl}\rho}$$

This inspired guess is a series solution:

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

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):

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

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

so

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

and

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

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

Lecture 11: The Hydrogen Atom, Continued

Friday, February 07, 2020

From last lecture, we showed that

$$\psi = \sum_{l,m} Y_{l,m} R_{k,l}$$

where

$$R_{k,l} = \frac{U_{k,l}}{r}$$

We then rescaled our units to $\rho = \frac{r}{a_0}$:

$$U_{k,l} = e^{-\lambda_{k,l}\rho} y_{k,l}$$

where

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

We then defined $\hat{k} + l = \frac{1}{\lambda_{k,l}} = n$ and showed that $\hat{k} > 0$ and is finite. Finally, we will define

$$y_{n=1} = C_0 \rho$$

such that

$$R_{n=1} = \frac{C_0 e^{-\frac{r}{a_0}}}{a_0}$$

This enumerates all the degeneracies of state. However, we have also ignored spin, so each of these states will have an additional degenerate state. We've also ignored spin-orbit and spin-spin coupling. In chemistry, we typically label states by $n = 1, 2, 3, \cdots$ and $l = 0, 1, 2, \cdots = s, p, d, f, \cdots$. Linear superpositions of degenerate states are eigenstates of the Hamiltonian, so we can form hybrid orbitals by combining different degenerate states. Remember that there is the additional degeneracy from the spherical harmonics, so for $n = 2$ (for example), $l = 0$ has one degenerate state while $l = 1$ has three from the spherical harmonic degeneracies in $m = -1, 0, +1$.

Now that we know the hydrogen atom at this basic level, we can talk about the effects of perturbations to see what happens when we do consider certain interactions like spin-spin coupling.

0.8 Time Independent Perturbation Theory

$$H = H_0 + \lambda H_I$$

where H_I has no *explicit* time dependence and $\lambda << 1$. Suppose that

$$H_0 \left|\phi_0^{(n)}\right\rangle = E_0^{(n)} \left|\phi_0^{(n)}\right\rangle$$

We would like to be able to solve for

$$(H_0 + \lambda H_I) \left|\phi^{(n)}\right\rangle = E^{(n)} \left|\phi^{(n)}\right\rangle$$

In practice, this is difficult and typically impossible. Instead of solving this exactly, we will expand the wave function as

$$\left|\phi^{(n)}\right\rangle = \left[\left|\phi_0^{(n)}\right\rangle + \sum_{k \neq n} C_k^{(n)} \left|\phi_0^{(k)}\right\rangle\right] N(\lambda)$$

As long as H_0 is a self-adjoint operator, any function that is square-integrable can be decomposed into an infinite series of its eigenvectors. The goal is now to try to solve for the $C_k^{(n)}$ factors:

$$C_k^{(n)} = \lambda C_k^{(n)[1]} + \lambda^2 C_k^{(n)[2]} + \cdots$$

and

$$E^{(n)} = E_0^{(n)} + \lambda E_1^{(n)} + \cdots$$

so that

$$(H_0 + \lambda H_I)\left[\left|\phi_0^{(n)}\right\rangle + \lambda C_k^{(n)[1]} \left|\varphi_0^{(k)}\right\rangle\right] = (E_0^{(n)} + \lambda E_1^{(n)})\left[\left|\phi_0^{(n)}\right\rangle + \lambda C_k^{(n)[1]} \left|\varphi_0^{(k)}\right\rangle\right] + \mathcal{O}(\lambda^2)$$

Finally, we match powers of λ on both sides of the equation:

$$\lambda^0 \to H_0 \left|\phi_0^{(n)}\right\rangle = E_0^{(n)} \left|\phi_0^{(n)}\right\rangle$$
$$\lambda^1 \to H_0 C_k^{(n)[1]} \left|\phi_0^{(k)}\right\rangle + H_I \left|\phi_0^{(n)}\right\rangle = E_1^{(n)} \left|\phi_0^{(n)}\right\rangle + E_0^{(n)} C_k^{(n)[1]} \left|\phi_0^{(k)}\right\rangle$$

Let's take this second equation and project onto the ground state $\left\langle\phi_0^{(n)}\right|$ and use the fact that $n \neq k \implies \left\langle\phi_0^{(n)}\middle|\phi_0^{(k)}\right\rangle = 0$. We are left with

$$\left\langle\phi_0^{(n)}\right| H_I \left|\phi_0^{(n)}\right\rangle = \left\langle\phi_0^{(n)}\right| E_1^{(n)} \left|\phi_0^{(n)}\right\rangle$$

So we find that, to first order,

$$E_1^{(n)} = \left\langle\phi_0^{(n)}\right| H_I \left|\phi_0^{(n)}\right\rangle = \Delta E^{(n)} \text{ at } \mathcal{O}(\lambda)$$

Let's now project onto another $\left\langle\phi_0^{(m)}\right|$ where $m \neq n$:

$$E_0^{(k)} C_k^{(n)[1]} \overbrace{\left\langle\phi_0^{(m)}\middle|\phi_0^{(k)}\right\rangle}^{\delta_{mk}} + \left\langle\phi_0^{(m)}\right| H_I \left|\phi_0^{(n)}\right\rangle = E_0^{(n)} C_k^{(n)[1]} \overbrace{\left\langle\phi_0^{(m)}\middle|\phi_0^{(k)}\right\rangle}^{\delta_{mk}}$$

so

$$E_0^{(m)} C_m^{(n)[1]} + \left\langle\phi_0^{(m)}\right| H_I \left|\phi_0^{(n)}\right\rangle = E_0^{(n)} C_m^{(n)[1]}$$

We now solve for the coefficient:

$$C_m^{(n)[1]} = \frac{\left\langle\phi_0^{(m)}\right| H_I \left|\phi_0^{(n)}\right\rangle}{E_0^{(n)} - E_0^{(m)}}$$

We can now write down the leading-order correction to the wave function:

$$\left|\phi^{(n)}\right\rangle = \left[\left|\phi_0^{(n)}\right\rangle + \sum_{n\neq m} \frac{\left\langle\phi_0^{(m)}\right| H_I \left|\phi_0^{(n)}\right\rangle}{E_0^{(n)} - E_0^{(m)}} \left|\phi_0^{(m)}\right\rangle\right] N(\lambda)$$

Lecture 12: Time-Independent Perturbation Theory

Monday, February 10, 2020

Last time, we found that, for

$$H = H_0 + \lambda H_I$$
$$\Delta E_n = \left\langle\phi_n^{(0)}\middle| H_I \middle|\phi_n^{(0)}\right\rangle$$

and

$$\Delta \left|\phi_n\right\rangle == \sum_{m\neq n} \frac{\left\langle\phi_m^{(0)}\middle| H_I \middle|\phi_n^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}} \left|\phi_m^{(0)}\right\rangle$$

Notice that we have switched the conventional indices from last lecture. Just use this from now on. The upper (0) means these are the unperturbed things.

What happens to this last equation if we have a degeneracy? Diagonalize the Hamiltonian such that

$$\langle m|H_I|n\rangle \propto \delta_{nm}$$

Let's say that $H_I = \bar{p} \cdot \vec{\mathbf{E}}$ where $\bar{p}$ is the dipole moment, which is the leading-order energy term for a hydrogen atom. If we put the electric field along the z-direction, the dipole moment will be $\bar{p} = -ez$ so

$$H_I = -ezE$$

Consider $n = 1$:

$$\Delta E_{n=1} = \langle 1,0,0|-ez|1,0,0\rangle\, E$$

$$\langle 0,0|z|0,0\rangle = 0 \quad \text{since}$$
$$\pi^{-1} z \pi = -z \quad \text{and} \quad \pi\,|0,0\rangle = \pm\,|0,0\rangle$$
$$\langle 0,0|\pi\pi^{-1} z \pi\pi^{-1}|0,0\rangle = (\pm)\,\langle 0,0|-z|0,0\rangle\,(\pm) = -\,\langle 0,0|z|0,0\rangle = 0$$

where π is the parity operator.

For the higher states, we will use the fact that

$$\pi\,|l,m\rangle = (-1)^l\,|l,m\rangle$$

For $n = 2$, $l = 0, 1$, so

$$\Delta\,|\phi_{n=2}\rangle = \sum_{m,n} \frac{\langle m|z|n\rangle}{E_n - E_m} Ee\,|m\rangle$$

Now there are four degenerate states, $\{|0,0\rangle, |1,-1\rangle, |1,0\rangle, |1,+1\rangle\}$. We will now try to diagonalize the system in terms of these states. First,

$$\langle l,m|z|l'm'\rangle \propto \delta_{mm'}$$

$[L_z, z] = 0$ so $\langle lm|[L_z,z]|l'm'\rangle = 0$, so

$$0 = \langle lm|L_z z|l'm'\rangle - \langle lm|zL_z|l'm'\rangle = (m-m')\hbar\,[\,\langle lm|z|l'm'\rangle]$$

so $\Delta m = 0$ for $H_I \sim z$. Also, $\Delta l \neq 0$ since if the l's are the same, the states are orthogonal.

$l'm' \to$	(0,0)	(1,-1)	(1,0)	(1,1)
(0,0)	0	0	λ	0
(1,-1)	0	0	0	0
(1,0)	λ	0	0	0
(1,1)	0	0	0	0

We claim $\langle lm|z|l'm'\rangle = \langle l'm'|z|lm\rangle$ because the operators are all Hermitian. Now we need to diagonalize this. First we will change the order of the basis a bit:

$l'm' \to$	(0,0)	(1,0)	(1,1)	(1,-1)
(0,0)	0	λ	0	0
(1,0)	λ	0	0	0
(1,1)	0	0	0	0
(1,-1)	0	0	0	0

Let's now define $\xi_1 = \frac{1}{\sqrt{2}}\,[|0,0\rangle + |1,0\rangle]$ and $\xi_2 = \frac{1}{\sqrt{2}}\,[|0,0\rangle - |1,0\rangle]$, which are the eigenvectors of this matrix. Therefore, we can define a new basis $\{\xi_1, \xi_2, |1,1\rangle, |1,-1\rangle\}$ where

$$z = \begin{pmatrix} \hat{\lambda} & & & \\ & -\hat{\lambda} & & \\ & & 0 & \\ & & & 0 \end{pmatrix}$$

Referring back to our original equation for the perturbed energy, we can now see that these new states, ξ_1 and ξ_2 are not degenerate to $|1,1\rangle$ and $|1,-1\rangle$, but in fact have $\Delta E = \pm_{1,2}\hat{\lambda} = \pm 3a_0 E$ (the last equality requires the full calculation of the matrix element).

0.9 Selection Rules

For an operator O, what values of n, l, and m give

$$\langle nlm|O|n'l'm'\rangle \neq 0?$$

For example, in the case of $O = z$, we just showed that $\Delta m = 0$ using the fact that $[L_z, z] = 0$. For Δl, we need to use the fact that

$$\left[L^2, \left[L^2, z\right]\right] = 2\hbar^2\left\{z, L^2\right\}$$

Taking the matrix elements of both sides, we get a relationship between l and l'. The right-hand side gives us:

$$\langle nlm|2\hbar^2\left\{z, L^2\right\}|n'l'm'\rangle = (2\hbar^2)\hbar^2\left[(l'\,|l'+1\rangle) + (l\,|l+1\rangle)\right]\langle nlm|z|n'l'm'\rangle$$

The left-hand side gives

$$\begin{aligned}\langle nlm|L^2(L^2z - zL^2) - (L^2z - zL^2)L^2|n'l'm'\rangle = \hbar^2\langle nlm|z|n'l'm'\rangle\,[&(l(l+1))^2 \\ &- l(l+1)l'(l'+1) \\ &- l(l+1)l'(l'+1) \\ &+ (l'(l'+1))^2]\end{aligned}$$

These sides must be equal, so we can cancel the matrix elements and equate

$$(l+l')(l+l'+1)((l-l')^2 - 1) = 0$$

The possible solutions are $(l - l') = \pm 1$. We could also have $l = l' = 0$, but we previously ruled this out by using a parity argument. Therefore, $\Delta l = \pm 1$.

Lecture 13: Perturbations of the Hydrogen Atom
Wednesday, February 12, 2020

0.10 Fine Structure of Hydrogen

0.10.1 Relativistic Correction

Let's call our expansion parameter $\lambda \equiv \frac{v}{c}$, the scaled velocity of the electron in an orbit. Recall that the virial theorem tells us that $KE \sim PE$, so $m_e v^2 \sim \frac{e^2}{r} \sim \frac{e^2}{a_0} = \frac{e^4 m_e}{\hbar^2}$. Dividing both sides by c^2, we find that

$$\frac{v^2}{c^2} \sim \frac{e^4}{\hbar c^2} \sim \alpha^2$$

where $\alpha \approx \frac{1}{137}$ is defined as the fine structure constant.

The Schrödinger equation was not built to do relativistic corrections (we need the Dirac equation for this), but we can use it to get a handle on sources of relativistic corrections. We know the relativistic energy that we should see from a free particle:

$$E^2 = \vec{\mathbf{p}}^2c^2 + m^2c^4 = mc^2\left[1 + \frac{\vec{\mathbf{p}}^2}{2m^2c^2} + \frac{\vec{\mathbf{p}}^4}{8m^4c^4}\right]$$

The first term is proportional to the free-particle Hamiltonian, but the next relativistic correction will be

$$H_I = \frac{\vec{\mathbf{p}}^4}{8m_e^3c^2} \sim \frac{v^4}{c^4} \sim \alpha^4$$

Recall that $E_0 \sim mc^2\alpha^2$ so

$$\frac{H_I}{E_0} \sim \alpha^2$$

There are two more corrections at this order.

0.10.2 Spin-Orbit Interaction

If we have an electron moving in the electric field of the proton, we also need to include the effect of a magnetic field that the electron sees because it is moving quickly through this field. The electron itself has spin, which is like a magnetic moment, and this interacts with this apparent magnetic field:

$$\vec{\mathbf{E}} = \frac{\vec{\mathbf{x}}}{r}\frac{\partial \Phi}{\partial r} \qquad \Phi = -\frac{e^2}{r}$$

$$\vec{\mathbf{B}} = -\frac{\vec{\mathbf{v}}}{c} \times \vec{\mathbf{E}}$$

$$H = -\frac{e\vec{\mathbf{S}}}{mc} \cdot \vec{\mathbf{B}} = -\frac{e}{mc^2}\vec{\mathbf{S}} \cdot (\vec{\mathbf{v}} \times \vec{\mathbf{x}})\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\Phi \qquad \Phi = -\frac{e^2}{r}$$

This is not really correct, because this is the magnetic field seen by a boosted inertial observer, and the electron is not moving at constant velocity (it's moving around the proton in some way, so the velocity vector must be changing). Interestingly, if you do this correctly with the Dirac equation, there's just an extra factor of 2:

$$H_I = \frac{1}{2m^2c^2}\vec{\mathbf{S}} \cdot \vec{\mathbf{L}}\frac{e^2}{r^3}$$

0.10.3 Darwin Term

Due to fluctuations (Compton wavelength) the electron itself isn't a point in space. If you try to probe an electron at smaller distances than this wavelength, you will necessarily create other electrons through pair production. The Compton wavelength of the electron goes like $\lambda_C = \frac{\hbar c}{m} \sim \frac{100\text{MeV} \cdot \text{Fermi}}{0.5\text{MeV}}$. We won't take up class time writing down the derivation of this correction:

$$H_D = \frac{\pi e^2 \hbar^2}{2m_e^2 c^2}\delta^{(3)}(\vec{\mathbf{r}})$$

0.10.4 Calculating the Spin-Orbit Contribution

Typically the wave function is divided into a spatial and a spin space:

$$|\psi\rangle = |\psi_s\rangle \otimes |\chi\rangle$$

and we want to find $E_1 = \langle H_I \rangle$. We can write this as

$$\left\langle \frac{1}{r^3}\vec{\mathbf{L}} \cdot \vec{\mathbf{S}} \right\rangle = \langle \psi_s | \frac{L_a}{r^3} | \psi_s \rangle \ \langle \chi | S_a | \chi \rangle$$

Note that we can write

$$\vec{\mathbf{S}} \cdot \vec{\mathbf{L}} = \frac{1}{2}(\vec{\mathbf{S}} + \vec{\mathbf{L}})^2 - \frac{\vec{\mathbf{S}}^2}{2} - \frac{\vec{\mathbf{L}}^2}{2} = \frac{1}{2}\left[\vec{\mathbf{J}}^2 - \vec{\mathbf{S}}^2 - \vec{\mathbf{L}}^2\right]$$

We would like to work in a basis which diagonalizes $\vec{\mathbf{J}}$, the total angular momentum. How do we add angular momentum? Before we go into the theory, let's just do an example. The simplest example possible is adding two spin-$\frac{1}{2}$ particles.

Example. Suppose we have a wave function of two particles:

$$|\chi\rangle = |\chi_1\rangle \otimes |\chi_2\rangle$$

What is the total spin? We always have a choice of basis, so we want to take all the operators which commute and diagonalize them. We have two choices of mutually commuting operators. We know that $\left[\vec{\mathbf{S}}_1, \vec{\mathbf{S}}_2\right] = 0$, so we can choose the set

$$\{\vec{\mathbf{S}}_1^2, S_{1z}, \vec{\mathbf{S}}_2^2, S_{2z}\}$$

However, we really want to diagonalize $(\vec{\mathbf{S}}_1+\vec{\mathbf{S}}_2)^2$. $\vec{\mathbf{S}}_{1,2}^2$ are the Casimir operators so they commute with everything, and it turns out the final set of commuting observables is

$$\{(\vec{\mathbf{S}}_1+\vec{\mathbf{S}}_2)^2, \vec{\mathbf{S}}_1^2, \vec{\mathbf{S}}_2^2, (S_{1z}+S_{2z})=S_z^T\}$$

There are four possible states in our Hilbert space: $\{|++\rangle, |--\rangle, |+-\rangle, |-+\rangle\}$ (where $|\pm\rangle$ corresponds to $S_z=\pm\frac{\hbar}{2}$). We want to transform into the second basis. For the first two states, have $S_z^T\{|++\rangle, |--\rangle\}\to\{\hbar,-\hbar\}$. We know that the states go from $-l$ to l, and the largest l we could have is $\frac{1}{2}+\frac{1}{2}=1$, so we assign $|++\rangle$ with $S_z^T\sim 1$ as the highest state. Next, we get the other states using raising and lowering operators:

$$S_{T_-}=S_{1_-}+S_{2_-}=(S_{1x}-\imath S_{1y})+(S_{2x}-\imath S_{2y})$$

Recall that in general, these ladder operators act on the system as

$$J_\pm|jm\rangle=\sqrt{(j\mp m)(j\pm m+1)}\hbar\,|j,m\pm 1\rangle$$

Let's get the next state down in the ladder:

$$S_{T_-}|++\rangle=(S_{1_-}+S_{2_-})|++\rangle$$

$$S_{1_-}|+\rangle=\left[\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)\right]^{\frac{1}{2}}\hbar\,|-\rangle=\hbar\,|-\rangle$$

and similarly with S_{2_-}. We therefore find that

$$S_{T_-}|++\rangle=\hbar\,[|+-\rangle+|-+\rangle]$$

If the $|++\rangle$ state is $|1,1\rangle$, the next lowest state will be $|1,0\rangle$, so

$$|1,0\rangle=\frac{1}{\sqrt{2}}\,[|+-\rangle+|-+\rangle]$$

$\diamond$

Lecture 14: Addition of Angular Momentum, Continued

Friday, February 14, 2020

Recall our original motivation:

$$\vec{\mathbf{L}}\cdot\vec{\mathbf{S}}=\frac{1}{2}\left(\vec{\mathbf{J}}^2-\vec{\mathbf{L}}^2-\vec{\mathbf{S}}^2\right)$$

We decided to start with the simplest example, which is to just add two spins (rather than spin and angular momentum). We start by trying to figure out the maximum total spin, which for two spin-$\frac{1}{2}$ particles is $\pm\left(\frac{1}{2}+\frac{1}{2}\right)=\pm 1$. We are starting in the basis of $\vec{\mathbf{S}}_1^2, \vec{\mathbf{S}}_2^2, S_{1z}, S_{2z}$ and trying to get into the basis $\vec{\mathbf{S}}_{\text{tot}}^2=\vec{\mathbf{S}}^2, \vec{\mathbf{S}}_1^2, \vec{\mathbf{S}}_2^2, S_{1z}+S_{2z}=S_z$. We decided that the maximum spin is

$$(S^2)=\hbar^2 1(1+1)$$

such that the highest state in this basis is $|1,1\rangle$:

$$|1,1\rangle=|++\rangle$$

We then use the lowing operators to get the other states. Just to be clear, in the original basis, we don't really care about $\vec{\mathbf{S}}_{1,2}^2$ because it's the same for all basis elements. We label our basis by $|S_{1z},S_{2z}\rangle=|\pm,\pm\rangle$. In the addition state, we are representing our states by $|S,S_z\rangle$.

We then showed that the lowering operator $S_-=(S_{1_-}+S_{2_-})$ acting on the $|1,1\rangle$ state gives us

$$|1,0\rangle=\frac{1}{\sqrt{2}}\,[|+-\rangle+|-+\rangle]$$

Now let's act on this state with the lowering operator on the $|1,0\rangle$ state:

$$S_- |S, S_z\rangle = \hbar\sqrt{(S+S_z)(S-S_z+1)}\,|S, S_z-1\rangle$$

$$S_- |1,0\rangle = (S_{1-} + S_{2-})\frac{1}{\sqrt{2}}\left[|+-\rangle + |-+\rangle\right]$$

$$\sqrt{1+1}\,|1,-1\rangle = \frac{1}{\sqrt{2}}\left[|--\rangle + |--\rangle\right]$$

so

$$|1,-1\rangle = |--\rangle$$

We know there must be one more state, since there are four states in the original basis. We know that this state should be labeled $|0,0\rangle$, and we can find it by ensuring it's orthogonal to all of the other states. The total spin must be 0, so

$$|0,0\rangle = a\,|+-\rangle + b\,|-+\rangle$$

since these are the only states with zero total spin.

$$\langle 0,0|1,0\rangle = 0 \implies a = -b$$

so

$$|0,0\rangle = N\left[|+-\rangle - |-+\rangle\right]$$

and by convention,

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left[|+-\rangle - |-+\rangle\right]$$

Now we have our four states in two different bases. The groupings of these states form irreducible representations. The original basis is reducible, since a general rotation will mix all four states. However, a rotation cannot change the total angular momentum, so there is one three-dimensional irreducible representation comprised of the states $|1,1\rangle, |1,0\rangle, |1,-1\rangle$ but the state $|0,0\rangle$ is invariant under rotations and forms a one-dimensional irreducible representation:

$$e^{\imath\vec{\mathbf{S}}\cdot\hat{\mathbf{n}}\theta}\,|0,0\rangle = |0,0\rangle$$

This state is called the "singlet" state and the other three are called the "triplet" states for obvious reasons. In this basis, every rotation matrix will look like

$$\begin{pmatrix} A_{3\times3} & \\ & B_{1\times1} \end{pmatrix}$$

Mathematically, we write this relationship as

$$\frac{1}{2}\otimes\frac{1}{2} = 1\oplus 0$$

The tensor product part means that

$$R(\theta)[\chi_i\chi_j] = (R(\theta)\chi_i)(R(\theta)\chi_j)$$

The action on a tensor sum acts like the block-diagonal operator in a different basis. Let's now consider a more general case. Suppose we want to add a general $\vec{\mathbf{J}}_1$ and $\vec{\mathbf{J}}_2$. We would expect that

$$J_{\max} = J_1 + J_2 \qquad J_{\min} = J_1 - J_2$$

and we have two different bases:

$$\vec{\mathbf{J}}_1^2, J_{1z}, \vec{\mathbf{J}}_2^2, J_{2z} \qquad ((a))$$

and

$$\vec{\mathbf{J}}^2, \vec{\mathbf{J}}_1^2, \vec{\mathbf{J}}_2^2, J_z \tag{(b)}$$

We want to find coefficients C_{J,J_z} such that

$$|J_1, J_2, J_{1z}, J_{2z}\rangle = \sum_{J,J_z} C_{J,J_z} |J, J_z, J_1, J_2\rangle$$

or equivalently

$$|J, J_z, J_1, J_2\rangle = \sum_{J_{1z},J_{2z}} C_{J_{1z},J_{2z}} |J_1, J_2, J_{1z}, J_{2z}\rangle$$

In Sakurai's notation, we use $M \equiv J_z$ and $m_{1,2} \equiv J_{(1,2)z}$. The coefficients C_{m_1,m_2} are known as the Clebsch-Gordon coefficients. In general,

$$|J, M; J_1, J_2\rangle = \sum_{m_1,m_2} |J_1, J_2, m_1, m_2\rangle \langle J_1, J_2, m_1, m_2|J, M; J_1, J_2\rangle$$

so

$$C_{m_1,m_2} = \langle J_1, J_2; m_1, m_2|J, M, J_1, J_2\rangle \equiv \langle m_1, m_2|J, M\rangle$$

In our group-theory notation,

$$J_1 \otimes J_2 = (J_1 + J_2) \oplus (J_1 + J_2 - 1) \oplus \cdots \oplus (J_1 - J_2)$$

The total number of states should be equal on both sides. On the left-hand side, we have $J_1 \otimes J_2$, and in J_1 there are $2J_1 + 1$ states (same for J_2) so there are $(2J_1 + 1)(2J_2 + 1)$ total states. On the right-hand side, we have $\sum_{J=J_{\min}}^{J_{\max}}(2J + 1)$ or

$$\sum_{J=J_1-J_2}^{J_1+J_2} (2J + 1) = \sum_{J=0}^{J_1+J_2} (2J + 1) - \sum_{J=0}^{J_1-J_2} (2J + 1)$$

In general, a sum

$$\sum_{n=0}^{a} n = \frac{1}{2}a(a + 1)$$

Using (Gauss') result, we have

$$2\left[\frac{1}{2}(J_1 + J_2)(J_1 + J_2 + 1)\right] + (J_1 + J_2 + 1) - \left[2\left[\frac{1}{2}(J_1 - J_2)(J_1 - J_2 + 1)\right] + (J_1 - J_2 + 1)\right] = (2J_1 + 1)(2J_2 + 1)$$

which agrees with the first result.

From our previous example with spin, we know that

$$|0, 0\rangle = \frac{1}{\sqrt{2}} [|+-\rangle - |-+\rangle]$$

so

$$C_{\frac{1}{2},-\frac{1}{2}} = \frac{1}{\sqrt{2}}$$

and

$$C_{-\frac{1}{2},\frac{1}{2}} = -\frac{1}{\sqrt{2}}$$

Lecture 15:
Wednesday, February 19, 2020

Recall that in the spin-orbit coupling correction, we wanted to calculate $\vec{\mathbf{L}}\cdot\vec{\mathbf{S}} = \frac{1}{2}\left[\vec{\mathbf{J}}^2 - \vec{\mathbf{L}}^2 - \vec{\mathbf{S}}^2\right]$. We need to write our states in a basis in which the Hamiltonian is diagonalized, and to do this, we had a method of writing out states using Clebsch-Gordan coefficients.

Recall that

$$J_{\max} = j_1 + j_2 \qquad J_{\min} = |j_1 - j_2|$$

Let's now show why $1 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2}$. Recall the number of states is $2j+1$, so there are the same number of states on either side of this equation. To move from the basis $|j_1, j_2; m_1, m_2\rangle$ to $|J, M, j_1, j_2\rangle$, we need to use the Clebsch-Gordan coefficients:

$$|J, M; j_1, j_2\rangle = \sum_{m_1, m_2} C_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle$$

To calculate these coefficients, we start with the highest state. In this case, in our "added" space is $\left|\frac{3}{2}, \frac{3}{2}\right\rangle$ (we suppress j_1 and j_2 since it is the same on both sides of that equation). We set this equal to the highest state in the "multiplied" space:

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = \left|m_1 = 1, m_2 = \frac{1}{2}\right\rangle$$

We then use the lowering operator on both sides till we cannot go farther. We could additionally start with the lowest state $\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = \left|-1, -\frac{1}{2}\right\rangle$ and use the raising operator.

Finally, we find states with lower J using orthogonality.

0.11 Hydrogen Atom Corrections

Darwin term: $\frac{\pi^2 e^2 \hbar^2}{2m^2c^2}\delta^{(3)}(\vec{\mathbf{r}})$

Kinetic energy correction: $-\frac{\vec{\mathbf{p}}^4}{8m^3c^2}$

Spin orbit coupling: $\frac{e^2}{2m^2c^2\vec{\mathbf{r}}^3}(\vec{\mathbf{S}}\cdot\vec{\mathbf{L}}) = \frac{\hbar^2 e^2}{4m^2c^2\vec{\mathbf{r}}^3}\left[j(j+1) - l(l+1) - s(s+1)\right]$

To calculate the expected energy shifts due to each of these terms, we know that to first order, we need to find the expectation values of these terms with the unperturbed wave functions. For

These can all be derived with the Hellmann-Feynman theorem:

Theorem 0.11.1 (Hellmann-Feynman Theorem)**.**

$$\frac{\mathrm{d}E_\lambda}{\mathrm{d}\lambda} = \left\langle \frac{\mathrm{d}H_\lambda}{\mathrm{d}\lambda} \right\rangle \qquad \text{(Hellmann-Feynman Theorem)}$$

For $\left\langle \frac{1}{r} \right\rangle$, we can use $l = e$ and take derivatives of the unperturbed Hamiltonian with respect to e. For $\left\langle \frac{1}{r^2} \right\rangle$, we allow $\lambda = l$ and let l be continuous rather than discrete so that we can take the derivatives. Additionally, we have to use the fact that $n = j_{\max} + l + 1$. For $\left\langle \frac{1}{r^3} \right\rangle$ and for any further expectation values, we can use the Kramers-Pasternack recurrence relation:

$$4(q+1)\left\langle r^q \right\rangle - 4n^2(2q+1)\left\langle r^{q-1} \right\rangle + n^2 q\left[(2l+1)^2 - q^2\right]\left\langle r^{q-2} \right\rangle = 0 \quad \text{(Kramers-Pasternack Relation)}$$

For the three expectation values which we care about, we find:

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{a_0 n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{a_0^2 n^3 \left(l + \frac{1}{2}\right)}$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{2}{a_0^3 n^3 l(l+1)(2l+1)}$$

We can use these formulae to calculate some of the low-energy expectation values:

$$\left\langle \frac{1}{r} \right\rangle_{1s} = \frac{1}{a_0} \qquad \left\langle \frac{1}{r} \right\rangle_{2s} = \frac{1}{4a_0} \qquad \left\langle \frac{1}{r} \right\rangle_{2p} = \frac{1}{4a_0}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{1s} = \frac{2}{a_0^2} \qquad \left\langle \frac{1}{r^2} \right\rangle_{2s} = \frac{1}{4a_0^2} \qquad \left\langle \frac{1}{r^2} \right\rangle_{2p} = \frac{1}{12a_0^2}$$

and

$$\left\langle \frac{1}{r^3} \right\rangle_{2p} \frac{1}{24a_0^3}$$

Let's calculate the shift for the $1s$ state:

Taking the expectation of the Darwin term will give us the energy shift:

$$\Delta E_D = \frac{\pi^2 e^2 \hbar^2}{2m^2c^2} \left[\left\langle \delta^{(3)}(\vec{\mathbf{r}}) \right\rangle \right] = \frac{\pi^2 e^2 \hbar^2}{2m^2c^2} |\psi_{1s}(0)|^2 = \frac{mc^2\alpha^4}{2}$$

For the kinetic energy correction, we can write

$$-\frac{\vec{\mathbf{p}}^4}{8m^3c^2} = -\left(\frac{\vec{\mathbf{p}}^2}{2m}\right)^2 \frac{1}{2mc^2} = -\frac{1}{2mc^2}\left(H_0 + \frac{e^2}{r}\right)^2$$

so

$$\Delta E_{KE} = -\frac{1}{2mc^2}\left[E_n^2 + \frac{2e^2 E_n}{\langle r \rangle} + \frac{e^4}{\langle r^2 \rangle}\right] = -\frac{1}{2}mc^2\alpha^4\left[\frac{5}{4}\right]$$

Finally, for spin-orbit coupling, we don't actually need to use any of the work we previously did learning to add angular momenta. This is because, for the $1s$ state, $l = 0$, so $J = L + S$ must give us $j = \frac{1}{2}$ (since $s = \frac{1}{2}$). Therefore, the spin-orbit term cancels for the $1s$ state and there is no correction to the energy.

Together, the Darwin term and kinetic energy correction together give us,

$$\Delta E_{1s} = -\frac{1}{8}mc^2\alpha^4$$

Lecture 16:
Friday, February 21, 2020

In the $n = 2$ case, the $2s$ and (three) $2p$ states will split (by the Darwin and Spin-Orbit terms) into three states, labeled by total angular momentum. The $2p_{3/2}$ state moves up, $2p_{1/2}$ goes down, and $2s_{1/2}$ stays the same. By numerical coincidence, the Kinetic Energy correction will merge these two lowest states back together, but in general all three of the states will be shifted down below the original, unperturbed energy.

These three corrections define the "fine" structure. The "hyperfine" structure has to do with interactions with the proton spin (spin-spin coupling and some spin-orbit coupling from the proton). We typically write the magnetic moment of the electron as

$$\vec{\mathbf{M}}_e = \mu_e \vec{\mathbf{S}} \qquad \mu_e = \frac{q}{2m_e c}$$

In terms of units, the Coulomb potential is

$$-\frac{q^2}{4\pi\epsilon_0 r} = \frac{e^2}{r}$$

where ϵ_0 is the vacuum electric permittivity, so $q^2 = e^2(4\pi\epsilon_0)$. Interestingly,

$$\mu_p = \frac{g_p q}{2m_p} \qquad g_p = 5.6$$

This factor g_p is a result of the proton not being an elementary particle. Technically, you could also define $g_e = 2$, but in our definition we've absorbed this into one of our terms (really the ratio is the thing that matters). Typically we write

$$\vec{\mathbf{M}}_p = \mu_p \vec{\mathbf{I}}$$

so that we don't confuse the spin of the electron and the proton.

We expect to see at least two effects from this new spin. First, there should be a similar spin-orbit correction from the proton, and additionally, there should be another term from spin-spin coupling between the two particles. Without proof, we will write down the Hamiltonian of the hyperfine structure:

$$\begin{aligned} H_{\text{HF}} = &-\frac{\mu_0}{4\pi}\left[\frac{q}{m_e \vec{\mathbf{R}}^3}\vec{\mathbf{L}}\cdot\vec{\mathbf{M}}_p \right. && ((\text{a})) \\ &+\frac{1}{\vec{\mathbf{R}}^3}\left[3(\vec{\mathbf{M}}_e\cdot\hat{\mathbf{n}})(\vec{\mathbf{M}}_p\cdot\hat{\mathbf{n}}) - \vec{\mathbf{M}}_p\cdot\vec{\mathbf{M}}_e\right] && ((\text{b})) \\ &\left.+\frac{8\pi}{3}\vec{\mathbf{M}}_e\cdot\vec{\mathbf{M}}_p\delta^3(\vec{\mathbf{R}})\right] && ((\text{c})) \end{aligned}$$

The final term comes from the fact that the proton is not a point-like particle, but rather made of constituent quarks. We believe that these corrections should be on the same order as $\alpha^4\frac{m_e}{m_p}(m_e c^2)$. If we assume the radius goes like a_0, we can see that the first term of the Hamiltonian has dimensions like

$$\frac{\mu_0 q\hbar^2}{m_e a_0^3}\frac{q}{m_p}$$

where one $\hbar$ comes from the $\vec{\mathbf{L}}$ operator and the other comes from $\vec{\mathbf{M}}_p$.

$$\mu_0 q^2 \sim \frac{q^2}{\epsilon_0 c^2} \sim \frac{e^2}{c^2}$$

so

$$\sim \frac{e^2}{c^2}\frac{\hbar^2}{m_e m_p}\frac{1}{\left[\frac{\hbar^2}{m_e e^2}\right]^3} = \frac{e^9}{c^2\hbar^4}\left(\frac{m_e}{m_p}\right)m_e\frac{c^2}{c^2} = \left(\frac{e^2}{\hbar c}\right)^4\left(\frac{m_e}{m_p}\right)m_e c^2 = \alpha^4\frac{m_e}{m_p}m_e c^2$$

We could go through the same exercise with the last two terms of the Hamiltonian to find the same relative dimensionality. Let's now see how the hyperfine perturbation effects the energy levels.

First, let's look at the $1s$ state (which really has two states which are degenerate due to spin). For the (a) term, $\vec{\mathbf{L}}\cdot\vec{\mathbf{M}}_p = 0$ since $l = 0$. For the (b) term, we have $\hat{\mathbf{n}} \equiv \hat{\mathbf{r}}$, the vector between the electron and proton.

$$\Delta E_{(b)}\left\langle 1s\right|\frac{1}{r^3}\left[3\vec{\mathbf{M}}_e\cdot\hat{\mathbf{r}}\times\vec{\mathbf{M}}_p\cdot\hat{\mathbf{r}} + \vec{\mathbf{M}}_p\cdot\vec{\mathbf{M}}_e\right]\left|1s\right\rangle$$

Let's consider the spatial part:

$$\left(\int\frac{\mathrm{d}^3x}{r^3}|\psi_{1s}(\vec{\mathbf{x}})|^2\left[3\hat{\mathbf{r}}_i\hat{\mathbf{r}}_j - \delta_{ij}\right]\right)\left\langle(M_e)_i(M_p)_j\right\rangle$$

Suppose we have an integral which is some function of x dotted into the z-direction.

$$\int \mathrm{d}^3x\, f(\vec{\mathbf{x}}\cdot\vec{\mathbf{A}})x_i = \alpha A_i$$

because we need an index on both sides, and we are integrating over x so the only thing left to put an index on is A. For

$$\int \mathrm{d}^3x\, f(\vec{\mathbf{x}}\cdot\vec{\mathbf{A}})x_ix_j = \alpha\delta_{ij} + \beta A_iA_j$$

because we need both indices on both sides, and the only things we have available are A and the δ function. For three indices, this gets harder, since you can include things like the Levi-Civita symbol.

$$\int \mathrm{d}^3x\, f(\vec{\mathbf{x}}\cdot\vec{\mathbf{A}}, \vec{\mathbf{x}}\cdot\vec{\mathbf{B}})x_i = \alpha A_i + \beta B_i$$

As a final example, consider

$$\int \mathrm{d}^3x\, f(\vec{\mathbf{x}}\cdot\vec{\mathbf{A}}, \vec{\mathbf{x}}\cdot\vec{\mathbf{B}})x_ix_j = \alpha A_iB_j + \beta A_jB_i + \gamma\delta_{ij} + \rho A_iA_j + \sigma B_iB_j = \alpha[A_iB_j + A_jB_i] + \gamma\delta_{ij} + \rho A_iA_j + \sigma B_iB_j$$

The left side is symmetric under exchange of i and j, so the right hand side also must be. Symmetries have to be conserved by the equal sign. For example, If $\vec{\mathbf{A}} = -\vec{\mathbf{A}}$, the first two terms cancel.

Using this reasoning, since $\psi_{1s}(\vec{\mathbf{x}})$ is spherically symmetric,

$$\int \mathrm{d}^3x\, \frac{1}{r^3}|\psi_{1s}(\vec{\mathbf{x}})|^2\left[3\hat{\mathbf{r}}_i\hat{\mathbf{r}}_j - \delta_{ij}\right] = A\delta_{ij}$$

If we then multiply both sides by δ_{ij}, we find that this integral is 0. Therefore, for the $1s$ state, there is no contribution from the (b) term.

For the (c) term,

$$\vec{\mathbf{M}}_e\cdot\vec{\mathbf{M}}_p\delta^3(\vec{\mathbf{R}})\left(\frac{-\mu_0}{4\pi}\right)\left(\frac{8\pi}{3}\right) = -\frac{q^2\mu_0}{3m_em_p}g_p\left[\vec{\mathbf{S}}\cdot\vec{\mathbf{I}}\right]$$

This is similar to the spin-orbit case, so we want to use a diagonalized basis (a basis of total spin):

$$\left[\vec{\mathbf{S}}\cdot\vec{\mathbf{I}}\right] = \frac{1}{2}\left[\underbrace{(\vec{\mathbf{S}}+\vec{\mathbf{I}})^2}_{\vec{\mathbf{J}}^2} - \vec{\mathbf{S}}^2 - \vec{\mathbf{I}}^2\right]$$

From our analysis of addition of vector spaces, $\frac{1}{2}\otimes\frac{1}{2} = 1\oplus 0$, so for $s1$, we have

$$H_{(c)} = -\frac{\mu_0q^2g_p\hbar^2}{12m_em_p}\left[\vec{\mathbf{J}}^2 - \frac{3}{4}\times 2\right]\delta^3(\vec{\mathbf{R}})$$

where we will have $J = 1$ and $J = 0$ splitting. The difference in the splitting corresponds to the 21cm line that is frequently used in cosmology.

Lecture 17: Tensor Operators
Monday, February 24, 2020

0.12 Tensor Operators

A tensor is something which transforms like a tensor. In the same vein, it is a representation of a group. A tensor is something which has some indices, and those indices label which representation it transforms under. For example, Cartesian tensors have indices which run over the three dimensions.

$$T_{ijk\ldots}, \quad i,j,k,\cdots\in\{0,1,2\}$$

whereas a spherical tensor can be represented as

$$T_{lm}$$

This uses an irreducible representation—there are no other ls or ms in this tensor. Under the group SU(2), such a tensor transforms as

$$O_l{}^m \to U O_l{}^m U^{-1}$$

in the same way that

$$|lm\rangle \to U\,|lm\rangle$$

$$O^s{}_l\,|l',m\rangle$$

transforms under the action of $l \otimes l'$:

$$O^s{}_l\,|l'm\rangle \to \left[UO^s{}_l U^{-1}\right]\left[U\,|l'm\rangle\right]$$

We can write this in terms of Wigner rotation matrices:

$$O^s{}_l\,|l'm\rangle \to \left(D^l_{s,s'}(\hat{\mathbf{n}},\theta)O^{s'}{}_l\right)\left(D^{l'}_{m,\hat{m}}\,|l'\hat{m}\rangle\right)$$

To clarify, a rotation can be written as

$$\begin{aligned} e^{-\imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta}\vec{\mathbf{x}}e^{\imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta} &= \vec{\mathbf{x}} - \imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta\vec{\mathbf{x}} + \vec{\mathbf{x}}\cdot(\imath\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta) + \cdots \\ &= \vec{\mathbf{x}} - \imath[\vec{\mathbf{L}}\cdot\hat{\mathbf{n}}\theta]\vec{\mathbf{x}} + \ldots \end{aligned}$$

but equivalently, we already know that the net action of this is a rotation of the coordinates: $R(\theta)x$.

From our previous analysis, the reducible representation $l \otimes l'$ breaks up into a tensor sum of irreducible representations:

$$l \otimes l' = |l + l'| \oplus \cdots \oplus |l - l'|$$

We can use our knowledge of addition of angular momentum to say something about this new state. Consider

$$J_z[O_l{}^s\,|l'm\rangle] = \hbar(s+m)O_l{}^s\,|l'm\rangle$$

This first term is a tensor product of the operator and the vector, so we know that the action will be an addition in terms of the irreducible representations labeled by s and m. The fact that O is an operator rather than a state is *almost* irrelevant. For the time being, it behaves in the exact same way as a state.

The maximum weight state for this particular tensor product is $O_l{}^l\,|l',l'\rangle$. This transforms like $|l,l;l',l'\rangle \equiv |l+l',l+l'\rangle$ so,

$$O_l{}^l\,|l',l'\rangle = K_{J=l+l'}\,|l+l',l+l'\rangle$$

The reason it is only proportional to this and not exactly equal can be shown by an example. Suppose we are in this maximum-weight state and there is an additional quantum number, α, which can be used to label the states:

$$O_l{}^l\,|l',l';\alpha\rangle = K_{l+l'}\,|l+l',l+l'\rangle$$

Now K must depend on α, since we arrive at the states on the right purely through group theory which doesn't take α into account. The Hilbert space on the right doesn't have anything to do with α. We can write this in general as

$$O_l{}^s\,|j,m;\alpha\rangle = \sum_{J=|l-j|}^{|l+j|} K_J(\alpha)\,|J,M\rangle \quad \underbrace{\langle J,M|l,s;j,m\rangle}_{\text{Clebsch-Gordan Coefficients}}$$

Let's now project this onto a different state:

$$\langle j'm';\beta|\,O_l{}^s\,|j,m;\alpha\rangle = K_j\,\langle j',m'|l,s;j,m\rangle$$

We require $m' = s + m$ since $M = s + m$ is required for the Clebsch-Gordan coefficients to be nonzero. Now what is this coefficient K_j?

$$K_J \left|J, l+m\right\rangle = \sum_\beta K_{\alpha\beta} \left|J, l+m; \beta\right\rangle$$

Therefore, taking the above matrix element means that K_j has to know about both α and β:

$$K_{\alpha\beta} = \left\langle J, \beta\right| \left|O\right| \left|J', \alpha\right\rangle$$

This is the standard notation for the "reduced matrix element". From here, we derive the Wigner-Eckart Theorem:

$$\left|J, M'; \beta\right\rangle O_l{}^s \left|j, m; \alpha\right\rangle = \delta_{M', s+m} \left\langle J, M' | j, m, l, s\right\rangle \left\langle J; \beta\right| \left|O_l\right| \left|j; \alpha\right\rangle \qquad \text{(Wigner-Eckart Theorem)}$$

Let's do an example that will hopefully clarify this.

Example. Suppose we go and measure the value of some matrix element in an experiment.

$$\left|\frac{1}{2}, \frac{1}{2}; \alpha\right\rangle Z \left|\frac{1}{2}, \frac{1}{2}; \beta\right\rangle = A$$

We want to then predict the value of

$$\left|\frac{1}{2}, \frac{1}{2}; \alpha\right\rangle X \left|\frac{1}{2}, -\frac{1}{2}; \beta\right\rangle = B$$

X transforms like $l = 1$ in Cartesian coordinates. Let's first write our operator in spherical coordinates, rotate it, and find the solution. The Z operator transforms like $Y_l^{m=0}$, whereas

$$X = \frac{1}{\sqrt{2}} \left[Y_{l=1}^{m=-1} - Y_{l=1}^{m=1}\right]$$

Only the second term will contribute:

$$\left\langle \frac{1}{2}, \frac{1}{2}; \alpha \right| X \left|\frac{1}{2}, -\frac{1}{2}; \beta\right\rangle = \left|\frac{1}{2}, \frac{1}{2}; \alpha\right\rangle - \frac{1}{\sqrt{2}} Y_{l=1}^{m=1} \left|\frac{1}{2}, -\frac{1}{2}; \beta\right\rangle$$

Technically there's also a radial component, but it's the same for Z so they will cancel. Let's now use Wigner-Eckart theorem:

$$\left\langle \frac{1}{2}, \frac{1}{2}; \alpha \right| X \left|\frac{1}{2}, -\frac{1}{2}; \beta\right\rangle = -\frac{1}{\sqrt{2}} \left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|1, \frac{1}{2}; 1, -\frac{1}{2}\right\rangle \left\langle \frac{1}{2}; \alpha \right| \left|Y_{l=1}^{m=1}\right| \left|\frac{1}{2}; \beta\right\rangle$$

We know that

$$A = \left\langle \frac{1}{2}, \frac{1}{2}; \alpha \right| Y_1^0 \left|\frac{1}{2}, \frac{1}{2}; \beta\right\rangle = \left\langle \frac{1}{2}, \frac{1}{2} \right| 1, 0; \frac{1}{2}, \frac{1}{2}\right\rangle \left\langle \frac{1}{2}; \alpha \right| \left|Y_l\right| \left|\frac{1}{2}; \beta\right\rangle$$

Therefore, the ratio of the two matrix elements is

$$\frac{\left\langle \frac{1}{2}, \frac{1}{2}; \alpha \right| Z \left|\frac{1}{2}, \frac{1}{2}; \beta\right\rangle}{\left\langle \frac{1}{2}, \frac{1}{2}; \alpha \right| X \left|\frac{1}{2}, -\frac{1}{2}; \beta\right\rangle} = \frac{\left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|1, 0; \frac{1}{2}, \frac{1}{2}\right\rangle}{-\frac{1}{\sqrt{2}} \left\langle \frac{1}{2}, \frac{1}{2} \right| 1, \frac{1}{2}; 1, \frac{1}{2}\right\rangle} = 1$$

so $A = B$. ◇

Lecture 18:
Wednesday, February 26, 2020

Recap from last lecture: We can represent an object x in a Cartesian basis x_i, $i = 1, 2, 3$ or in a spherical basis x_a, $a = 1, 0, -1$ if if it is a representation of the rotation group (vectors, for example). We can transform both states and operators under the action of the group:

$$\left|\psi\right\rangle \to U \left|\psi\right\rangle$$

and

$$O \to UOU^{-1}$$

Let's try to relate the Cartesian and spherical bases. First, consider states. We know that the state $|i=3\rangle = |m=0\rangle$ by our definitions. They are both eigenstates of L_z with $L_z |m=0\rangle = 0$. Under a rotation around the z-axis, the state $|i=3\rangle$ transforms infinitesimally as

$$|i=3\rangle \to U(\hat{\mathbf{n}} = \hat{\mathbf{e}}_3, \theta) |i=3\rangle \approx (1 - \imath\theta L_z) |i=3\rangle = |i=3\rangle$$

by definition, so $L_z |i=3\rangle = 0$. Next, let's rotate around the x-axis, first in Cartesian coordinates:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \sim \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ -\theta \\ 0 \end{bmatrix}$$

since the rotation matrix is approximately (for small θ),

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{bmatrix} \approx \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\theta \\ 0 & \theta & 1 \end{bmatrix}$$

Therefore, the infinitesimal rotation of $|i=3\rangle$ is $\delta_x(\theta) |i=3\rangle = -\theta |i=2\rangle$.

In the spherical basis, we have

$$\begin{aligned} e^{-\imath L_x \theta} |m=0\rangle \approx |m=0\rangle - \imath\theta L_x |m=0\rangle &\approx \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} - \imath\theta \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \\ &= |m=0\rangle - \frac{\imath\theta}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \\ &= |m=0\rangle - \frac{\imath\theta}{\sqrt{2}} [|m=1\rangle + |m=-1\rangle] \end{aligned}$$

All together,

$$\begin{aligned} \delta_x(\theta) |i=3\rangle &= -theta |i=2\rangle \\ \delta_x(\theta) |m=0\rangle &= -\frac{\imath\theta}{\sqrt{2}} [|m=1\rangle + |m=-1\rangle] \end{aligned}$$

so we can conclude that

$$|i=2\rangle = \frac{\imath}{\sqrt{2}} [|m=1\rangle + |m=-1\rangle]$$

We could do the same manipulation around the y-axis and find that

$$|i=1\rangle = \frac{1}{\sqrt{2}} [|m=-1\rangle - |m=1\rangle]$$

We can then use these results to show that

$$|m=\pm 1\rangle = \mp \frac{1}{\sqrt{2}} [\hat{\mathbf{x}} \pm \imath\hat{\mathbf{y}}]$$

We have just determined the relationship between the bases using states. Now let's do the same thing using operators:

$$O \to UOU^{-1} \approx (1 - \imath\theta\hat{\mathbf{n}} \cdot \vec{\mathbf{L}}) O (1 + \imath\theta\hat{\mathbf{n}} \cdot \vec{\mathbf{L}}) = O - \imath\theta \left[\vec{\mathbf{L}}, O\right]$$

Therefore, the group action on an operator is the commutator. Again, we define $X_{m=0} \equiv X_{i=3}$ because both are invariant under rotations about the z-axis.

$$[J_\pm, X_{m=0}] = \sqrt{2}\hbar X_\pm$$

since this is the action of the raising and lowering operators. Now let's do the same action in the Cartesian basis:

$$\begin{aligned}[J_x \pm \imath J_y, X_{i=3}] &= [(\vec{\mathbf{r}} \times \vec{\mathbf{p}})_x \pm \imath(\vec{\mathbf{r}} \times \vec{\mathbf{p}})_y, z] \\ &= [r_i p_j \epsilon_{ijx}, z] \pm \imath[r_i p_j \epsilon_{ijy}, z] \\ &= r_i[p_j, z]\epsilon_{ijx} \pm \imath r_i[p_j, z]\epsilon_{ijy}\end{aligned}$$

$r_i p_j$ is zero unless $i = j$, but $\epsilon_{ijx} = 0$ when $i = j$, and r commutes with z, so we can pull it out of the commutator in the final step above.

Together, we have

$$\begin{aligned}[J_x \pm \imath J_y, X_{i=3}] &= r_i\hbar(-\imath)\epsilon_{izx} + \imath r_i(-\imath\hbar)\epsilon_{izy} \\ &= y\hbar(-\imath)\epsilon_{yzx} \pm x\hbar\epsilon_{xzy} \\ &= (\mp x - \imath y)\hbar\end{aligned}$$

We can then equate these results:

$$X_{m=\pm 1} = \frac{1}{\sqrt{2}}\left(\mp X_{X_{i=1}} - \imath X_{i=2}\right)$$

0.13 Recap: Wigner-Eckart Theorem

$$\langle lm, \alpha| O_L^s |l'm', \beta\rangle$$

is only nonzero if $m = s + m'$.

$$\langle lm, \alpha| O_L^s |l'm', \beta\rangle = \langle lm|Ls; l'm'\rangle \langle l, \alpha| |O_L| |l', \beta\rangle$$

Suppose we know

$$A = \left\langle \frac{1}{2}\frac{1}{2}\alpha \middle| z \middle| \frac{1}{2}\frac{1}{2}\beta \right\rangle$$

and we are interested in calculating

$$\left\langle \frac{1}{2}\frac{1}{2}\alpha \middle| x \middle| \frac{1}{2}, -\frac{1}{2}\beta \right\rangle = B$$

With Wigner-Eckart, we can write

$$A = \left\langle \frac{1}{2}\frac{1}{2} \middle| 1, 0; \frac{1}{2}\frac{1}{2} \right\rangle \left\langle \frac{1}{2}\alpha \middle| |z| \middle| \frac{1}{2}\beta \right\rangle$$

and

$$B = \left\langle \frac{1}{2}\frac{1}{2}\alpha \middle| \frac{1}{\sqrt{2}}[x_{m=1} + \imath x_{m=-1}] \middle| \frac{1}{2}, -\frac{1}{2}\beta \right\rangle$$

The $x_{m=-1}$ matrix element vanishes from our knowledge that $m = s + m'$ from above, and $-1 - \frac{1}{2}$ doesn't equal $\frac{1}{2}$ but $1 - \frac{1}{2}$ does:

$$B = \left\langle \frac{1}{2}\frac{1}{2}\alpha \middle| \frac{1}{\sqrt{2}} x_{m=1} \middle| \frac{1}{2}, -\frac{1}{2}\beta \right\rangle$$

Using Wigner-Eckart, we can now write

$$B = \left\langle \frac{1}{2}\frac{1}{2}\middle| 1,1;\frac{1}{2},-\frac{1}{2}\right\rangle \left\langle \frac{1}{2}\alpha\middle| |x| \middle|\frac{1}{2}\beta\right\rangle$$

but x and z are both $l=1$ states, so the reduced matrix elements must be the same thing, since it only depends on the total l of the operator. Therefore

$$\frac{A}{B} = \frac{\left\langle \frac{1}{2}\frac{1}{2}\middle|1,0;\frac{1}{2},\frac{1}{2}\right\rangle|}{-\frac{1}{\sqrt{2}}\left\langle \frac{1}{2}\frac{1}{2}\middle|1,1;\frac{1}{2},-\frac{1}{2}\right\rangle} = 1 \implies A = B$$

Lecture 19: Interaction of Particles in Electromagnetic Fields
Friday, February 28, 2020

0.14 Electrons in Electromagnetic Fields

In quantum mechanics, a wave cannot change in a static field, but we know that particles do move in static B and E fields. This means the A field must be important to the Hamiltonian:

$$H = \frac{\left(\vec{\mathbf{p}} - \frac{e}{c}\vec{\mathbf{A}}\right)^2}{2m} + e\Phi$$

Right now, we haven't shown why this is true, but we will do this later using symmetries. If we take this to be the action, let's calculate the rate of change of the x operator:

$$\begin{aligned}\imath\hbar\dot{x}_i &= [x_i, H] \\ &= \frac{1}{2m}\left[x_i, \vec{\mathbf{p}}^2 - \frac{e}{c}\left[\vec{\mathbf{p}}\cdot\vec{\mathbf{A}} + \vec{\mathbf{A}}\cdot\vec{\mathbf{p}}\right] + \frac{e^2}{c^2}\vec{\mathbf{A}}^2\right] + [x_i, e\Phi]\end{aligned}$$

In general, $\vec{\mathbf{A}}$ and Φ are operators which depend on x, so $[p, A] \neq 0$. In fact, $[x_i, p_j A_j] = [x_i, p_j]A_j = \imath\hbar A_i$ Therefore,

$$[x_i, H] = \frac{1}{2m}\left[\overbrace{\left[x_i, \vec{\mathbf{p}}^2\right]}^{2\imath\hbar p_i} - \frac{e}{c}\left[\left[x_i, \vec{\mathbf{p}}\cdot\vec{\mathbf{A}}\right] + \left[x_i, \vec{\mathbf{A}}\cdot\vec{\mathbf{p}}\right]\right] + \cancelto{0}{\left[x_i, \frac{e^2}{c^2}\vec{\mathbf{A}}^2\right]}\right] + \cancelto{0}{[x_i, e\Phi]}$$

$$\imath\hbar\dot{x} = \frac{\imath\hbar}{m}\left[p_i - \frac{e}{c}A_i\right]$$

so

$$m\dot{x}_i = \left[p_i - \frac{e}{c}A_i\right] = \Pi_i \qquad \text{(Kinematic Momentum)}$$

As opposed to the conjugate momentum p_i, which is the generator of translations ($e^{\imath\vec{\mathbf{p}}\cdot\vec{\mathbf{d}}}|\vec{\mathbf{x}}\rangle = \left|\vec{\mathbf{x}} + \vec{\mathbf{d}}\right\rangle$ or $e^{\imath\vec{\mathbf{p}}\cdot\vec{\mathbf{d}}}F(\vec{\mathbf{x}})e^{-\imath\vec{\mathbf{p}}\cdot\vec{\mathbf{d}}} = F(\vec{\mathbf{x}} + \vec{\mathbf{d}})$).

$$[\Pi_i, \Pi_j] = \left[p_i - \frac{e}{c}A_i, p_j - \frac{e}{c}p_j\right] = -\frac{e}{c}\left[[A_i, p_j] + [p_i, A_j]\right] = -\frac{e}{c}\left[\imath\hbar\partial_j A_i - \imath\hbar\partial_i A_j\right]$$

We can rewrite this using $\epsilon_{ijk}\epsilon_{abk} = \delta_{ia}\delta_{jb} - \delta_{ib}\delta_{ja}$:

$$\begin{aligned}[\Pi_i, \Pi_j] &= \frac{e}{c}\epsilon_{ijk}\imath\hbar B_k \\ &= \frac{e}{c}\epsilon_{ijk}(\partial_a A_b \epsilon_{abk})\imath\hbar \\ &= \frac{e}{c}\left[\delta_{ia}\delta_{jb} - \delta_{ib}\delta_{ja}\right]\partial_a A_b \imath\hbar \\ &= \frac{e}{c}\left[\partial_i A_j - \partial_j A_i\right]\imath\hbar\end{aligned}$$

If we think about Lorentz transformations, they form a group. Adding Lorentz transforms creates another, they all have an inverse, they're obviously associable, and there's an identity (doing nothing). We call this the Lorentz group $\mathrm{SO}(1,3)$. However, if we boost an electric field, it doesn't remain as an electric field, it mixes with the magnetic field. E cannot possibly be an irreducible representation of the Lorentz group. We have to combine the magnetic and electric field into one multiplet so they can transform as an irreducible representation of the group. When we look at the A field, $A_\mu = (\Phi, \vec{\mathbf{A}})$, this forms a representation of the Lorentz group. Gauge invariance tells us that $A_\mu(x) = A_\mu(x) + \partial_\mu \lambda(x)$. All observables must be gauge invariant, because it wouldn't make sense for the value to be different depending on what gauge we pick. We can write down the gauge-invariant, antisymmetric, two-form (it is an irrep of $\mathrm{SO}(1,3)$ since it is antisymmetric),

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

Under a gauge transformation, this goes to

$$F_{\mu\nu} \to [\partial_\mu(A_\nu + \partial_\nu\lambda) - \partial_\nu(A_\mu + \partial_\mu\lambda)] = F_{\mu\nu} + \partial_\mu\partial_\nu\lambda - \partial_\nu\partial_\mu\lambda = F_{\mu\nu}$$

We can see that the elements of this tensor tell us about the fields:

$$F_{0i} = \partial_0 A_i - \partial_i A_0 = \frac{1}{c}\partial_t A_i - \partial_i \Phi = E_i$$

where $i = 1, 2, 3$. We can also get the components of the B field:

$$F_{ij} = \frac{1}{2}\epsilon_{ijk} B_k = \partial_i A_j - \partial_j A_i$$

The Schrödinger equation for the Hamiltonian we wrote down at the beginning is

$$\imath\hbar\partial_t |\psi\rangle = \frac{\left(p_i - \frac{e}{c}A_i\right)^2}{2m} |\psi\rangle + e\Phi |\psi\rangle$$

This must be gauge invariant, but under a gauge transformation, $A_i \to A_i + \partial_i\lambda$ and $\Phi \to \Phi - \frac{1}{c}\dot{\lambda}$. The state itself transforms like

$$|\psi\rangle \to e^{\imath\frac{e}{\hbar c}\lambda(x,t)} |\psi\rangle$$

Since λ is a singlet of the Lorentz group (a scalar).

Therefore, the momentum term will transform like

$$P_i \left[e^{\frac{\imath e}{\hbar c}\lambda}\psi\right] = -\imath\hbar\partial_i \left[\frac{\imath e}{\hbar c}\partial_i\lambda\right] e^{\frac{\imath e}{\hbar c}\lambda} + e^{\frac{\imath e}{\hbar c}\lambda}\partial_i\psi$$

so

$$p_i \to p_i + \frac{e}{c}\partial_i\lambda$$

Therefore, the momentum term transformation under a gauge transformation will cancel out the effect from the transformation of A_i. There is still the contribution from the Φ term:

$$\imath\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left[e^{\frac{\imath e}{\hbar c}\lambda}\psi\right] = -\frac{e}{c}\dot{\lambda}\psi e^{\frac{\imath e}{\hbar c}\lambda} + \imath\hbar e^{\frac{\imath e}{\hbar c}\lambda}\frac{\mathrm{d}\psi}{\mathrm{d}t}$$

So the time derivative on the left side of the Schrödinger equation cancels out the Φ contribution. Therefore, gauge invariance fixes the Hamiltonian in this form. Now technically, the state itself transforms like it does because gauge transformations are part of the U(1) group, which is the group of phases, so the state must transform by a phase.

If we want to calculate $\ddot{x} = [\dot{x}, H]$, this is given by

$$\frac{\imath\hbar e}{2mc}\left[\dot{\vec{\mathbf{x}}} \times \vec{\mathbf{B}} - \vec{\mathbf{B}} \times \dot{\vec{\mathbf{x}}}\right] + \frac{e}{m}\vec{\mathbf{E}}$$

Lecture 20: Electromagnetic Interactions, Continued

Monday, March 02, 2020

Last time, we said that, neglecting spin, gauge invariance restricts the Hamiltonian to have the form

$$H = \frac{\left(\vec{\mathbf{p}} - \frac{e}{c}\vec{\mathbf{A}}\right)^2}{2m} + e\Phi$$

Now we want to study how atoms interact with the electromagnetic field considering this Hamiltonian. Let's assume that the wavelength of the radiation is much larger than the Bohr radius ($\lambda >> a_0$) and use the multipole expansion with static fields. In electrostatics, the electric field only depends on the scalar potential Φ, so

$$\Delta E_E \approx \int |\psi(x)|^2 e\Phi(x)\,\mathrm{d}^3x$$

since, to first order, $\Delta E \approx \langle nlm|\, H_I\, |nlm\rangle$. We can Taylor expand the perturbation as:

$$e\Phi(\vec{\mathbf{x}}, 0) = e\Phi(\vec{\mathbf{0}}, 0) + e\vec{\mathbf{x}}\vec{\partial}\Phi(\vec{\mathbf{0}}, 0) + ex_ix_j\partial_i\partial_j\Phi(\vec{\mathbf{0}}, 0) + \cdots$$

We can ignore the first term, since in the static case, this is a constant, so it will not effect the Hamiltonian (as long as gravity is not involved):

$$\Delta E_E = e\,\langle nlm|\,\vec{\mathbf{x}}\,|nlm\rangle\left(-\vec{\mathbf{E}}(0)\right) = \langle nlm|\,\vec{\mathbf{d}}\cdot\vec{\mathbf{E}}\,|nlm\rangle$$

where $\vec{\mathbf{d}} = -e\vec{\mathbf{x}}$. We know that both ls can't be $l = 0$, since $\vec{\mathbf{d}}$ is an $l = 1$ operator and $1 \otimes 0 = 1$, which is orthogonal to $l = 0$. The next term is

$$ex_ix_j\partial_i\partial_j\Phi = (?)_{ij}\partial_iE_j$$

x_ix_j is symmetric so it is not irreducible. We need to subtract the trace:

$$\begin{aligned}
&= \left[e\left(x_ix_j - \frac{1}{3}\delta_{ij}\vec{\mathbf{x}}^2\right) + \frac{e}{3}(\delta_{ij}\vec{\mathbf{x}}^2)\right]\partial_iE_j \\
&= Q_{ij}\partial_iE_j + \frac{e}{3}\delta_{ij}\vec{\mathbf{x}}^2\partial_iE_j
\end{aligned}$$

but the second term is $\frac{e}{3}\vec{\mathbf{x}}\vec{\partial}\cdot\vec{\mathbf{E}}(0)$ which vanishes due to Gauss' law. Therefore

$$H = \int \vec{\mathbf{d}}\cdot E + Q_{ij}\partial_iE_j$$

with $Q_{ij} = e\left(x_ix_j - \frac{1}{3}\delta_{ij}\vec{\mathbf{x}}^2\right)$ defining the quadrupole moment.

Say we wanted to evaluate a particular quadrupole moment, $\langle nlm|\, Q_{xx}\, |nlm\rangle$. First, we need to convert this into spherical coordinates with indices $-1, 0, 1$:

$$Q_{xx} = \hat{\mathbf{e}}_x^a\hat{\mathbf{e}}_x^bQ_{ab}$$

where

$$\hat{\mathbf{e}}_1 = -\frac{1}{\sqrt{2}}\left[\hat{\mathbf{e}}_x + \imath\hat{\mathbf{e}}_y\right]$$

$$\hat{\mathbf{e}}_{-1} = \frac{1}{\sqrt{2}}\left[\hat{\mathbf{e}}_x - \imath\hat{\mathbf{e}}_y\right]$$

We can solve for $\hat{\mathbf{e}}_x = \frac{1}{\sqrt{2}}\left[-\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_{-1}\right]$. From here, we can (abuse notation to) say $\hat{\mathbf{e}}_x^1 = -\frac{1}{\sqrt{2}}$ and $\hat{\mathbf{e}}_x^{-1} = \frac{1}{\sqrt{2}}$. We can now write Q_{xx} as

$$Q_{xx} = \left[-\frac{1}{\sqrt{2}}\right]^2\left[Q_{1,1} + Q_{-1,-1} - Q_{1,-1} - Q_{-1,1}\right]$$

Each of the indices transform as $l = 1$, and the indices are the m's. Therefore, Q_{11} transforms as $|11;11\rangle$, $Q_{1,-1}$ transforms as $|11;1,-1\rangle$, and so on. We can therefore write

$$\langle nlm|\, Q_{xx}\, |nlm\rangle = \frac{1}{2}\langle nlm|\, Q_{11} + Q_{-1,-1} - Q_{1,-1} - Q_{-1,1}\, |nlm\rangle$$

The first two terms must have vanishing expectation values, since $m = 1 + 1 + m$ or $m = -1 - 1 + m$ don't add up. We can write $Q_{1,-1}$ as

$$|1,1;1,-1\rangle = \sum_{J,M} |JM\rangle \langle JM|1,1;1,-1\rangle$$

and $Q_{-1,1}$ as

$$|1,-1;1,1\rangle = \sum_{J,M} |JM\rangle \langle JM|1,-1;1,1\rangle$$

From here, we could derive the nonzero matrix elements. However, we don't really need to do this entire decomposition, since we know that if Q_{ij} is symmetric and traceless, it must transform as $l = 2$. Therefore the $l = 0$ matrix element must be zero, since $2 \otimes 0 = 2$ and $l = 1 \neq l = 2$ (the states are orthogonal). However, for $l = 1$, we have $2 \otimes 1 = 3 \oplus 2 \oplus 1 \oplus 0$, so there are nonzero matrix elements.

Next, let's find what the magnetic part of the energy shift is.

$$H = \frac{\left(\vec{\mathbf{p}} - \frac{e}{c}\vec{\mathbf{A}}\right)^2}{2m} \to -\frac{e}{2m}\left[\vec{\mathbf{p}}\cdot\vec{\mathbf{A}} + \vec{\mathbf{A}}\cdot\vec{\mathbf{p}}\right] + \frac{e^2}{2mc^2}\vec{\mathbf{A}}^2$$

The second term is repressed by an additional factor of $\frac{1}{c}$, so let's only consider a non-relativistic case. If we expand $\vec{\mathbf{A}}$, $\vec{\mathbf{A}}(0)$ doesn't depend on x, so it commutes with $\vec{\mathbf{p}}$:

$$H = -\frac{e}{2mc}\left[2\vec{\mathbf{p}}\cdot\vec{\mathbf{A}}(0,t) + p_i x_j \partial_j A_i + (\vec{\mathbf{x}}\cdot\vec{\partial})A_i p_i\right]$$

The lowest order energy shift is proportional to the matrix elements

$$\langle nlm|\, \vec{\mathbf{p}}\cdot\vec{\mathbf{A}}(0,t)\, |nlm\rangle$$

$$\langle\vec{\mathbf{p}}\rangle = \left\langle\frac{\mathrm{d}\vec{\mathbf{x}}}{\mathrm{d}t}\right\rangle = \frac{1}{\imath\hbar}\langle E|\,[x,H]\,|E\rangle = \frac{1}{\imath\hbar}\left[\langle x\rangle\,(E-E)\right] = 0$$

so the first term in the multipole expansion vanishes.

A Short Diversion (Nugget)

$$\langle p|\,[x,p]\,|p\rangle = \imath\hbar\,\langle p|p\rangle = \imath\hbar$$

but

$$\langle p|\,[x,p]\,|p\rangle = \langle p|\,xp - px\,|p\rangle = \langle p|\,x\,|p\rangle\,(p-p) = 0$$

Great.

The next term in the expansion is

$$\langle nlm|\, p_i x_j \partial_j A_i(0) + x_j \partial_j A_i(0) p_i\, |nlm\rangle = \langle nlm|\, p_i x_j \partial_j A_i + x_j p_i \partial_j A_i\, |nlm\rangle$$

We can write

$$p_i x_j = x_j p_i - [p_i, x_j] = x_j p_i - \imath\hbar\delta_{ij}$$

so we can rewrite our operator as

$$2x_j p_i \partial_j A_i + \imath\hbar(\vec{\partial}\cdot\vec{\mathbf{A}})$$

When we're done, this needs to be proportional to the magnetic field, since we must be gauge invariant. We'll finish this in the next lecture.

Lecture 21: Time Dependent Perturbation Theory
Wednesday, March 04, 2020

In the last lecture, we looked at electrostatics and expanded the action. We said that if $\mathbf{A}$ varies on a scale larger than a_0, we can use the multipole expansion:

$$A \to A(0,0) + \vec{\mathbf{x}} \cdot \vec{\partial} \vec{\mathbf{A}} + \frac{1}{2} x_i x_j \partial_i \partial_j \vec{\mathbf{A}} + \cdots$$

and

$$\Phi \to \Phi(0,0) + \vec{\mathbf{x}} \cdot \vec{\partial} \Phi + \frac{1}{2} x_i x_j \partial_i \partial_j \Phi$$

where the second terms are the dipole terms, the third are the quadrupole, and so on. The first terms vanish in the static case, since they are just constants and the fields depend on the derivatives of these potentials. We also showed that the quadrupole moment must be traceless and symmetric, and it is in the 2 representation of SO(3).

0.15 Time Dependent Perturbation Theory

$$H = H_0 + V(t)$$

$$H_0 |n\rangle = E_n |n\rangle$$

Any arbitrary state can be decomposed in this way (in the Schrödinger picture, where the states, not the operators, evolve in time):

$$|\alpha, t\rangle_S = \sum_n C_n(t) e^{-\imath E_n t/\hbar} |n\rangle$$

where $\lim_{V \to 0} C_n(t) = C_n$. This limit motivates us to define

$$|\alpha\rangle_I = e^{\imath H_0 t/\hbar} |\alpha\rangle_S$$

where the I stands for the interaction picture. Recall that in the Heisenberg picture, states are time independent and operators are time dependent, but in the interaction picture, the states evolve according to $V = H_I$ while the operators evolve according to H_0:

$$\imath\hbar \frac{\partial}{\partial t} |\alpha\rangle_I = \imath\hbar \frac{\partial}{\partial t} \left[e^{\imath H_0 t/\hbar} |\alpha\rangle_S \right] = -H_0 e^{\imath H_0 t/\hbar} |\alpha\rangle_S + e^{\imath H_0 t/\hbar} \underbrace{\left(\imath\hbar \frac{\partial}{\partial t} |\alpha\rangle_S \right)}_{(H_0+V)|\alpha\rangle}$$

We can use the Schrödinger equation on the last part:

$$\imath\hbar \frac{\partial}{\partial t} |\alpha\rangle_I = e^{\imath H_0 t/\hbar} \left[-H_0 + (H_0 + V) \right] |\alpha\rangle_S = V |\alpha\rangle_I$$

We could run through an analogous description of the operators in this interaction picture to find that

$$\imath\hbar \frac{\partial}{\partial t} O_I = [O_I, H_0]$$

The point is that we can split up the total time evolution $e^{\imath(H_0+V)t/\hbar} |\psi\rangle$ into a part that acts on the state and a part that acts on the operator $\to e^{\imath H_0 t/\hbar} \left(e^{\imath V t/\hbar} |\psi\rangle \right)$.

We will now decompose the interaction picture states in terms of energy eigenstates in the interaction picture.

$$|\alpha, t\rangle_I = \sum_n C_n(t) |n, t\rangle_I$$

We want to solve for the $C_n(t)$ factors:

$$\imath\hbar\frac{\partial}{\partial t}\left|\alpha,t\right\rangle_I = V_I(t)\left|\alpha,t\right\rangle_I = \imath\hbar\sum_n \dot{C}_n\left|n,t\right\rangle_I + \imath\hbar\sum_n C_n(t)\frac{\partial}{\partial t}\left|n,t\right\rangle_I$$

Now let's project this onto a particular eigenstate $\langle m|n\rangle = \delta_{mn}$ and insert the identity $\sum_{m'}\left|m'\right\rangle\left\langle m'\right|$:

$$\imath\hbar\dot{C}_m = \sum_{m'}\left\langle m\right|V_I(t)\left|m'\right\rangle\underbrace{\left\langle m'|\alpha,t\right\rangle_I}_{C_{m'}(t)}$$

Therefore

$$\imath\hbar\dot{C}_m = \sum_{m'}\left\langle m\right|V_I(t)\left|m'\right\rangle C_{m'}(t)$$

Lecture 22: Time Dependent Perturbation Theory, Continued.

Wednesday, March 18, 2020

In our last lecture, we were discussing perturbations of the following form:

$$H = H_0 + \lambda W(t)$$

In the interaction picture, states evolve according to

$$\imath\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle_I = \lambda W_I(t)\left|\psi\right\rangle_I$$

where

$$W_I(t) = e^{-\imath H_0 t/\hbar}W(t)e^{\imath H_0 t/\hbar}$$

The states evolve according to the interaction Hamiltonian while the operators evolve according to the unperturbed (free) Hamiltonian. In the limit where $\lambda \to 0$, the states don't evolve and only the operators evolve. The advantage of this is that if we take $\lambda << 1$, we can expand in λ. Let's now project a time independent eigenstate of H_0 onto this interaction picture equation and insert an identity using the basis states m of the free Hamiltonian:

$$\imath\hbar\frac{\partial}{\partial t}\left\langle n|\psi\right\rangle_I = \sum_m\left\langle n\right|W_I\left|m\right\rangle\left\langle m|\psi\right\rangle_I$$

where $H_0\left|n\right\rangle = E_0^{(n)}\left|n\right\rangle$.

Let's decompose the state $\left|\psi\right\rangle_I$ as

$$\left|\psi\right\rangle_I = \left|\alpha,t_0,t\right\rangle = \sum_n c_n(t)\left|n\right\rangle$$

We can now write our time-dependent Schrödinger equation as

$$\imath\hbar\dot{c}_n(t) = \sum_m W_{nm}c_m(t)e^{\imath\omega_{mn}t}$$

where

$$W_{nm} = \left\langle n|W_I|m\right\rangle = \left\langle n|e^{\imath H_0 t/\hbar}WVe^{-\imath H_0 t/\hbar}|m\right\rangle = \left\langle n|W|m\right\rangle e^{\imath(\omega_n-\omega_m)t}$$

and $\omega_{nm} = \omega_n - \omega_m$.

This formulation gives a set of differential equations which are typically not solvable. However, we can see that this works by considering solvable systems.

Example. Consider a two-state system with states $|1\rangle$ and $|2\rangle$:

$$H_0 = E_1 |1\rangle \langle 1| + E_2 |2\rangle \langle 2|$$

We can introduce some interaction potential

$$V(t) = \gamma e^{\imath\omega t} |1\rangle \langle 2| + \gamma e^{-\imath\omega t} |2\rangle \langle 1|$$

Therefore, we can write the complete Hamiltonian as

$$H = \begin{bmatrix} E_1 & \gamma e^{\imath\omega t} \\ \gamma e^{-\imath\omega t} & E_2 \end{bmatrix}$$

Using the equations we constructed above, we find the following set of differential equations:

$$\imath\hbar\dot{c}_1 = \gamma e^{\imath t(\omega+\omega_{12})} c_2(t)$$
$$\imath\hbar\dot{c}_2 = \gamma e^{-\imath t(\omega+\omega_{12})} c_1(t)$$

Let's suppose that at $t = 0$, $c_1(0) = 1$ and $c_2(0) = 0$. This is a statement that the system starts entirely in the $|1\rangle$ state. In the second homework problem, we will show that

$$|c_2|^2 = \frac{\gamma^2}{\hbar^2} \frac{1}{\left[\frac{\gamma^2}{\hbar^2} + \frac{(\omega+\omega_{12})^2}{4}\right]} \sin^2\left(\left(\frac{\gamma^2}{\hbar^2} + \frac{(\omega+\omega_{12})^2}{4}\right)^{1/2} t\right)$$

Additionally, we know that $|c_1|^2 + |c_2|^2 = 1$, so knowing $|c_2|^2$. If we look at the $\sin^2(\cdots)$ portion, we see that the maximal probability of the state occurs when $\omega = \omega_2 - \omega_1$, the "resonance". In the first oscillation, the state of the system goes from $|1\rangle$ to $|2\rangle$. We can call this absorption. In the "dip" in the $\sin^2(\cdots)$, the state is oscillating back to $|1\rangle$, and we could call this emission. The system is absorbing and emitting energy in a cyclical fashion.

If we study the maximum value of $|c_2(t)|^2$ as a function of ω, we can see that it will peak at ω_{21} and die off as $\omega \to 0$ and $\omega \to \infty$. ◇

Let's now look at an implementation of this model using spins.

Example.

$$H_0 = -\vec{\mu}_e \cdot \vec{\mathbf{B}}_0$$

where $|mu|_e = \frac{e\hbar}{2mc}$ and $\vec{\mathbf{B}}_0 - B_0\hat{\mathbf{e}}_z$. This is just the Hamiltonian of an electron in a magnetic field. Let's now add a transverse field which is oscillating in the z-plane:

$$V(t) = -\vec{\mu} \cdot \Delta\vec{\mathbf{B}}$$

where $\vec{\mu} = \frac{e}{mc}\vec{\mathbf{S}}$ and $\Delta\vec{\mathbf{B}} = B_1 [\hat{\mathbf{e}}_x \cos(\omega t) + \hat{\mathbf{e}}_y \sin(\omega t)]$.

Therefore,

$$V(t) = -\frac{e\hbar B_1}{2mc} \begin{bmatrix} 0 & \cos(\omega t) + \imath \sin(\omega t) \\ \cos(\omega t) - \imath \sin(\omega t) & 0 \end{bmatrix}$$

In analogy to the toy model above, we can define $\gamma \equiv \frac{e\hbar}{2mc}$. The resonant frequency is then $\omega_{21} = \frac{e\hbar}{mc} B_0$. This is the general idea behind MRI technology, where the resonant frequency is typically tuned to that of water. Water is chosen because being able to see the differences in concentration of water can very precisely determine the type of tissue. ◇

We just found exact solutions for these systems. However, this is not always possible. We need to find a way to approximate these solutions similar to the way we constructed time-independent perturbation theory:

$$c_n(t) = c_n^{(0)} + c_n^{(1)} + c_n^{(2)} + \cdots$$

scaling in powers of λ. We can write our system of differential equations as

$$\imath\hbar \begin{bmatrix} \dot{c}_1 \\ \vdots \\ \dot{c}_n \end{bmatrix} = \begin{bmatrix} V_{11} & V_{12}e^{\imath\omega_{12}t} & \cdots \\ \vdots & \vdots & \\ \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix}$$

We assume we know the exact state at $t = 0$:

$$c_i(t) = \delta_{i,(n=1)}$$

such that

$$c^{(0)}_{(n=1)} = 1$$

At leading order, only c_1 is non-vanishing, and

$$\imath\hbar\dot{c}^{(1)}_1 = V_{11}\underbrace{c^{(0)}_1}_{1}$$

Let's now continue to solve the system using the time evolution operator. We can again write our states as

$$|\alpha, t_0; t\rangle_I = U_I(t, t_0)\,|\alpha, t_0; t_0\rangle$$

and the Schrödinger equation tells us that

$$\imath\hbar\frac{\partial}{\partial t}\,|\psi\rangle_I = V_I(t)\,|\psi\rangle_I$$

where $|\psi\rangle_I = |\alpha, t_0; t\rangle_I$. Plugging this in, we really want to solve

$$\imath\hbar\frac{\partial}{\partial t}U_I = V_I(t)U_I(t)$$

Additionally, $U(t_0, t_0) = 1$. We can formally solve this equation as

$$U_I(t, t_0) = \frac{1}{\imath\hbar}\int_{t_0}^{t} \mathrm{d}t'\, V_I(t')U_I(t', t_0)$$

This is known as an integral equation. We obviously can't solve it directly, since we don't know U_I, so we can approximate the solution iteratively. First, expand U_I:

$$U_I = U_I^{(0)} + U_I^{(1)} + U_I^{(2)} + \cdots$$

$$U_I^{(1)} = \frac{1}{\imath\hbar}\int_{t_0}^{t} \mathrm{d}t'\, V_I(t')\underbrace{U_I^{(0)}}_{1}$$

To next order, we write

$$U_I^{(2)} = \frac{1}{\imath\hbar}\int_{t_0}^{t} \mathrm{d}t'\, U_I^{(1)}(t', t_0)V_I(t') = \frac{1}{\imath\hbar}\int_{t_0}^{t} \mathrm{d}t'\, \frac{1}{\imath\hbar}V_I(t')\int_{t_0}^{t'} \mathrm{d}t''\, V_I(t'')$$

We could continue this to whatever arbitrary order we want. There is a way of writing down the exact formal solution:

$$U_I = Te^{\frac{1}{\hbar}\int_{t_0}^{t} V_I(t')\mathrm{d}t'}$$

Suppose we had a matrix that depends on t and we exponentiate it:

$$e^{\int A(t)\mathrm{d}t}$$

In the past, we wrote

$$e^A = \sum_n \frac{1}{n!}A^n$$

but we have no guarantee that $[A(t), A(t')] = 0$ (and in general, these do not commute). The T is the "time-ordering" operator. We ran out of time in the lecture, but we will quickly discuss this in the next lecture.

Lecture 23: Time-Dependent Perturbation Theory

Friday, March 20, 2020

In the previous lecture, we introduced the time-ordering operator T:

$$U_I(t, t_0) = Te^{-\frac{\imath}{\hbar}\int_{t_0}^{t} V_I(t')\mathrm{d}t'}$$

with

$$T\{A(x)B(y)\} \equiv \begin{cases} A(x)B(y) & t_x > t_y \\ \pm B(y)A(x) & t_y > t_x \end{cases}$$

This reproduces the exact iterative solution.

Given the initial state $|i\rangle = |i, t_0, t_0\rangle_I$, we can find the time evolution of this state as

$$|i, t_0, t\rangle = U_I(t, t_0)\,|i\rangle = \sum_n c_n(t)\,|n\rangle$$

We can ask what is the probability of ending up in the state $|m\rangle$:

$$\Pr(i \to m) = \left|c_m^{(0)} + c_m^{(1)} + \cdots\right|^2$$

Our initial condition is $c_m^{(0)} = \delta_{mi}$, and using our iterative method, we find that

$$c_m^{(1)} = -\frac{1}{\hbar}\int_{t_0}^{t} \langle n|V_I(t')|i\rangle\,\mathrm{d}t' = \langle m|V_I|i\rangle$$

and

$$U_I^{(1)} = \frac{1}{\imath\hbar}\int_{t_0}^{t} \mathrm{d}t'\,V_I(t')$$

Example. For example, consider the potential

$$V(t) = \begin{cases} 0 & t < 0 \\ V & t \geq 0 \end{cases}$$

We can do the integral for $c_m^{(1)}$:

$$\begin{aligned} c_m^{(1)} &= -\frac{\imath}{\hbar}\int_{t_0}^{t} \langle n|\,e^{\imath H_0 t'/\hbar} V e^{-\imath H_0 t'/\hbar}\,|i\rangle\,\mathrm{d}t' = -\frac{\imath}{\hbar}\,\langle n|V|n\rangle \int_{t_0}^{t} e^{\imath\omega_{ni}t'}\,\mathrm{d}t' \\ &= -\frac{\imath}{\hbar}\,\langle n|V|i\rangle \left[\frac{1}{\imath\omega_{mi}}\left[e^{\imath\omega_{mi}t} - e^{\imath\omega_{ni}t_0}\right]\right] \end{aligned}$$

so

$$|c_m(t)|^2 = \frac{4|V_{mi}|^2}{|E_m - E_i|^2}\sin^2\left(\frac{(E_m - E_i)t}{2\hbar}\right)$$

where $V_{mi} \equiv \langle m|V|i\rangle$ and $\omega = \frac{E_m - E_i}{\hbar}$. This is a sinc function in ω with the middle peak height proportional to t^2. We see as we wait longer and longer, the probability of transition away from the initial state goes to zero, $E_m \to E_i$. Why is this true? When we have time dependence, energy is not in general conserved, but if we were given a system in which we turn on an interaction which is constant in time, after a while, that "turning on" step won't really matter. In reality, if we were to cut off the interaction at small t, the frequency of energy added to the system is proportional to $\frac{1}{t} = \omega$. This results in the time-energy uncertainty principle,

$$\Delta\omega\Delta t \sim 1 \implies \Delta t\Delta E \leq \hbar$$

$\diamond$

Typically we are interested in states where the final state is continuum, electron scattering for example. The end state of the electron is not bound or quantized. In such cases, we define the density of states, $\rho(E)$ such that $\rho(E)\,\mathrm{d}E$ is the number of states which have energy at $E + \Delta E$. In the continuum,

$$\sum_n |c_n|^2 = \int \mathrm{d}E_n\, \rho(E_n) |c_n|^2$$

At lowest order in perturbation theory,

$$\sum_n |c_n|^2 = \int \mathrm{d}E_n\, \rho(E_n) \frac{4|V_{ni}|^2}{|E_n - E_i|^2} \sin^2\left(\frac{(E_n - E_i)t}{2\hbar}\right)$$

As $t \to \infty$,

$$\frac{1}{|E_n - E_i|} \sin^2\left(\frac{(E_n - E_i)t}{2\hbar}\right) \to \frac{\pi t}{2\hbar}\delta(E_i - E_n)$$

so

$$\lim_{t\to\infty} \int \mathrm{d}E_n\, \rho(E_n) \left|c_n^{(1)}\right|^2 = \frac{2\pi}{\hbar} |V_{ni}|^2 \rho(E_n) t$$

we can define the time derivative of this as

$$\Gamma_{i\to[n]} = \frac{2\pi}{\hbar} |V_{ni}|^2 \rho(E_n) \qquad \text{(Fermi's Golden Rule)}$$

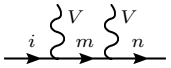
where the brackets mean i "near" n:

$$\Gamma_{i\to n} = \frac{2\pi}{\hbar} |V_{ni}|^2 \delta(E - E_n)$$

This is still for constant V, we will go back to $V \sim e^{\imath\omega t}$ soon. To next order, we are interested in

$$\begin{aligned}
\langle n| T\left[e^{-\frac{\imath}{\hbar}\int_{t_0}^t V_I(t')\mathrm{d}t'}\right] |i\rangle &= \left(-\frac{\imath}{\hbar}\right) \frac{1}{2!} \cdot 2 \int_0^t V_I(t')\,\mathrm{d}t' \int_0^{t'} V_I(t'')\,\mathrm{d}t''\, |i\rangle \\
&= -\frac{1}{\hbar^2} \sum_m \langle n| \int_0^t V_I(t')\,|m\rangle \langle m| \int_0^{t'} V_I(t'')\,\mathrm{d}t''\,|i\rangle \\
&= -\frac{1}{\hbar^2} \sum_m |V_{nm}|^2 |V_{mi}|^2 \int_0^t e^{\imath\omega_{nm}t'}\,\mathrm{d}t' \int_0^{t'} e^{\imath\omega_{mi}t''}\,\mathrm{d}t'' \\
&= \frac{\imath}{\hbar} \sum_m \frac{V_{nm}V_{mi}}{(E_m - E_i)} \int_0^t \left[e^{\imath\omega_{ni}t'} - e^{\imath\omega_{mn}t'}\right] \mathrm{d}t'
\end{aligned}$$

Notice that $E_m \neq E_i$. $|m\rangle$ is some intermediate state. We are taking some initial state i, scattering it off the potential to state m, and it ends up in the final state n. It appears energy conservation is violated at second order!The state m is a "virtual state". There is a short time energy violation, but there is no way to measure this energy violation in this virtual fluctuation.



Lecture 24: Time-Dependent Perturbation Theory, Continued

Monday, March 23, 2020

Let's look at how Fermi's Golden Rule changes under a harmonically oscillating potential (rather than a step function).

$$V = Ve^{\imath\omega t} + V^\dagger e^{-\imath\omega t}$$

$$c_n^{(1)} = \frac{1}{\imath\hbar}\int_0^t \left(V_{ni}e^{\imath\omega t'} + V_{ni}^\dagger e^{-\imath\omega t'}\right)\mathrm{d}t'$$

Recall that our electromagnetic interactions have the form

$$\begin{aligned} H &= \frac{(\vec{\mathbf{p}} - e/c\vec{\mathbf{A}})^2}{2m} + e\Phi(x) \\ &= \frac{\vec{\mathbf{p}}^2}{2m} - \frac{e}{2mc}\left(\vec{\mathbf{A}}\cdot\vec{\mathbf{p}} + \vec{\mathbf{p}}\cdot\vec{\mathbf{A}}\right) + \mathcal{O}\big(A^2\big) + e\Phi(x) \end{aligned}$$

Recall we have the freedom to choose our gauge, so let's use the Coulomb gauge:

$$\vec{\boldsymbol{\nabla}}\cdot\vec{\mathbf{A}} = 0$$

so

$$\vec{\mathbf{p}}\cdot\vec{\mathbf{A}} = ()$$

Let's write $\vec{\mathbf{A}} = 2A_0\vec{\epsilon}\cos\big(\frac{\omega}{c}(\hat{\mathbf{n}}\cdot\vec{\mathbf{x}}) - \omega t\big)$ where $\vec{\epsilon}$ is the polarization and $\hat{\mathbf{n}}$ is the direction of motion. By Maxwell's equations, $\hat{\mathbf{n}}\cdot\vec{\epsilon} = 0$.

$$A_\mu = (\Phi, \vec{\mathbf{A}}) = (0, \epsilon_x, \epsilon_y, 0)$$

for a wave propagating in the $\hat{\mathbf{z}}$ direction. We can write our interaction Hamiltonian as

$$H_I = -\frac{e}{mc}A_0\vec{\mathbf{p}}\cdot\vec{\epsilon}\left[e^{\imath(\ldots)} + e^{-\imath(\ldots)}\right]$$

Now we employ Fermi's golden rule:

$$\Gamma_{i\to n} = \frac{2\pi}{\hbar}\frac{e^2}{m^2c^2}|A_0|^2\left|\langle n|e^{\imath(\cdots)}|i\rangle\right|^2\delta(E_n - E_i - \hbar\omega)$$

where we include $\hbar\omega$ because we are now absorbing one quantum of light. We need to figure out how to calculate this matrix element (there's a similar problem in the homework). First, let's find the absorptive cross-section, the energy absorbed per unit time divided by the flux. Recall that the energy density is

$$U \equiv \frac{1}{2}\left[\frac{\vec{\mathbf{E}}^2}{8\pi} + \frac{\vec{\mathbf{B}}^2}{8\pi}\right] = \frac{1}{2\pi}\frac{\omega^2}{c}|A_0|^2$$

The energy flux is just cU, so

$$\sigma_{\text{abs}} = \frac{(\hbar\omega)\frac{2\pi}{\hbar}\left(\frac{e^2}{m^2c^2}\right)\left|\langle n|e^{\imath(\cdots)}|i\rangle\right|^2|A_0|^2}{\frac{1}{2\pi}\frac{\omega^2}{c^2}|A_0|^2}\delta(E_i + \hbar\omega - E_n)$$

Now we can use the multipole approximation:

$$\langle n|e^{\imath\left(\underbrace{\hat{\mathbf{n}}\cdot\vec{x}\frac{\omega}{c}}_{\frac{\hat{\mathbf{n}}\cdot\vec{\mathbf{x}}}{\lambda}} - \omega t\right)}|i\rangle$$

We can expand around λ:

$$e^{\imath\left(\hat{\mathbf{n}}\cdot\vec{\mathbf{x}}\frac{\omega}{c}\right)} \approx 1 + \imath\hat{\mathbf{n}}\cdot\vec{\mathbf{x}}\frac{\omega}{c} + \cdots$$

so

$$\sigma_{\text{abs}} = \left(\frac{e^2}{\hbar c}\right)\frac{4\pi^2\hbar}{m^2\omega}\left|\langle n|\vec{\epsilon}\cdot\vec{\mathbf{p}}|i\rangle\right|^2\delta(E_{\text{in}} - E_{\text{out}})$$

If we take the polarization to be along the x-axis (while $\hat{\mathbf{n}}$ is along the $\hat{\mathbf{z}}$ direction), we get the matrix element $\langle n|p_x|i\rangle$. Recall there is no monopole moment for the Hydrogen atom, but why don't we see the dipole moment as the leading order term? What is this momentum element? Notice that

$$[H, x] = -\frac{\imath\hbar\vec{\mathbf{p}}}{m}$$

so we can rewrite

$$\langle n|p_x|i\rangle = \frac{m}{\imath\hbar}\langle n|[x, H_0]|i\rangle = \frac{m}{\imath\hbar}(E_i - E_n)\langle n|x|i\rangle = \imath m\omega_{ni}\langle n|x|i\rangle$$

which looks more like the expected dipole operator. Now let's look at this in terms of the $|l, m\rangle$ basis. Recall in this basis, the selection rules for $\langle l'm'|\, x\, |lm\rangle$ make $m' = m \pm 1$ since x is an operator with $l = 1$ and $\Delta l = 0, \pm 1$ by a parity argument.

$$\sigma_{\text{abs}} = 4\pi\alpha\omega_{ni}|\langle n|x|i\rangle|^2\delta(\omega - \omega_{ni})$$

This is interesting, because every time $\omega = \omega_{ni}$, the cross-section diverges. Physically, there are effects which smear out this δ-function, and in particular you can approximate the function as a Lorentzian

$$\delta(\omega - \omega_{ni}) = \lim_{\gamma\to 0}\left(\frac{\gamma}{2\pi}\right)\frac{1}{\left((\omega - \omega_{ni})^2 + \frac{\gamma^2}{4}\right)}$$

Physically, this is due to collisional broadening. When you do this experiment, you'd have to scatter light off of a cloud of hydrogen gas, and those atoms are all moving, so the relative energy of the photon depends on which particle you're looking at. Therefore, you will see some distribution with the width proportional to the temperature. The other source of this is the finite lifetime of the states, which we will discuss in the next lecture. When you integrate over σ, you get the total absorption cross section:

$$f_{ni} = \frac{2m\omega_{ni}}{\hbar}|\langle n|x|i\rangle|$$

$$\begin{aligned}
\sum_n f_{ni} &= \sum_n \frac{2m\omega_{ni}}{\hbar}|\langle n|x|i\rangle|^2 = \sum_n \frac{1}{2}\left(\frac{2m}{\hbar}\right)[\langle n|[H_0, x]|i\rangle\ \langle i|x|n\rangle + \text{Hermitian conjugate}] \\
&= \sum_n \frac{1}{2}\left(\frac{2m}{\hbar}\right)\left[\langle i|x|n\rangle\ \langle n|-\frac{\imath\hbar}{m}p_x|i\rangle + \text{h.c.}\right] \\
&= \frac{m}{\hbar}\left[\langle i|xp|i\rangle\left(-\frac{\imath\hbar}{m} + \text{h.c.}\right)\right] \\
&= \langle i|[x, p]|i\rangle = 1 \qquad \text{(Thomas-Reiche-Kuhn Sum Rule)}
\end{aligned}$$

which is an incredible result (which has roots in probability conservation).

$$\int_{\text{abs}}^{\text{tot}}(\omega)\,\mathrm{d}\omega = 2\pi^2 c\frac{e^2}{mc^2}$$

LECTURE 25: TIME-DEPENDENT PERTURBATION THEORY: UNSTABLE STATES
Wednesday, March 25, 2020

0.16 Unstable States

So far we've been calculating probabilities to transition to another state ($i \to n$). Now we want to talk about the probability of staying in a particular state ($i \to i$). Recall that at second order in perturbation theory, we found that

$$c_n^{(2)} = \frac{\imath}{\hbar}\sum_m \frac{V_{nm}V_{mi}}{E_m - E_i}\int_0^t \left(e^{\imath\omega_{mi}t'} - e^{\imath\omega_{nm}t'}\right)\mathrm{d}t'$$

Notice this value is singular when $E_m = E_i$, which means this formula isn't very useful to calculate probabilities of $i \to i$. The reason for this is because we derived this formula assuming the interactions turn on instantaneously, which is never possible. Instead, let's adiabatically turn on the potential:

$$V(t) = e^{\eta t} V$$

and take the limit as $\eta \to 0$.

$$\begin{aligned} c_n^{(1)} &= -\frac{\imath}{\hbar} \lim_{t_0 \to -\infty} \int_{t_0}^{t} e^{\eta t'} e^{\imath \omega_{ni} t'} V_{ni} \, \mathrm{d}t' \\ &= -\frac{\imath}{\hbar} \frac{V_{ni}}{\eta + \imath \omega_{ni}} e^{\eta t + \imath \omega_{ni} t} \end{aligned}$$

so

$$\left| c_n^{(1)} \right|^2 = \frac{1}{\hbar^2} \frac{|V_{ni}|^2 e^{2\eta t}}{(\eta^2 + \omega_{ni}^2)}$$

$$\lim_{\eta \to 0} \mathrm{d}t \left| c_n^{(1)} \right|^2 = \frac{2\eta e^{2\eta t} |V_{ni}|^2}{\hbar^2 (\eta^2 + \omega_{ni}^2)}$$

We would imagine this would go to 0, but in reality,

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2 + \omega_{ni}^2} = \pi \delta(\omega_{ni})$$

so

$$\lim_{\eta \to 0} \mathrm{d}t \left| c_n^{(1)} \right|^2 = \frac{2\pi}{\hbar} |V_{ni}|^2 \delta(E_n - E_i)$$

Again, we regain the Fermi Golden Rule, and η is irrelevant using this η derivation. Now let's examine the second-order:

$$\begin{aligned} c_n^{(2)}(t) &= \langle n | \left(-\frac{\imath}{\hbar} \right)^2 \int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t'''} \mathrm{d}t'' \, V_I(t') V_I(t'') \, |i\rangle \\ &= \sum_m \langle n | \left(-\frac{\imath}{\hbar} \right)^2 \int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t''} \mathrm{d}t'' \, V_I(t') \, |m\rangle \langle m| \underbrace{V_I}_{= e^{\imath H_0 t} V e^{-\imath H_0 t}} (t'') \, |i\rangle \\ &= \sum_m \left(-\frac{\imath}{\hbar} \right)^2 \int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t''} \mathrm{d}t'' \, e^{\imath \omega_{nm} t' + \eta t'} V_{nm} \int_{t_0}^{t'} \mathrm{d}t'' \, e^{\imath \omega_{mi} t'' + \eta t''} V_{mi} \\ &= \sum_m \left(-\frac{\imath}{\hbar} \right)^2 \int_{t_0}^{t} \mathrm{d}t' \, e^{\imath \omega_{nm} t' + \eta t'} (-\imath)(V_{nm})(V_{mi}) \frac{e^{\imath \omega_{mi} t' + \eta t'}}{(\omega_{mi} - \imath \eta)} \\ (n = i) &= \sum_m \left(-\frac{\imath}{\hbar} \right)^2 (-\imath) \int_{t_0}^{t} \mathrm{d}t' \, \frac{e^{2\eta t'}}{(\omega_{mi} - \imath \eta)} \\ &= \left(\frac{\imath}{\hbar^2} \right) \int_{t_0}^{t} \frac{e^{2\eta t'} |V_{ii}|^2}{(-\imath \eta)} \, \mathrm{d}t' + \frac{\imath}{\hbar^2} \int_{t_0}^{t} \sum_{m \neq i} \frac{e^{2\eta t'} |V_{im}|^2}{(\omega_{mi} - \imath \eta)} \, \mathrm{d}t' \\ c_i(t) &= 1 - \frac{\imath}{\hbar} \frac{V_{ii}}{\eta} e^{\eta t} - \left(-\frac{\imath}{\hbar} \right)^2 \frac{|V_{ii}|^2 e^{2\eta t}}{2\eta^2} + \frac{\imath}{\hbar^2} \sum_{m \neq i} \frac{|V_{im}|^2 e^{2\eta t}}{(2\eta)(\omega_{mi} - \imath \eta)} \end{aligned}$$

We want to know about the stability of this state, so let's take the time derivative:

$$\begin{aligned} \dot{c_i}(t) &= -\frac{\imath}{\hbar} V_{ii} + \frac{1}{\hbar^2} |V_{ii}| + \frac{\imath}{\hbar^2} \sum_{m \neq i} \frac{|V_{im}|^2}{(\omega_{mi} - \imath \eta)} \\ \frac{\dot{c_i}}{c_i} &= \frac{-\frac{\imath}{\hbar} V_{ii} + \frac{1}{\hbar^2} |V_{ii}| + \frac{\imath}{\hbar^2} \sum_{m \neq i} \frac{|V_{im}|^2}{(\omega_{mi} - \imath \eta)}}{\left(1 - \frac{\imath}{\hbar^2} \frac{V_{ii}}{\eta} \right)} \\ &= -\frac{\imath}{\hbar} V_{ii} + \frac{\imath}{\hbar} \sum_{m \neq i} \frac{|V_{im}|^2}{(\omega_{mi} - \imath \eta)} \end{aligned}$$

so

$$c_i(t) = e^{-\imath\Delta_i t/\hbar}$$

where

$$\Delta = V_{ii} + \frac{\imath}{\hbar}\sum_{i\neq m}\frac{|V_{im}|^2}{(\omega_{mi} - \imath\eta)} = \underbrace{V_{ii}}_{\Delta^{(1)}} - \underbrace{\frac{\imath}{\hbar}\sum_{m\neq i}\frac{|V_{im}|^2}{(\omega_i - \omega_m + \imath\eta)}}_{\Delta^{(2)}}$$

so to first order, $\Delta \to \Delta E_i = \langle i|V|i\rangle$ and we obtain the typical result

$$c_i(t) = e^{-\frac{\Delta E_i t}{\hbar}}$$

What happens with the second-order term?

$$\begin{aligned}\Delta^{(2)} &= \sum_{m\neq i}\frac{|V_{im}|^2}{(E_i - E_m + \imath\eta)} \\ &= \sum_{m\neq i}\Pr\left(\frac{|V_{im}|^2}{E_i - E_m}\right) - \imath\pi\delta(E_i - E_m)|V_{im}|^2\end{aligned}$$

where here, by $\Pr(\,\cdot\,)$ we mean the principal part:

$$\Pr(f(x)) = \lim_{\delta\to 0}\int_{-\infty}^{\delta} f(x)$$

$$|c_i|^2 = e^{2\Delta_I t/\hbar} = e^{-\Gamma t/\hbar}$$

where Γ is the width of the state:

$$\tau = \frac{\hbar}{\Gamma}$$

What this is telling us is if we have some initial state and Δ has an imaginary part, we will see spontaneous emission from this state down to a lower state.

If we have a particle, even a fundamental particle, the mass of the particle has some uncertainty because of the uncertainty in the energy, $\Delta E\tau = 0$.

Lecture 26: The Classical Limit

Friday, March 27, 2020

Recall the differences between classical and quantum mechanics. In classical mechanics, we work in phase space rather than the quantum Hilbert space, and states are points in phase space rather than rays in Hilbert space. The classical Hamiltonian equations can be written in terms of Poisson brackets:

$$\dot{x} = \{x, H\} \qquad \dot{p} = \{p, H\}$$

where

$$\{A, B\} = \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}$$

with $A(p, x)$ and $B(p, x)$ and $\{x, p\} = 1$.

We compare this with quantum mechanics, where the equations of motion are defined by the commutator rather than the Poisson bracket and we can use the Schrödinger equation to say how states evolve.

Classically, any function of x and p is an observable, but in quantum we know that observables are Hermitian operators. Of course, in classical, it makes sense to know x and p at the same time, but in quantum, our observables are statistical:

$$\langle O\rangle = \int \psi^*(x)O^\dagger\,\mathrm{d}x$$

Given a quantum system, we should be able to get the classical result as $\hbar \to 0$ while turning our quantum Hamiltonian into a classical Hamiltonian by converting the operators into classical variables. Notice that doing this the other way there is an ambiguity. If $H = f(p, x)$, we need to convert to a function of operators, but how do we know which ordering to use (since the variables commute in classical mechanics). However, given a quantum system, we can uniquely determine the classical limit (just not the other way around).

To understand the classical limit of a quantum system, we can think back to the idea of the wave-particle duality of quantum mechanics. A wave function like $\psi(x)$ behaves like a wave. We can define $\rho = |\psi|^2$ as the probability density, and if this is propagating like a wave, we know that there should probably be some conservation rule to prevent the distribution from going to zero or diverging:

$$\frac{\partial \rho}{\partial t} - \vec{\boldsymbol{\nabla}} \cdot \vec{\mathbf{J}} = 0$$

where $\vec{\mathbf{J}}$ is the probability current.

$$\imath\hbar \frac{\partial \rho}{\partial t} = \imath\hbar \left[\left(\frac{\partial \psi^*}{\partial t} \right) \psi + \psi^* \left(\frac{\partial \psi}{\partial t} \right) \right] = [(-H\psi^*)\psi + \psi^* H \psi]$$

Using $V = V^*$, we can write this as

$$\begin{aligned} \imath\hbar \frac{\partial \rho}{\partial t} &= - \left(\frac{-nabla^2}{2m} \psi^* \right) \psi + \psi^* \left(- \frac{nabla^2}{2m} \right) \psi \\ &= \frac{\vec{\mathbf{nabla}}}{2m} \cdot \left[\psi^* \vec{\boldsymbol{\nabla}} \psi - (\vec{\boldsymbol{\nabla}} \psi^*) \psi \right] \end{aligned}$$

so

$$\vec{\mathbf{J}} = \frac{\hbar}{2\imath m} \left[\psi^* (\vec{\boldsymbol{\nabla}} \psi) - (\vec{\boldsymbol{\nabla}} \psi^*) \psi \right] = \frac{\hbar}{m} \operatorname{Im} \left[\psi^* \vec{\boldsymbol{\nabla}} \psi \right]$$

We can put any wave function into the form

$$\psi(x, t) = \sqrt{\rho(x, t)} e^{\imath S(x,t)/\hbar}$$

where $\rho \in \mathbb{R}^+$ and $S \in \mathbb{R}$. In terms of this parameterization,

$$\vec{\mathbf{J}} = \frac{\rho}{m} \vec{\boldsymbol{\nabla}} S$$

Thinking in this way, we want to find the classical limit of wave mechanics. There are two distinct ways to do this, geometric optics and wave optics. Here we are thinking about the canonical electromagnetic waves. Geometric optics correspond to particle-like behavior (reflection, refraction) while wave optics correspond to wavelike behavior (interference, diffraction). The wave optics description already contains the wavelike behavior of a quantum state, so we want to find the geometric optics limit. In the case where the wavelength is much smaller than the thing it's interacting with, it scatters like a ray. We expect the classical limit of quantum mechanics to behave the same way when the de Broglie wavelength is much less than the gradient of some potential the state is interacting with.

We can solve the classical equations of motion by finding a change of variables $(p, q) \to (P, Q)$ such that Q is a cyclic variable—H does not depend on it. This is useful because then the equations will read

$$\dot{P} = 0 \qquad \dot{Q} = P$$

so $P = P_0$ and $Q = P_0 t + Q_0$.

If you find such a coordinate transform, you can easily solve the system for some initial conditions. Let's consider a trivial example:

Example.

$$H = \frac{\vec{\mathbf{p}}^2}{2m} + V(\vec{\mathbf{x}}^2)$$

If we change variables to $\{r, \theta, \varphi\}$, θ and φ are cyclic, so we know that $\theta = \omega t + \theta_0$ and similar for φ, since $V(\vec{\mathbf{x}}^2) = V(r)$. ◇

More generally, we would like to transform coordinates from $Q_i = Q_i(q_i, p_i, t)$, $P_i = P_i(q_i, p_i, t)$ in a restricted way to preserve the form of Hamilton's equations. In other words, we want the equations of motion in the new system to be

$$\dot{Q} = \frac{\partial H'}{\partial P} \qquad \dot{P} = \frac{\partial H'}{\partial Q}$$

which is just the Poisson bracket formulation with $\frac{\partial Q}{\partial Q} = \frac{\partial P}{\partial P} = 1$. Such transformations are called canonical.

$$p\dot{q} - H = P\dot{Q} - H' + \frac{\mathrm{d}}{\mathrm{d}t}F$$

F is called the generating function the transformation. $F = F(q, Q, p, P, t)$, but for now let's choose $F(q, Q, t)$:

$$p\dot{q} - H = P\dot{Q} - H' + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial Q}\dot{Q}$$

since q and Q are independent variables, we can equate the like parts on either side of the equation to find that

$$\frac{\partial F}{\partial q} = p \qquad P = -\frac{\partial F}{\partial Q}$$

and

$$H = H' - \frac{\partial F}{\partial t}$$

Lecture 27: Canonical Transformations
Monday, March 30, 2020

Disclaimer

I missed the beginning of this lecture, so the following notes might not make much sense.

Consider a generating functional which is now a function of q and P: $F(q, P)$. We want to choose F such that $H' = 0$. If this is true,

$$\begin{aligned} p\dot{q} - H = P\dot{Q} - H + \frac{\mathrm{d}F}{\mathrm{d}t} &= -\dot{P}Q - H' + \frac{\mathrm{d}F}{\mathrm{d}t} \\ &= -\dot{P}Q - H' + \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial P}\dot{P} \end{aligned}$$

so we get that

$$Q = \frac{\partial F}{\partial P} \qquad p = \frac{\partial F}{\partial q}$$

and

$$-H = -H' + \frac{\partial F}{\partial t}$$

We want $H' = 0$, so

$$\frac{\partial F}{\partial t} + H = 0$$

If we then convert p, we get

$$H(q, p) = H(q, \frac{\partial F}{\partial q})$$

so

$$\frac{\partial F(q, P)}{\partial t}_{H}(q, \frac{\partial F}{\partial q}) = 0$$

or

$$\frac{\partial F(q, \alpha, t)}{\partial t} + H(q, \frac{\partial F}{\partial q}) = 0 \qquad \text{(Hamilton-Jacobi Equation)}$$

Often we write $F \equiv S$ and call it Hamilton's principal function. More generally,

$$H(q_1, \cdots, q_n, \frac{\partial S}{\partial q_1}, \cdots, \frac{\partial S}{\partial q_n}, t) + \frac{\partial S}{\partial t} = 0$$

Example. Let's do an example with a simple harmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$$

By our Hamilton-Jacobi Equation, we have

$$0 = \frac{1}{m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2}m\omega^2 q^2 + \frac{\partial S}{\partial t}$$

We can make an ansatz $S \equiv w - \alpha t$ where W is called the characteristic function. We can now solve for this W:

$$W = \sqrt{2m\alpha}\int \mathrm{d}q \left[1 - \frac{m\omega^2 q^2}{2\alpha}\right]^{1/2}$$

We can make $Q = \frac{\partial S}{\partial \alpha} = \beta\sqrt{\frac{2m}{\alpha}}\int \mathrm{d}q \frac{1}{\left[1-\frac{m\omega^2 q^2}{2\alpha}\right]^{1/2}}$, so

$$\beta = \sqrt{\frac{2m}{\alpha}}\int \mathrm{d}q \frac{1}{\left[1 - \frac{m\omega^2 q^2}{2\alpha}\right]^{1/2}}$$

and

$$t + \beta = \frac{1}{\omega}\sin^{-1}\left[q\sqrt{\frac{2\alpha}{m\omega^2}}\right]$$

or

$$q = \frac{1}{\omega}\sin^{-1}(\omega t + \beta)\sqrt{\frac{2\alpha}{m\omega^2}}$$

◇

Remember that we started with the assumption that

$$\psi = \sqrt{\rho}e^{\imath S/\hbar}$$

If we plug this into the Schrödinger equation, we find

$$-\frac{\hbar^2}{2m}\left[\nabla^2\sqrt{\rho} + \frac{2\imath}{\hbar}(\vec{\boldsymbol{\nabla}}\sqrt{\rho})\cdot(\vec{\boldsymbol{\nabla}}\sqrt{\rho}) - \frac{1}{\hbar^2}\sqrt{\rho}(\vec{\boldsymbol{\nabla}}S)^2 + \frac{\imath}{\hbar}\sqrt{\rho}\nabla^2 S\right] + \sqrt{\rho}V = \imath\hbar\left[\frac{\partial\sqrt{\rho}}{\partial t} + \frac{1}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right]$$

Let's keep only the leading order terms in $\hbar$, since we want to take $\hbar \to 0$:

$$\frac{\sqrt{q}}{2m}(\vec{\boldsymbol{\nabla}}S)^2 + \sqrt{\rho}V = \imath\sqrt{\rho}\frac{\partial S}{\partial t}$$

or

$$\frac{(\vec{\boldsymbol{\nabla}}S)^2}{2m} + V - \imath\frac{\partial S}{\partial t} = 0$$

The solutions to this equation are "wave functions" in the semi-classical limit as $\hbar \to 0$. What this says is that the length of the wave function should be much less than the scale of the potential. This is often referred to as the WKB approximation.

Lecture 28: The W.K.B. Approximation

Wednesday, April 01, 2020

The idea we are using is a coordinate transform that makes the Hamiltonian zero, such that the coordinates are constants of motion. We write the Hamilton-Jacobi equation as

$$H\left(q, \frac{\partial S}{\partial q}\right) + \frac{\partial S}{\partial t} = 0$$

We showed how to find S for the trivial Harmonic oscillator. Then we linked this to quantum by writing our wave function as

$$\psi = \sqrt{\rho} e^{\imath S/\hbar}$$

Now we are going to explore the W.K.B Approximation. If H is a constant, we can make the ansatz

$$S = W - Et$$

where W is Hamilton's principle function. If we write out the Hamilton-Jacobi equation, we now get

$$\frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + V(q) = E$$

where we used the fact that $p = \frac{\partial S}{\partial q} = \frac{\partial W}{\partial q}$. Now we can simply solve for W:

$$W = \int \sqrt{(E - V(q))(2m)}\, \mathrm{d}q$$

Let's see if we can use this to find our wave function. Remember that

$$\psi = \sqrt{\rho} e^{\imath S/\hbar} = \sqrt{\rho} e^{\imath W/\hbar + \imath E t/\hbar}$$

If this is an eigenstate of energy, $\frac{\partial \rho}{\partial t} = 0$ and by conservation of probability, $\frac{\partial \rho}{\partial t} + \vec{\boldsymbol{\nabla}} \cdot \vec{\mathbf{j}} = 0$, so

$$\vec{\boldsymbol{\nabla}} \cdot (\psi^* \vec{\boldsymbol{\nabla}} \psi) = 0 = \vec{\boldsymbol{\nabla}} \cdot (\rho \vec{\boldsymbol{\nabla}} S)$$

so

$$\rho \frac{\partial W}{\partial q} = \rho \sqrt{2m(E - V(q))} = \text{const}$$

so

$$\rho \sim \frac{1}{\sqrt{2m(E - V(q))}}$$

Therefore, our wave function, up to normalization, is

$$\psi \sim \frac{1}{(E - V(q))^{1/4}} e^{\frac{\imath}{\hbar}\int \mathrm{d}q' \sqrt{2m(E - V(q))}} e^{-\imath E t/\hbar}$$

This is the W.K.B. Approximation. Where is it valid? Recall that when we plugged our wave function into the Schrödinger equation and dropped higher-order $\hbar$ terms, we found that

$$\hbar \left| \frac{\mathrm{d}^2 W}{\mathrm{d}q^2} \right| << \left| \frac{\mathrm{d}W}{\mathrm{d}q} \right|^2$$

tells us when the W.K.B Approximation is valid (when we can take $\hbar \to 0$). If we put our expression for W in here, we find

$$W = \int \mathrm{d}q' \sqrt{2m(E - V(q'))}$$

$$\frac{\mathrm{d}W}{\mathrm{d}q} = \sqrt{2m(E - V(q))}$$

$$\frac{\mathrm{d}^2 W}{\mathrm{d}q^2} = \frac{m \frac{\mathrm{d}V}{\mathrm{d}q}}{\sqrt{2m(E - V(q))}}$$

so the validity criteria becomes

$$\frac{\hbar}{\sqrt{2m(E - V(q))}} << \frac{2(E - V(x))}{\frac{\mathrm{d}V}{\mathrm{d}x}}$$

or

$$\frac{\frac{\mathrm{d}V}{\mathrm{d}q}}{2(E - V(q))} << \sqrt{2m(E - V(q))}/\hbar$$

The wavelength is $\frac{p}{\hbar} = \frac{1}{\lambda}$ we say that $p(q) = \sqrt{2m(E - V(q))}$ in the classical limit (since $E - V$ is the kinetic energy), so the criteria which must be met to use the W.K.B. Approximation is

$$\frac{1}{\lambda} >> \frac{\frac{\mathrm{d}V}{\mathrm{d}q}}{(\mathrm{KE})}$$

Suppose we wanted to calculate some bound-state energies using this approximation. We have a slight problem when $E \sim V(x_i)$, we call x_i the turning points. If we think of this as a classical problem, these turning points are where the particle turns around in the harmonic oscillator, but in quantum, we know that there is a nonzero probability of the particle escaping the potential when it reaches this reason. Our approximation will not work here, but we know that the wave function should decay exponentially when it is below the potential, while we should have an oscillating solution inside the potential. To do this, we solve the system outside and inside using W.K.B., but we have to switch the sign inside the square root (since outside the potential well we want $V - E$ not $E - V$). We then match these solutions at the turning points. We find an interesting property:

$$h\left(n + \frac{1}{2}\right) = \int_{x_1}^{x_2} \left[2m(E - V(q))\right]^{1/2} \mathrm{d}q \qquad n \in \mathbb{Z} \qquad \text{(Bohr-Sommerfeld Quantization)}$$

where $h = 2\pi\hbar$. This turns out to only be valid for large n because that is where the potential is much larger than the wavelength (this was originally derived using the idea that the orbits of electrons were quantized by how many wavelengths it takes to match the ends up for a particular orbit). Consider the following potential:

$$V(x) = A|x|$$

First, let's find the turning points. This is where $E = \pm A|x|$. Therefore, the Bohr-Sommerfeld quantization tells us

$$\left(n + \frac{1}{2}\right) h = \int_{-E/A}^{E/A} \sqrt{E - A|x|}\,\mathrm{d}x = 2\int_0^{E/A} \sqrt{E - Ax}\,\mathrm{d}x$$

so

$$E_n = \left[\frac{A}{\sqrt{2m}\frac{3}{4}\left(n + \frac{1}{2}h\right)}\right]^{2/3}$$

This can be solved exactly, and the eigenfunctions are Airy functions. It works to four significant digits for $n \geq 3$, which is incredibly well for an approximation (this is not necessarily the case for more generic models).

We will re-derive the semi-classical approximation when we cover the path integral formulation, and it will show us why the ansatz of the wave function had the form it did.

0.17 The Path Integral Formulation

The path integral formulation is an alternative interpretation of quantum mechanics which lets us do some calculations with great ease (but of course makes other problems harder). One important component is the propagator, which we know as the time evolution operator: $U(x_1, t_1; x_2, t_2)$. We know that the time evolution of a state can be written

$$|\psi(t)\rangle = \sum_n e^{-\imath E_n t/\hbar} |n\rangle \langle n|\psi(0)\rangle$$

If we project to the x basis, we find

$$\langle x|\psi(t)\rangle = \sum_n u_n(x) e^{-\imath E_n t/\hbar} c_n$$

where $c_n = \int \mathrm{d}^3x' \langle n|x'\rangle \langle x'|\psi(0)\rangle$ and $u_n(x) = \langle x|n\rangle$. We can write this as

$$\psi(t, x) = \int \mathrm{d}^3x'\, u_n(x) u_n^*(x') \psi(x', t = 0) e^{-\imath E_n t/\hbar} \equiv \int \mathrm{d}^3x'\, K(x, x', t, t') \psi(x', t = 0)$$

where

$$k(x,x';t,t') \equiv \sum_n u_n(x)u_n^*(x')e^{-\imath E_n(t-t')/\hbar}$$

is the propagator (although we usually set $t'=0$). Notice that if $t\to 0$, then $K(x,x';t,t')\to\delta^n(\vec{\mathbf{x}}-\vec{\mathbf{x}}')$ (for however many dimensions n we are working with). What's interesting about this propagator is that it contains all the information we need about the energy eigenstates. Let's take the Fourier transform of K where we set $x'=x$ and I will abbreviate $t'=0$ by not writing it:

$$\begin{aligned}\int \mathrm{d}t\, e^{\imath\omega t}K(x,x;t)\,\mathrm{d}x &= \int \mathrm{d}t\, e^{\imath\omega t}\sum_n u_n(x)u_n^*(x)e^{-\imath E_n t/\hbar}\\ &= \int \mathrm{d}t\sum_n \mathrm{d}x\,\langle n|x\rangle\,\langle x|n\rangle\, e^{-\imath\left(\frac{E_n t}{\hbar}-\omega t\right)}\\ &= \sum_n \int \mathrm{d}t\, e^{-\imath\left(\frac{E_n t}{\hbar}-\omega t\right)}\\ &= \sum_n (2\pi)\delta\left(\frac{E_n}{\hbar}-\omega\right)\end{aligned}$$

so knowing the propagator pretty much solves the system exactly. Let's calculate the propagator for a free particle:

$$K(x,x';t) = \int \mathrm{d}p\,\frac{1}{2\pi\hbar}e^{\imath px/\hbar}e^{-\imath px'/\hbar}e^{-\imath\frac{p^2}{2m}t/\hbar} = \sqrt{\frac{m}{2\pi\imath\hbar t}}e^{\frac{\imath m(x-x')^2}{2\hbar t}}$$

Lecture 29: The Path Integral

Friday, April 03, 2020

When we last left off, we were discussing the propagator

$$k(x_f,t_f;x_i,t_i) = \sum_n u_n(x_f)u_n^*(x_i)e^{-\imath E_n\Delta t/\hbar}$$

We did this by starting with $\langle x_f t_f|x_i t_i\rangle$ and inserting a complete set f states. Notice the boundary condition, where $t_i\to t_f$ gives us

$$k(x_f,t_f;x_i,t_i) = \delta(x_i-x_f)$$

Physically, this is just saying that the probability of moving from x_i to x_f instantaneously is zero unless they're the same. If we consider

$$\int \mathrm{d}x\lim_{x'\to x}\sum_n e^{-E_n t/\hbar}\langle x|n\rangle\langle n|x'\rangle = \sum_n e^{-\imath E_n t/\hbar}\equiv G(t)$$

If we take $t\to -\imath\tau$, then

$$G(-\imath\tau) = \sum_n e^{-\tau E_n/\hbar}\sim\sum_n e^{-\beta H}$$

There seems to be some connection between quantum mechanics in real time and statistical mechanics in imaginary time. Last time we were working through calculating the propagator for a free particle.

$$\begin{aligned}k(x,x';\delta t) &= \int\frac{\mathrm{d}p}{2\pi}\langle x|p\rangle\langle p|x'\rangle\, e^{-\frac{\imath p^2\delta t}{2m\hbar}}\\ &= \int\frac{\mathrm{d}p}{2\pi}e^{\imath p(x-x')/\hbar}e^{-\frac{\imath p^2\Delta t}{2m\hbar}}\\ &= \sqrt{\frac{m}{2\pi\imath\hbar\Delta t}}e^{\frac{\imath m(x-x')^2}{2\hbar\Delta t}}\end{aligned}$$

0.17.1 The Propagator as a Green's Function of the Wave Equation

If we have some differential operator O where $O\varphi(x) = J(x)$. We can solve this by calculating the Green's function, which is defined as

$$OG(x, x') = \delta(x' - x)$$

Once we have this,

$$O[\varphi(x) = \int \mathrm{d}x'\, G(x - x')J(x')] = \int \mathrm{d}x'\, \delta(x - x')J(x') = J(x)$$

The Schrödinger equation can be written as

$$\left(\imath\hbar\frac{\partial}{\partial t} - H_0\right)|\psi\rangle = V\,|\psi\rangle$$

where $H = H_0 + V$. The Green's function is the propagator, so we want to find

$$\left(\imath\hbar\frac{\partial}{\partial t} - H_0\right)k(\vec{\mathbf{x}}_i, t_i; \vec{\mathbf{x}}_f, t_f) = \delta^3(xvece - \vec{\mathbf{x}}')\delta(t_i - \delta_f)$$

which would mean that

$$\psi(x, t) = \int \mathrm{d}^3x'\, k(x, x'; \Delta t)V$$

Now if we operate with the differential operator, we see that the Schrödinger equation is satisfied. We can find k by solving the equation with the δ function, and the easiest way to do this is in momentum space, where the equation we want to solve is

$$\left(\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m}\right)K(\vec{\mathbf{p}}, \omega) = \frac{1}{(2\pi)^4}$$

so

$$k(\vec{\mathbf{p}}, \omega) = \frac{1}{(2\pi)^4}\frac{1}{\left(\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m}\right)}$$

However, this equation has a pole in it, so the inverse Fourier transform is not well-defined. We have to do this in a careful way:

$$k(x_f - x_i; t_f - t_i) = \int \frac{\mathrm{d}^3p\,\mathrm{d}\omega}{(2\pi)^4}\frac{e^{\imath\frac{\vec{\mathbf{p}}\cdot\Delta x}{\hbar} - \imath\omega\Delta t}}{\hbar\omega - \frac{\vec{\mathbf{p}}^2}{2m} \pm \imath\epsilon}$$

We need to integrate around the pole in either the lower half-plane or the upper half=plane. If $t_f < t_i$, the probability should be zero, so if $\Delta t < 0$, $k = 0$ to preserve causality. By the Jordan curve theorem, we want to close in the lower half-plane.

$$k = -\frac{2\pi i}{(2\pi)^4}\int \mathrm{d}^3p\, e^{\frac{\imath\vec{\mathbf{p}}\cdot\Delta\vec{\mathbf{x}}}{\hbar} + \frac{\imath\vec{\mathbf{p}}^2}{2m\hbar}\Delta t}$$

which gives us the same result as when we calculated the free-particle propagator before.

0.17.2 The Path Integral

Dirac said that the probability amplitude should be related to the integral of the Lagrangian due to the time difference:

$$\langle x_f, t_f | x_i, t_i\rangle \sim e^{\imath\int L\mathrm{d}t}$$

We can do this by breaking up the path in $x - t$ space into many infinitesimal steps:

$$\langle x_f, t_f|\int \mathrm{d}^3x\,|x, t_f - \epsilon\rangle\,\langle x, t_f - \epsilon|\cdots|x_i, t_i\rangle$$

or

$$\langle x_f, t_f | x_i t_i \rangle = \lim_{n\to\infty} \int \mathrm{d}^3 x_1 \cdots \mathrm{d}^3 x_n \, \langle x_1, t_f | x_1, t_f - \epsilon \rangle \, \langle x_1, t_f - \epsilon | x_2, t_2 - 2\epsilon \rangle \cdots$$

where $n\epsilon = t_f - t_i$. Each one of these steps can be written as

$$\langle x_m | x_{m+1} \rangle - \frac{\imath\epsilon}{\hbar} \langle x_m | \, H \, | x_{m+1} \rangle$$

We know that

$$\langle x_m | \, f(x) \, | x_{m+1} \rangle = f(x_m)\delta(x_m - x_{m+1}) \equiv \frac{f(x_m + x_{m+1})}{2} \int \frac{\mathrm{d}p}{(2\pi)\hbar} e^{\frac{\imath p(x_m - x_{m+1})}{\hbar}}$$

If we do this as a function of p, we get

$$\langle x_m | \, f(p) \, | x_{m+1} \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} f(p) e^{\imath p(x_m - x_{m+1})/\hbar}$$

so that

$$\langle x_m + 1 | \, e^{-\imath\epsilon H/\hbar} \, | x_m \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} e^{-\imath\epsilon H\left(\frac{x_m - x_{m+1}}{2}, p\right)}$$

We then have to repeat this over an over for each small step:

$$\left[\prod_{k=1}^{N} \int \mathrm{d}x_k \, \frac{\mathrm{d}p_k}{2\pi\hbar}\right] e^{\imath \sum_k p_k(x_{k+1} - x_k) - \imath\epsilon H\left(\frac{x_{k+1} - x_k}{2}, p_k\right)}$$

In the limit as $N \to \infty$, $\epsilon \to 0$ and $N\epsilon = t_f - t_i$, we can write this as

$$\int Dx(t) Dp(t) e^{\imath \int_{t_i}^{t_f} p\dot{x} - H} = \langle x_f, t_f | x_i, t_i \rangle$$

as long as $x(t_i) = x_i$ and $x(t_f) = x_f$. This is what's known as a functional integral. We are integrating over all possible functions of time (that's what $Dx(t)$ refers to, rather than $\mathrm{d}x$). You can recognize the exponential as the Lagrangian.

Lecture 30: The Path Integral, Continued

Monday, April 06, 2020

We can write the phase space version of the path integral as

$$\langle x_f t_f | x_i t_i \rangle = \int Dx(t) Dp(t) e^{\imath \int_0^t p\dot{x} - H}$$

We essentially have an action

$$S = \int \mathrm{d}t \, [p\dot{x} - H(p, x)]$$

Take the special case where the potential does not depend on the momentum:

$$H = \frac{p^2}{2m} + V(x)$$

Here, the momentum integral is Gaussian:

$$\begin{aligned}
\int Dx(t) \int Dp(t) e^{\imath \int -\frac{p^2}{2m} + p\dot{x} + V(x)} &= \int Dx(t) \int Dp(t) e^{\imath \int -\frac{1}{2m}(p - m\dot{x})^2 + \frac{1}{2}m\dot{x}^2 + V(x)} \\
&\quad p \to p + mx \\
&= \int Dx(t) \int Dp(t) \mathbf{J} e^{\imath \int_0^T \left(\frac{p^2}{2m} + \frac{1}{2}m\dot{x}^2 - V(x)\right)} \\
&= \hat{\mathbf{N}} \int Dx(t) e^{\imath \int_0^T L \mathrm{d}t}
\end{aligned}$$

where $\hat{\mathbf{N}}$ is a normalization constant from the Gaussian integral which we will determine later. Let's do an example with a free particle. We split up the path into a number of time steps $\Delta t + \epsilon$ with $N\epsilon = T_{\text{tot}}$ and we take the limit as $N \to \infty$ and $\epsilon \to 0$. Our amplitude then becomes

$$\begin{aligned}\langle x_f t_f | x_i t_i \rangle &= \lim \int \mathrm{d}x_1 \dots \mathrm{d}x_{N-1}\, e^{\imath \sum_{i=1}^{N-1} \frac{\epsilon}{2} \frac{m}{\hbar} \frac{(x_i - x_{i+1})^2}{\epsilon^2}} \\ \sqrt{\frac{m}{2\hbar\epsilon}} x_i \to y_i& \\ &= \lim \int \mathrm{d}y_1 \dots \mathrm{d}y_{N-1} \left(\frac{2\hbar\epsilon}{m}\right)^{\frac{N-1}{2}} e^{\imath \sum_{i=1}^{N-1} (y_i - y_{i+1})^2}\end{aligned}$$

Consider $\int \mathrm{d}y_1$:

$$\begin{aligned}\int \mathrm{d}y_1\, e^{\imath\left((y_1-y_0)^2 + (y_2-y_1)^2 + \dots\right)} &= \int \mathrm{d}y_1\, e^{\imath(y_0^2+y_2^2)} e^{-2\imath y_1 y_0 - 2\imath y_2 y_1 + 2y_2^2 \dots} \\ &= e^{\imath(y_0^2+y_2^2)} \int \mathrm{d}y_1\, e^{2(y_1^2 - y_1(y_0+y_2))} \\ &= e^{\imath(y_0^2+y_2^2)} \int \mathrm{d}y_1\, e^{-2\imath\left(y_1 - \frac{(y_0+y_2)}{2}\right)^2} e^{-2\imath\frac{(y_0+y_2)^2}{4}} \\ &= e^{\imath(y_0^2+y_2^2)} e^{-\frac{\imath}{2}(y_0+y_2)^2} \int \mathrm{d}y_1\, e^{2\imath y_1^2} \\ &= e^{\frac{\imath}{2}(y_0-y_2)^2} \left(\frac{\imath\pi}{2}\right)^{1/2}\end{aligned}$$

Doing the $\mathrm{d}y_2$ integration, we can start to see the pattern:

$$\begin{aligned}\left(\frac{\imath\pi}{2}\right)^{1/2} \int \mathrm{d}y_2\, e^{\frac{\imath}{2}(y_0-y_2)^2} e^{\imath(y_2-y_3)^2} &= \left(\frac{\imath\pi}{2}\right)^{1/2} \left(\frac{2\pi\imath}{3}\right)^{1/2} e^{-\frac{(2y_3^2+y_0^2)}{2\imath}} e^{\frac{(y_0+2y_3)}{6\imath}} \\ &= \left(\frac{\imath\pi}{3}\right)^{1/2} e^{-\frac{\imath}{3}(y_3-y_0)^2}\end{aligned}$$

We can see that repeating this process will turn these 3's into N's, so our final result will be

$$\begin{aligned}\hat{\mathbf{N}} \left(\frac{\imath\pi}{N^{1/2}}\right)^{\frac{N-1}{2}} e^{\imath(y_N-y_0)^2/N} \left(\frac{2\hbar\epsilon}{m}\right)^{\frac{N-1}{2}} &= \hat{\mathbf{N}} \left(\frac{2\hbar\epsilon}{m}\right)^{\frac{N-1}{2}} \left(\frac{2\hbar\epsilon}{m}\right)^{\frac{N-1}{2}} \frac{(\imath\pi)^{\frac{N-1}{2}}}{N^{1/2}} e^{\frac{\imath m(x_0-x_N)^2}{2\hbar T_{\text{tot}}}} \\ \langle x_t t_t | x_i t_i \rangle &= \hat{\mathbf{N}} \left[\frac{2\pi\imath\hbar\epsilon}{m}\right]^{N/2} \left(\frac{m}{2\pi\imath\hbar T}\right) e^{\frac{\imath(x_0-x_N)^2}{2\hbar T}}\end{aligned}$$

We can fix $\hat{\mathbf{N}}$ by saying that as $t_f \to t_i$, this whole thing should be $\delta(x_f - x_i)$. We know that the following can act as a definition of the δ function (a Gaussian integral with vanishing variance):

$$\lim_{T\to 0} \frac{m}{2\pi\imath\hbar T} e^{\frac{\imath\Delta x^2}{m} 2\hbar T} = \delta(x_f - x_i)$$

so

$$\hat{\mathbf{N}} = \left[\frac{2\pi\hbar\epsilon\imath}{m}\right]^{-N/2}$$

so we end up with

$$\langle x_f t_f | x_i t_i \rangle = \left(\frac{m}{2\pi\imath\hbar T}\right) e^{\frac{\imath m(x_0-x_N)^2}{2\hbar T}}$$

which is what we got using canonical methods. In general, you cannot solve the path integral in closed form, although there are various special cases where you can solve it, for instance, any potential which is quadratic (or of lower order) in x. There are also other systems known as integrable systems, but those are more of the exception rather than the rule. We can now do some examples of things that would be incredibly painful without the path integral. The path integral sort of explains the classical limit.

$$\langle x_t t_t | x_i t_i \rangle \sim Dx(t) e^{\imath S/\hbar}$$

If we think of these paths as functions of t, we are imagining integrations over many different paths. However, there is a classically preferred path which extremizes the action. If you consider nearby paths and suppose S is large in units of $\hbar$, then on average, nearby paths around the preferred classical path will cancel each other out. However, in the region that $\frac{\partial S}{\partial x} \sim 0$, the classical path will dominate and the nearby paths will not cancel out. The farther away from the classical path, the more the phase will vary, and those paths will typically average out to zero if the action is much larger than $\hbar$. Now remember there are systems which just inherently don't act classically. The low n states of the hydrogen atom are not classical, and the reason is because the action is much smaller than $\hbar$. If we want large phases, $H >> \hbar$. To do this, we could just make the kinetic energy much larger than the potential energy, or $\frac{KE>>PE}{\hbar}$. When we were studying the WKB approximation, we found this condition: $\frac{\hbar\frac{\partial V}{\partial x}}{E-V} << \frac{1}{\lambda} \sim [(E-V)(2m)]^{1/2}$. Notice that if $E >> V$, this condition will be met as long as $\frac{\partial V}{\partial x}$ is not too large. This is called the Eikonal limit.

LECTURE 32: BERRY'S PHASE
Friday, April 10, 2020

0.18 The Adiabatic Approximation

Theorem 0.18.1. *Adiabatic Theorem Take some system in an energy eigenstate and turn on a time dependence by allowing one of the parameters in the Hamiltonian to be time dependent ($\lambda \to \lambda(t)$). For instance, a particle in a box of size L and letting $L \to L(t)$, where we grow or shrink the size of the box in time. If $|\psi\rangle = |n, L\rangle$ at $t = 0$, then as we propagate in time, if the parameter is changing slowly enough, the system will stay in the same eigenstate, but an eigenstate of the new Hamiltonian: $t > 0 \implies |\psi\rangle = |n, L(t)\rangle$.*

To prove this, suppose we have the Schrödinger equation on a state

$$\imath\hbar\frac{\partial}{\partial t}|\alpha, t\rangle = H|\alpha, t\rangle$$

where

$$|\alpha, t\rangle = \sum_n c_n(t)e^{\imath\theta_n(t)}|n\rangle$$

If H is independent of time, then

$$|\alpha, t\rangle = \sum_n c_n e^{-\imath E_n t/\hbar}|n\rangle$$

where $c_n = \langle n|\alpha, t = 0\rangle$ or $\theta_n(t) = -E_n t/\hbar$.

However, if we allow for this additional time dependence, we would write

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,\mathrm{d}t'$$

This is an inspired guess based on the time-independent limit. Now we can apply the Schrödinger equation:

$$\imath\hbar\frac{\partial}{\partial t}|\alpha, t\rangle = \sum_n(\imath\hbar)\left[\dot{c}_n(t)|n\rangle + c_n(t)(\imath\dot{\theta}_n(t))|n, t\rangle + c_n\frac{\partial}{\partial t}|n, t\rangle\right]e^{\imath\theta_n(t)}$$

where $\imath\dot{\theta}_n(t) = (-\imath)\hbar E_n(t)$. Therefore

$$\imath\hbar\frac{\partial}{\partial t}|\alpha, t\rangle = \sum_n e^{\imath\theta_n(t)}\imath\hbar\left[\dot{c}_n + \frac{E_n}{\hbar}c_n(t) + c_n\frac{\partial}{\partial t}\right]|n, t\rangle$$

and

$$H|\alpha, t\rangle = \sum_n c_n e^{\imath\theta_n}E_n|n, t\rangle$$

so this term cancels out. Let's project onto $\langle m,t|$

$$\imath\hbar\dot{c}_m e^{\imath\theta_m(t)} + \imath\hbar\sum_n c_n \langle m,t| e^{\imath\theta_n(t)} \frac{\partial}{\partial t}|n,t\rangle = \langle m,t| \sum_n c_n e^{\imath\theta_n} E_n |n,t\rangle = 0$$

so

$$\dot{c}_m = -\sum_m c_n \langle m,t| \frac{\partial}{\partial t}|n,t\rangle e^{\imath(\theta_n(t)-\theta_m(t))}$$

Note that if $\frac{\partial}{\partial t}|n\rangle = 0$, then $\dot{c}_m = 0$, which makes sense. We can break this up into two parts:

$$\dot{c}_m = -c_n \langle n,t| \frac{\partial}{\partial t}|n,t\rangle - \sum_{n\neq m} c_n \langle m,t| \frac{\partial}{\partial t}|n,t\rangle e^{\imath(\theta_n-\theta_m)}$$

For the second term, consider

$$\frac{\partial}{\partial t}\left[H|n,t\rangle\right] = \frac{\partial}{\partial t}\left[E_n(t)|n,t\rangle\right]$$
$$\dot{H}|n,t\rangle + H\frac{\partial}{\partial t}|n,t\rangle = \dot{E}_n(t)|n,t\rangle + E_n\frac{\partial}{\partial t}|n,t\rangle$$

If we then project onto $m \neq n$, we find

$$\left[\langle nt|\dot{H}|n,t\rangle + E_m(t)\langle m,t|\frac{\partial}{\partial t}|n,t\rangle\right] = E_n\langle m,t|\frac{\partial}{\partial t}|n,t\rangle$$

so

$$\langle m,t|\frac{\partial}{\partial t}|n,t\rangle = \frac{\langle m,t|\dot{H}|n,t\rangle}{E_n - E_m}$$

Now that we have this piece, we can insert it into our differential equation:

$$\dot{c}_m = -c_m\langle m,t|\frac{\partial}{\partial t}|m,t\rangle - \sum_{n\neq m} c_n \frac{\langle m,t|\dot{H}|n,t\rangle}{E_n - E_m} e^{\theta_n-\theta_m}$$

The adiabatic approximation is simply dropping the second term, which is a statement that the rate of change in H is much smaller than the natural frequencies associated with the energies of the states. We can solve this differential equation as

$$c_m = e^{\imath\gamma_m(t)}c_m(0)$$

where $\imath\gamma_m(t) = -\langle m,t|\frac{\partial}{\partial t}|m,t\rangle$. Now we can reinsert this into our equation for the wave function:

$$|\alpha,t\rangle = \sum_n c_n(0)e^{\imath\gamma_n(t)}e^{\imath\theta_n(t)}|n,t\rangle$$

where $\gamma_n \in \mathbb{R}$ is called the adiabatic phase. θ_n is the canonical phase from time evolution which we defined above. This adiabatic phase was known for a very long time, but the reason it is interesting is that it is purely geometric.

First, let's prove $\gamma_n \in \mathbb{R}$. Notice that if it weren't real, the wave function's norm would change, which would violate unitarity.

$$I = \int_0^t \langle n,t|\frac{\partial}{\partial t}|n,t\rangle$$

so

$$\begin{aligned}\operatorname{Im} I &= \int_0^t \left(\langle n,t|\frac{\partial}{\partial t}|nt\rangle - (\langle n,t|\frac{\partial}{\partial t}|n,t\rangle)^*\right)\\ &= \int_0^t \left(\langle n,t|\frac{H}{\imath\hbar}|n,t\rangle - \langle n,t|\frac{H}{\imath\hbar}|n,t\rangle\right)\end{aligned}$$

From this, it is easy to see that $\gamma_m^* = \gamma_m$

Now let's prove that Berry's phase is purely geometric. Suppose $H(\vec{\mathbf{R}}(t))$. Then

$$\langle n,t|\frac{\partial}{\partial t}|n,t\rangle = \langle n,t|\frac{\mathrm{d}\vec{\mathbf{R}}}{\mathrm{d}t}\frac{\mathrm{d}}{\mathrm{d}\vec{\mathbf{R}}}|n,t\rangle = \langle n,t|\dot{\vec{\mathbf{R}}}\cdot\vec{\boldsymbol{\nabla}}_R|n,t\rangle$$

$\vec{\mathbf{R}}$ is not a coordinate in space, it is a coordinate in the parameter space. In other words, we don't mean $\vec{\mathbf{R}} = (x,y,z)$, we mean that it could be anything, like the components of a magnetic field. From this we see that

$$\begin{aligned}\gamma_n &= \imath\int_0^t \langle n,t'|\vec{\boldsymbol{\nabla}}_R|n,t'\rangle\,\frac{\mathrm{d}\vec{\mathbf{R}}}{\mathrm{d}t'}\,\mathrm{d}t' \\ &= \imath\int_{\vec{\mathbf{R}}(0)}^{\vec{\mathbf{R}}(t)} \langle n,t'|\vec{\boldsymbol{\nabla}}_R|n,t'\rangle\cdot\mathrm{d}\vec{\mathbf{R}}\end{aligned}$$

If we call the matrix element $\vec{\mathbf{A}}$, then this phase looks like

$$e^{\imath\int_{R(0)}^{R(t)}\vec{\mathbf{A}}\cdot\mathrm{d}\vec{\mathbf{R}}}$$

What happens if we move in a closed loop? In this case, the adiabatic phase will give us

$$e^{\imath\oint\vec{\mathbf{A}}\cdot\mathrm{d}\vec{\mathbf{R}}} = e^{\imath\int(\vec{\boldsymbol{\nabla}}\times\vec{\mathbf{A}})\cdot\mathrm{d}a}$$

where a is the area of the surface we are working with. This is a bit of a cheat because Stoke's theorem is for three dimensions and the parameter space can have an arbitrary number of dimensions, but there is a generalization of Stoke's theorem that covers these cases. We can define $\vec{\mathbf{B}} = \vec{\boldsymbol{\nabla}}\times\vec{\mathbf{A}}$, so the phase is just

$$e^{\imath\Phi_B}$$

This is not a real "flux of a field", it is a mathematical name for something that looks like one. One of the things we will do is take a particle with spin and move it around in a magnetic field. As it turns out, it doesn't matter what path the particle takes, the only thing that effects the outcome is the angle between the plane of the path and the field. This is what it means to be geometric or topological. The mathematics doesn't care about the shape of the surface.

Lecture 33: Berry's Phase Continued

Monday, April 13, 2020

From last lecture, we found that if $H(t)\equiv H(\vec{\mathbf{R}}(t))$ where $\vec{\mathbf{R}}$ is some parameter-space vector and we let the system evolve adiabatically,

$$|n,t\rangle = e^{\imath\gamma_n(t)+\imath\theta_n(t)}\,|n,t=0\rangle$$

where

$$\imath\theta_n(t) = -\frac{\imath}{\hbar}\int^t E_n(t')\,\mathrm{d}t'$$

and

$$\gamma_n = \imath\int_{\vec{\mathbf{R}}(0)}^{\vec{\mathbf{R}}(t)}\mathrm{d}\vec{\mathbf{R}}\cdot\langle n,t|\,\vec{\boldsymbol{\nabla}}_R\,|n,t\rangle$$

We also discussed moving around closed loops in parameter space. We defined a fictitious vector potential $\vec{\mathbf{A}} = \imath\langle n,t|\,\vec{\boldsymbol{\nabla}}_R\,|n,t\rangle$, we can use Stoke's theorem to assert that

$$\gamma_n = \int\vec{\mathbf{B}}\cdot\hat{\mathbf{n}}\,\mathrm{d}A$$

where $\vec{\mathbf{B}}$ is a fictitious magnetic field associated with the vector potential:

$$\vec{\mathbf{B}} = \imath\sum_{n\neq m}\frac{\langle n,t|\,\vec{\boldsymbol{\nabla}}_R H\,|m,t\rangle\times\langle m,t|\,\vec{\boldsymbol{\nabla}}_R H\,|n,t\rangle}{(E_n-E_m)^2}$$

Let's work through an example.

Example. Take a spin in a (time-dependent, slow-moving) magnetic field:

$$H = -\frac{2\mu}{\hbar}\vec{\mathbf{S}}\cdot\vec{\mathbf{B}}(t)$$

with $\mu_e = \frac{eh}{2m_e c}$. Here, let's let our parameter-space be $\vec{\mathbf{R}} \equiv \vec{\mathbf{B}}$ (not to be confused with the fictitious magnetic field). Suppose the magnetic field starts in the $\hat{\mathbf{z}}$-direction:

$$\vec{\mathbf{R}}(t=0) \sim \hat{\mathbf{z}}$$

There are two energy states (aligned and anti-aligned):

$$E_\pm = \mp\mu\vec{\mathbf{R}}$$

and because we are moving adiabatically in $\vec{\mathbf{B}}$, the state will stay in one of these eigenstates. We can calculate the fictitious $\vec{\mathbf{B}}$-field. The denominator is

$$(E_\pm - E_\mp)^2 = 4\mu^2\vec{\mathbf{R}}^2$$

We also need the gradient of the Hamiltonian:

$$\vec{\boldsymbol{\nabla}}_R H = -\frac{2\mu}{\hbar}\vec{\mathbf{S}}$$

so

$$B_{n=\pm} = \imath\sum_n \frac{\langle n,t| - \frac{2\mu}{\hbar}\vec{\mathbf{S}}\,|m,t\rangle \times \langle m,t| - \frac{2\mu}{\hbar}\,|n,t\rangle}{(E_n - E_m)^2}$$

or

$$B_\pm = \sum_m \imath\,\langle\pm,t|\,\vec{\mathbf{S}}\,|m,t\rangle \times \langle m,t|\,\vec{\mathbf{S}}\,|\pm,t\rangle\left(\frac{4\mu^2}{4\mu^2\vec{\mathbf{R}}^2\hbar^2}\right)$$

Let's write $\vec{\mathbf{S}} = \frac{1}{2}(S_+ + S_-)\hat{\mathbf{x}} + \frac{1}{2\imath}(S_+ - \imath S_-)\hat{\mathbf{y}} + S_z\hat{\mathbf{z}}$. Remember the summation was over $n \neq m$, so really we have

$$B_\pm = \imath\,\langle\pm,t|\,\vec{\mathbf{S}}\,|\mp,t\rangle \times \langle\pm,t|\,\vec{\mathbf{S}}\,|\pm,t\rangle\,\frac{1}{\vec{\mathbf{R}}^2\hbar^2}$$

and

$$\langle\pm|\,\vec{\mathbf{S}}\,|\mp\rangle = \frac{\hbar}{2}\left[\hat{\mathbf{x}} \mp \imath\hat{\mathbf{y}}\right]$$

so

$$\vec{\mathbf{B}}_\pm = \frac{\imath}{4\vec{\mathbf{R}}^2}\left[(\hat{\mathbf{x}} \mp \imath\hat{\mathbf{y}}) \times (\hat{\mathbf{x}} \pm \imath\hat{\mathbf{y}})\right] = \mp\frac{\hat{\mathbf{z}}}{2\vec{\mathbf{R}}^2} = \mp\frac{\hat{\mathbf{R}}}{2\vec{\mathbf{R}}^2}$$

This is the fictitious B-field, not the real one in the problem. We can now calculate the geometric phase by calculating the flux through a surface which we traverse:

$$\gamma_\pm = \mp\int \frac{\hat{\mathbf{R}}\cdot\,\mathrm{d}\vec{\mathbf{a}}}{2\vec{\mathbf{R}}^2} = \mp\frac{1}{2}\Omega$$

where Ω is the solid angle of the surface. ◇

0.19 Hannay Angle

Suppose we have a pendulum in a box and we move the pendulum slowly compared to the period of the oscillations. As long as we do this, the pendulum will always swing parallel to the box. Suppose we are on the globe and have a pendulum at the north pole which is swinging N-S. If we then move down to the equator, along the equator a certain distance, and back up to the north pole, the pendulum will no longer be swinging in the N-S direction, but rather a direction rotated by the solid angle of the path. For instance, if we went around a certain angle from the our equator departure, the area will be $\frac{1}{2}4\pi R^2\frac{\theta}{2\pi} = R^2\theta$ and $\Omega = \frac{A}{R^2} = \theta$. It doesn't matter what path you take, if the solid angle is the same, you will get the same change in angle of rotation. This is called a non-holonomic process.

0.20 Bohm-Aharanov using Berry's Phase

The Hamiltonian for a charged particle in a magnetic field is

$$H = \frac{\left(\vec{\mathbf{P}} - \frac{e}{c}\vec{\mathbf{A}}\right)^2}{2m} + V(X)$$

When $\vec{\mathbf{B}} = 0$, $\vec{\boldsymbol{\nabla}} \times \vec{\mathbf{A}} = 0$. In our Schrödinger equation, we can define

$$|\psi'\rangle = e^{\imath \frac{e}{\hbar c} \int^{\vec{\mathbf{x}}} \vec{\mathbf{A}}(\vec{\mathbf{x}}') \cdot \mathrm{d}\vec{\mathbf{x}}} |\psi\rangle \equiv e^{\imath\gamma} |\psi\rangle$$

such that

$$\left(H = \frac{\vec{\mathbf{p}}^2}{2m} + V\right) |\psi_n'\rangle = E |\psi_n'\rangle$$

This only works when $\vec{\boldsymbol{\nabla}} \times \vec{\mathbf{A}} = 0$, because if we look at the integral over $\vec{\mathbf{A}}$, we see that if $\vec{\mathbf{A}} = \vec{\boldsymbol{\nabla}}\chi$, the result doesn't depend on the path. If it did depend on the path, this would be a problem, since it wouldn't be a well-defined function of x.

Consider a particle in a box:

$$H = \frac{\vec{\mathbf{p}}^2}{2m} + V(x)$$

Now $\vec{\mathbf{R}}(t)$ will be the physical position of the box, $\vec{\mathbf{R}}$. In this case,

$$H = \frac{\vec{\mathbf{p}}^2}{2m} - V(\vec{\mathbf{r}} - \vec{\mathbf{R}}(t))$$

If we now turn on an $\vec{\mathbf{A}}$ field, we get

$$\left(\frac{\vec{\mathbf{p}}^2}{2m} - V(\vec{\mathbf{r}} - \vec{\mathbf{R}}(t))\right) e^{\imath q} |\psi_n\rangle = E_n e^{\imath q} |\psi_n\rangle$$

Let's now calculate the fictitious $\vec{\mathbf{A}}$-field (which will turn out to be the real one):

$$\begin{aligned}\vec{\mathbf{A}} &\equiv \int \imath \, \mathrm{d}^3x \, \psi_n^*(r - R(t)) e^{-\imath q} \vec{\boldsymbol{\nabla}}_R \left(e^{\imath q} \psi_n(r - R(t))\right) \\ &= \imath \int \mathrm{d}^3x \left(\cancelto{0}{\psi_n^* \vec{\boldsymbol{\nabla}}_R \psi_n} + \frac{e}{c} \vec{\mathbf{A}}(R) \psi_n^* \psi_n\right)\end{aligned}$$

since $\langle \vec{\mathbf{p}} \rangle = 0$, so

$$\vec{\mathbf{A}}_{\text{fict}} = \frac{e}{\hbar c} \vec{\mathbf{A}}_{\text{real}}$$

so

$$\gamma_n = \frac{e}{\hbar c} \Phi_B$$

LECTURE 36: THE HELIUM ATOM
Wednesday, April 22, 2020

0.21 The Helium Atom

The helium atom has $Z = 2$, so we can write down the Hamiltonian as

$$H = \sum \frac{p_i^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

where r_1 and r_2 are the distances to each electron and r_{12} is the distance between electrons. The last term here is the repulsion between electrons, and we can write the wave function to leading order (in the $|nlm\rangle$ basis) as

$$|\psi\rangle = |100\rangle \times |100\rangle \times \underbrace{\chi_{\text{singlet}}}_{\frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]}$$

Additionally, the ground state energy will be $E = 8E_0 = -108.8\text{eV}$ where $E_0 = -13.6\text{eV}$. Experimentally, we find that it is actually -78.8eV, so we're off by around 20%. However, there's no reason to suspect that leading order is much larger than the next-order calculation (there's no reason why the repulsion term should be small). Let's now do first-order perturbation theory to see if we can get closer:

$$\begin{aligned}\Delta E &= |100\rangle \frac{e^2}{r_{12}} |100\rangle \\ &= |100\rangle \frac{e^2}{|\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|} |100\rangle = e^2 \int \frac{\mathrm{d}^3 r_1 \, \mathrm{d}^3 r_2 \, \varphi_{100}(r_1)\varphi_{100}(r_2)}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta)}}\end{aligned}$$

Recall that

$$\psi_{100}(r_1)\varphi_{100}(r_2) = \frac{Z^3}{\pi a_0^3} e^{-Z(r_1+r_2)/a_0}$$

We can write

$$\left[r_1^2 + r_2^2 - 2r_1 r_2 \cos(\theta)\right]^{-1/2} = \sum \frac{r_<^l}{r_>^{l+1}} P_l(\cos(\theta))$$

The r-integral isn't that tricky, but we need to figure out the θ integral. We can rewrite

$$P_l(\cos(\theta)) = \sum_m Y_{lm}(\theta_1, \varphi_1) Y_{lm}(\theta_2, \varphi_2) \left[\frac{4\pi}{2l+1}\right]$$

Remember that P_l and Y_{lm} are related by an overall coefficient with $m = 0$, so we can write

$$P_l(\cos(\theta)) = \langle \hat{\mathbf{n}}_2 | l, m = 0 \rangle \frac{2l+1}{4\pi}$$

Now the integral over θ becomes easy, since the angular part of φ_{100} is $Y_{00} = \frac{1}{\sqrt{4\pi}}$. The angular part will be

$$\sum_m \int \mathrm{d}\Omega_1 \, \mathrm{d}\Omega_2 \, Y_{lm}(\Omega_1) Y_{00}(\Omega_1) Y_{lm}^*(\Omega_2) Y_{00}(\Omega_2)$$

However, we know that

$$\int \mathrm{d}\Omega \, Y_{lm} = 4\pi \delta_{l,0} \delta_{m,0}$$

so this integral becomes trivial. Doing the integrals, we find that

$$\Delta E = \frac{5}{2} \left(\frac{e^2}{2a_0}\right)$$

so our corrected energy is

$$E = -74.8\text{eV}$$

which is much closer to the experimental value. Why does this work so well? No clue.

0.21.1 Excited States of Helium

The first excited state will have one electron in the ground state and the other in an excited state. The wave function is no longer constrained to the singlet state because the electrons have different quantum numbers.

$$E = E_{1s} + E_{\not<} + \Delta E$$

$$|\psi\rangle = \varphi_{100}(x_1)\varphi_{nlm}(x_2) \pm \varphi_{100}(x_2)\varphi_{nlm}(x_1)$$

where $+$ gives the wave function for the χ_{singlet} state (orthohelium) and $-$ gives the wave function for the χ_{triplet} state (parahelium).Recall that in the symmetric spatial wave function, fermions can sit on top of each other (so the repulsion term will be larger), and the singlet spin state is antisymmetric so it must be spatially symmetric, so the singlet state has a higher energy than the triplet state.

0.22 Multi-Particle Systems

It turns out that when you get large numbers of particles interacting, you get all kinds of neat effects, like superconductivity, the quantum Hall effect, and ferromagnets. Suppose we have N particles:

$$|\psi\rangle = |k_1\rangle\,|k_2\rangle\cdots|k_i\rangle\cdots|k_j\rangle\cdots|k_N\rangle$$

where k_i label eigenvalues of some observable.

$$P_{ij}\,|\psi\rangle = \pm\,|k_1\rangle\,|k_2\rangle\cdots|k_j\rangle\cdots|k_i\rangle\cdots|k_N\rangle$$

For example, consider three particles:

$$|\psi\rangle = \frac{1}{\sqrt{6}}\left[|k_1\rangle\,|k_2\rangle\,|k_3\rangle \pm (213) + (231) \pm (321) + (312) \pm (132)\right]$$

This is an eigenstate of P_{12}, P_{13}, and P_{23} with eigenvalues ± 1. If two states are identical ($k_2 = k_3$), $|\psi\rangle = 0$ for Fermions (this is the Pauli principle), and

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left[|k_1\rangle\,|k_2\rangle\,|k_2\rangle + (212) + (221)\right]$$

for Bosons. In general, this normalization factor is $\frac{\sqrt{N_1!}\sqrt{N_2!}\sqrt{N_2!}}{\sqrt{N!}}$ if $k_2 = k_3$, so

$$|\psi\rangle = \sum_\sigma \frac{\left|k_{\sigma(1)}\cdots\left|k_{\sigma(N)}\right\rangle\right\rangle}{\sqrt{N_1!\cdots N_N!}}$$

and for Fermions

$$|\psi\rangle = \frac{1}{\sqrt{N!}}\sum_\sigma (-1)^{\text{parity}}\,|k_1\cdots k_N\rangle$$

0.22.1 Fock States

Rather than drag around all these symmetrization factors, we instead turn to Fock states where we relabel $|k_1\cdots k_n\rangle$ as $|n_1 n_2\cdots\rangle$ where n_i is the number of particles in state i. For instance, $|k_1, k_1, k_2\rangle = |21\rangle$. Recall the raising and lowering operators. Let's introduce the notation $a_i^\dagger$ such that this creates a particle in the state k_i. Therefore, we can generate the Fock states as

$$a_i^\dagger\,|0\rangle = |1, 0\cdots\rangle \equiv |k_i\rangle$$

and generate other states like

$$a_{i=1}^\dagger a_{j=2}^\dagger\,|0\rangle = |1, 1, 0\cdots\rangle \equiv |k_1\rangle\,|k_2\rangle$$

We also must define the lowering operator $a_1\,|1, 0, 0\cdots\rangle = |0, 0, 0\cdots\rangle$ and $a_1\,|0\cdots\rangle = 0$. The nice part about this system is that statistics are automatic. If we create a two-particle system, $a_i^\dagger a_j^\dagger\,|0\rangle$, then the choice that $\left[a_i^\dagger, a_j^\dagger\right] = 0$, the state is automatically symmetric, whereas the choice that $\left\{a_i^\dagger, a_j^\dagger\right\} = 0$ generates antisymmetric states.

LECTURE 37: FOCK SPACE
Friday, April 24, 2020

At the end of the last lecture, we noticed that if we made the ladder operators commute, we automatically get Boson statistics, whereas anti-commutation (a Poisson bracket or alternatively, we can subscript the commutator with a + sign) gives Fermion statistics:

$$\left[[a_i, a_j]_\pm\right]^\dagger = \left[a_j^\dagger, a_i^\dagger\right]_\pm = 0$$

$$\left[a_i, a_j^\dagger\right] = \delta_{ij}$$

$$N_i = a_i^\dagger a_i$$

is the number of particles in the energy eigenstate enumerated by i.

Let's now consider hydrogen:

$$|\psi_0\rangle = \int \mathrm{d}^3x\, \psi_{nlm}(x) a_x^\dagger |0\rangle$$

We need to normalize it:

$$\langle\psi_0|\psi_0\rangle = \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \langle 0|\, a_{x'}\psi^*(x')\psi(x)a_x^\dagger\, |0\rangle = \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \psi^*(x')\psi^*(x)\delta^3(x-x') = \int \mathrm{d}^3x\, |\psi(x)|^2 = 1$$

$$|k\rangle = \sum_x |x\rangle\, \langle x|k\rangle$$

$$a_k = \sum_x \langle x|k\rangle\, a_x$$

$$|\psi\rangle = \int \mathrm{d}^3k\, \psi(k) a_k^\dagger\, |0\rangle$$

If the system is in a box, k is discrete:

$$\left[a_k, a_p^\dagger\right] = \delta_{p,k}$$

What is the probability of of being in the x_0 state?

$$\begin{aligned}
\Pr(x_0) &= |\, \langle 0|a_{x_0}|\psi\rangle|^2 \\
&= \left|\, \langle 0|a_{x_0} \int \mathrm{d}^3x\, \psi(x) a_x^\dagger |0\rangle \right|^2 \\
&= \left|\, \langle 0|\delta^3(x_0 - x)|0\rangle \right| = |\psi(x_0)|^2
\end{aligned}$$

This checks out with what we would expect.

Lets look at the Helium ground state (ignoring the Coulomb repulsion):

$$\int \mathrm{d}^3x\, \mathrm{d}^3y\, \psi_{100}(x)\psi_{100}(y) a_{x\uparrow}^\dagger a_{y\downarrow}^\dagger\, |0\rangle$$

What is the probability of finding one particle at x_0^1 and S_1 and one at x_2^2 and S_2?

$$\begin{aligned}
\left\langle x_{0,S_1}^1, x_{0,S_2}^2 \middle| \psi \right\rangle &= \int \mathrm{d}^3x, y\, \langle 0|\, a_{x_{0,S_1}^1} a_{x_{0,S_2}^2} a_{x\uparrow}^\dagger a_{y\downarrow}^\dagger\, |0\rangle\, \psi_{100}(x)\psi_{100}(y) \\
&= \int \left[\langle 0|\, a_{x_{0,S_1}^1} \delta^3(x_0^2 - x)\delta_{S_2,\uparrow} a_{y\downarrow}^\dagger\, |0\rangle - \langle 0|\, a_{x_{0,S_1}^1} a_{x\uparrow}^\dagger a_{x_{0,S_1}^2} a_{y\downarrow}^\dagger\, |0\rangle\right] \mathrm{d}^3x, y\, \psi_{100}(x)\psi_{100}(y) \\
&= \int \mathrm{d}^3x, y\, \{[\delta^3(x_0^1 - y)\delta(x_0^2 - x)\delta_{S_2,\uparrow}\delta_{\downarrow,S_1}] - [\delta^3(x_0^2 - y)\delta_{S_2,\downarrow}\delta^3(x_0^1 - x)\delta_{S_1,\uparrow}]\}\psi_{100}(x)\psi_{100}(y) \\
&= \psi_{100}(x_0^2)\psi_{100}(x_0^1)\delta_{S_2,\uparrow}\delta_{S_1,\downarrow} - \psi_{100}(x_0^1)\psi_{100}(x_0^2)\delta_{S_2,\downarrow}\delta_{S_1,\uparrow}
\end{aligned}$$

By choosing the proper commutation relation for the statistics of electrons, we get an anticommuting wave function as expected.

0.23 Operations on Fock Space

$$H_{\text{free}} = \sum_{\vec{\mathbf{k}}} \frac{\hbar^2 \vec{\mathbf{k}}^2}{2m} a_{\vec{\mathbf{k}}}^\dagger a_{\vec{\mathbf{k}}}$$

$$\vec{\mathbf{p}} = \sum_k \hbar \vec{\mathbf{k}} a_k^\dagger a_k$$

Some interesting properties of Bosons and Fermions are that Bosons fall into ground-state condensates while Fermions build a "sea" of states. How do we include interactions between the particles, which are obviously crucial? Suppose we have pairwise interactions:

$$H = \sum_{ij} \frac{1}{2} V_{ij} N_i N_j$$

where the 1/2 avoids double-counting. For electromagnetism, we have interactions of the form

$$\frac{e^2}{\vec{\mathbf{x}}_1 - \vec{\mathbf{x}}_2} \rho(x_1)\rho(x_2)$$

where our N_i's are the charge density and V_{ij} is the fraction term. Let's consider Fermions:

$$\begin{aligned} H &= \sum_{ij} \frac{1}{2} V_{ij} a_i^\dagger a_i a_j^\dagger a_j \\ &= \sum_{ij} \frac{1}{2} V_{ij} \left[-a_i^\dagger a_j^\dagger a_i a_j + a_i^\dagger a_j^\dagger \delta_{ij} \right] \\ &= \frac{1}{2} \sum_{i \neq j} V_{ij} N_i N_j + \frac{1}{2} \sum_i V_{ii} N_i (N_i - 1) \\ &= \frac{1}{2} \sum_{ij} N_i N_j - \frac{1}{2} \sum_i V_{ii} N_i \end{aligned}$$

This operator has a name:

$$\Pi_{ij} = N_i N_j - N_i \delta_{ij}$$

is called the pair distribution operator. Let's apply this to the Coulomb interaction.

$$H = \sum \frac{p_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j} \frac{e^{-\mu(x_i - x_j)}}{x_i - x_j} + \frac{e^2}{2} \int \mathrm{d}^3 x, x' \, \frac{\rho(x)\rho(x') e^{-\mu(x-x')}}{|x - x'|} - e^2 \int \mathrm{d}^3 x \sum_i \frac{\rho(x)}{|x - x_i|} e^{-\mu(x - x_i)}$$

where the final term is an additional positive charge density (since a lot of electrons together won't make for an interesting particle, the system will blow apart).

We will eventually take $\mu \to 0$. This is called a regulator. In the intermediate parts of this calculation, we will find some rather annoying divergences without it.

LECTURE 38: PROPERTIES OF MANY-BODY SYSTEMS
Monday, April 27, 2020

0.24 Coulomb Gas

In the last lecture we were discussing negatively charged Fermions in a positively charged background. We can write the classical Hamiltonian as

$$H = \sum_{i=1}^{\infty} \frac{p_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j} \frac{e^{-\mu|x_i - x_j|}}{|x_i - x_j|} + \frac{e^2}{2} \int \mathrm{d}^3 x, x' \, \frac{\rho(x)\rho(x')}{|x - x'|} e^{-\mu|x - x'|} - e^2 \sum_i \int \mathrm{d}^3 x \, \rho(x) \frac{e^{-\mu|x - x_i|}}{|x_i - x|}$$

The terms in order are the free particle kinetic energy, the pairwise interaction, the self-interaction of the background, and the interaction of the background with the electrons:

$$H = H_{\text{KE}} + H_{\text{Coulomb}} + H_{\text{Background}} + H_{\text{Background—Electrons}}$$

Since $\rho(x)$ is uniform, we can say $\rho(x) = \frac{N}{V}$ where N is both the number of electrons and the number of positive background charges, since we will assume the system is electrically neutral. In the end, we will take $\mu \to 0$ as we discussed in the last class.

$$\begin{aligned} H_{\text{bg}} &= \frac{e^2}{2} \int \mathrm{d}^3x, x' \left(\frac{N}{V}\right)^2 \frac{e^{-\mu|x-x'|}}{|x-x'|} \\ &= \frac{e^2}{2} \left(\frac{N}{V}\right)^2 V \int \frac{e^{-\mu r}}{r} (4\pi) r^2 \,\mathrm{d}r \\ &= \frac{e^2}{2} \left(\frac{N^2}{V}\right) (4\pi) \int_0^\infty e^{-\mu r} r \,\mathrm{d}r \\ &= (\ldots)(-\partial_\mu \int_0^\infty e^{-\mu r} \,\mathrm{d}r) \\ &= \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2} \end{aligned}$$

$$\begin{aligned} H_{\text{bg—e}} &= -e^2 \sum_i \int \mathrm{d}^3x \, \frac{\rho(x) e^{-\mu|x-x_i|}}{|x-x_i|} \\ &= -e^2 \frac{N}{V} \sum_i \int \frac{e^{-\mu|x-x_i|}}{|x-x_i|} \,\mathrm{d}^3x \\ &= -e^2 \frac{N}{V} \underbrace{\sum_i}_{N} \int_0^\infty 4\pi r e^{-\mu r} \\ &= -\frac{e^2 N^2}{V} \frac{4\pi}{\mu^2} \end{aligned}$$

so

$$H = H_{\text{KE}} + H_{\text{C}} - \frac{e^2 N^2}{2V} \left(\frac{4\pi}{\mu^2}\right)$$

Now we will quantize in the Fock space. This is often called second-quantization. What basis should we quantize in (momentum, energy, position)? Obviously we want to choose the simplest one. We can treat the Coulomb interaction as a perturbation and treat H_{KE} as leading order (we will have to justify this later), so we can choose the momentum basis:

$$H_{\text{KE}} = \sum_{k^2} a_k^\dagger a_k \frac{\hbar^2 k^2}{2m}$$

$$H_{\text{C}} = \frac{e^2}{2} \sum_{i \neq j} \frac{e^{-\mu|x_i - x_j|}}{|x_i - x_j|}$$

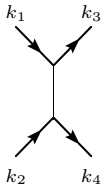
Last time we showed that we can write pairwise interactions as

$$V = \sum_{i \neq j} N_i N_j \frac{1}{2} V_{ij} + \sum_i \frac{1}{2} V_{ii} N_i (N_i - 1) = \frac{1}{2} \sum_{ij} a_i^\dagger a_j^\dagger a_i a_j$$

On the homework, we'll show that

$$V = \frac{1}{2} \sum_{k_1 \lambda_1} \cdots \sum_{k_4 \lambda_4} \langle k_1 \lambda 1, k_2 \lambda_2 | \, V \, | k_3 \lambda_3, k_4 \lambda_4 \rangle = \frac{e^2}{2V} \sum_{k_1 \lambda_1 \ldots k_4 \lambda_4} \delta_{k_1 + k_2, k_3 + k_4} \frac{4\pi}{q^2 + \mu^2} a_{k_1 \lambda_1}^\dagger \cdots a_{k_4 \lambda_4}^\dagger a_{k_1 \lambda_1} \cdots a_{k_4 \lambda_4}$$

where $q = k_1 - k_3$. This is just momentum conservation and represents a Feynman diagram:



Therefore

$$H = \sum_k a_k^\dagger a_k \frac{\hbar^2 k^2}{2m} + \frac{2^2}{2V}\sum_{k_i\lambda_i}(\cdots) - \frac{e^2N^2}{2V}\left(\frac{4\pi}{\mu^2}\right)$$

Let's solve this when $q = 0$ (no momentum is exchanged) or $k_1 = k_3 = k$ and $k_2 = k_4 = q$: The interaction term is now

$$\begin{aligned} H_{\mathrm{C}} &= \frac{e^2}{2V}\sum_{k,p}\sum_{\lambda_1,\lambda_2} a^\dagger_{k,\lambda_1}a^\dagger_{p,\lambda_2}a_{p,\lambda 3}a_{k,\lambda_4} \\ &= \frac{e^2}{2V}\sum\sum\left[N_{\lambda_1}(k)N_{\lambda_2}(p) - N_{\lambda_1}(k)\delta_{\lambda_1,\lambda_2}\right] \\ &= \frac{4\pi}{\mu^2}\frac{e^2}{2V}\left[N^2 - N\right] \end{aligned}$$

Due to the $q = 0$ interaction, $\frac{E}{N} = \frac{4\pi e^2}{\mu^2(2V)}$, and this exactly cancels the other divergent μ term. We will then remove the forward scattering term:

$$H = \sum_\lambda\sum_k a^\dagger_{\lambda k}a_{\lambda k}\frac{\hbar^2k^2}{2m} + 4\pi\frac{e^2}{2}\sum_{q\neq 0}\sum_{\lambda_i} a^\dagger_{k_1,lambda_1}a_{k_2,\lambda_2}a^\dagger_{k_3,\lambda_3}a_{k_4,\lambda_4}\frac{\delta_{k_1+k_2,k_3+k_4}}{q^2}$$

where the sum over $q = 0$ is the same as a sum over $k_1 \neq k_3$. Let's try to calculate the ground-state energy. We refer to the first term in this Hamiltonian as the one-particle operator or "free" operator and the second term the two-particle operator. It's easy to find the ground state for the first part, and then we can treat the Coulomb interaction as a perturbation. When can we do this? Counter-intuitively, the denser the gas is, the less important the Coulomb interaction becomes! Define r_0 as the typical inter-particle spacing. The potential energy will therefore go like PE $\sim \frac{e^2}{r_0}$. However, think about the kinetic energy: KE $\sim \frac{p^2}{2m}$. By the uncertainty principle, $px \sim \hbar$, so $p \sim \frac{\hbar}{x} \sim \frac{\hbar}{r_0}$. Then KE $\sim \frac{\hbar^2}{2mr_0^2}$! As we force particles into smaller and smaller regions, the uncertainty of p grows, which cases the kinetic energy to get smaller (much faster than the potential energy grows). If we want KE >> PE, we need $\frac{\hbar^2}{2mr_0^2} >> \frac{e^2}{r_0}$ or $r_0 << \frac{\hbar^2}{2me^2} = \frac{a_0}{2}$, so we expect our approximation to hold when

$$\frac{r_0}{a_0} \equiv r_s << 1$$

At leading order,

$$(H_0 = H_{\mathrm{KE}})\,|\Omega\rangle \equiv E_0\,|\Omega\rangle$$

the ground state is just filling up the Fermi sea, where we will call the highest energy state $E_F = \frac{\hbar^2k_F^2}{2m}$. The leading-order result is

$$N = \sum_{k,\lambda}\Theta(k_F - k) = \sum_\lambda \frac{1}{(2\pi)^3}\int \mathrm{d}^3k\, V\Theta(k - k_F) = (2V)(4\pi)\frac{1}{(2\pi)^3}\int_0^{k_F} k^2\,\mathrm{d}k = \frac{V}{3\pi^2}k_F^3$$

so

$$K_F = \left[\frac{3\pi N}{V}\right]^{1/3}$$

Therefore

$$E_0 = \underbrace{2}_{\text{spin}}\int^{k_F}\frac{V\,\mathrm{d}^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m} = \frac{V\hbar^2}{2m\pi^2}\frac{k_F^5}{5}$$

or

$$E_0 = \frac{e^2}{2a_0}N\frac{3}{5}\left[\frac{a_0\pi}{4}\right]^{2/3}\frac{1}{r_s^2}$$

This is divergent as $r_s \to 0$, which is true, since the momentum should diverge as we compress the system. We should hope that our first-order correction fixes this.

Lecture 40: Superconductivity

Friday, May 1, 2020

In the last lecture, we established that the necessary conditions for superconductivity were an attractive potential and a Fermi surface. Because of Pauli exclusion, the density of states is large on the Fermi surface, which is why superconductivity wouldn't work with Bosons. The next question we want to answer is, what is the ground state of a superconductor? If we had no interactions, we would get the typical Fermi sea, where the probability to find a particle with any given momentum is 1 up to k_F. Bardeen, Cooper, and Schriefer (B.C.S. Theory) won a Nobel prize by making an ansätz for the ground state. Cooper's calculation told us that there would be bound states of two electrons with opposite momentum (Cooper pairs), so BCS guessed that

$$|\psi\rangle = \prod_q \left[\cos(\theta_q)\,|0\rangle_q + \sin(\theta_q)\,|1\rangle_q\right]$$

where $|1\rangle_q$ corresponds to one electron with spin up and momentum $\vec{\mathbf{q}}$ and one electron with spin down and momentum $-\vec{\mathbf{q}}$. The $|0\rangle_q$ is not occupied while $|1\rangle_q$ is occupied:

$$|1\rangle_q = a^\dagger_{q\downarrow} a^\dagger_{-q\uparrow}\,|0\rangle$$

We can write the full wave function as

$$|\psi\rangle = e^{\imath \prod_q \theta_q a^\dagger_{q\uparrow} a^\dagger_{-q\downarrow}}\,|0\rangle$$

since $a^\dagger_q a^\dagger_q = 0$ because we want $\left\{a^\dagger_q, a^\dagger_q\right\} = 0$ for Fermions. Note that $\sin^2(\theta_q)$ is the probability to find a Cooper pair labeled by q. Our goal now is to find θ_q such that $E < E_{\text{free}}$ subject to $\langle N\rangle = N$. In this ground state, we can calculate the kinetic energy, so

$$H_0 = \sum_i \frac{\hbar^2 q^2}{2m}\sin^2(\theta_q)$$

We will define an interaction that takes our pairs labeled by q to pairs labeled by q' as

$$\hat{V}_{qq'}\,|0\rangle_q\,|1\rangle_{q'} = |1\rangle_q\,|0\rangle_{q'}$$

so that

$$\hat{V}_{qq'}\,|0\rangle_q\,|0\rangle_{q'} = 0 = \hat{V}_{qq'}\,|1\rangle_q\,|1\rangle_{q'}$$

so we can write the potential as

$$\hat{V} = \sum_{q,q'} a^\dagger_{q\downarrow} a^\dagger_{-q\uparrow} a_{q'\uparrow} a_{-q'\downarrow} V_{qq'}$$

$$\langle\psi|\hat{V}|\psi\rangle = \left[\left(\langle 0|_q \cos(\theta_q) - \imath\sin(\theta_q)\,|1\rangle_q\right)\left(\langle 0|_{q'}\cos\left(\theta_{q'} - \imath\sin(\theta_{q'})\,\langle 1|_{q'}\right)\right)\cdots\right]\hat{V}_{qq'}\,[(\text{conj})\,(\text{conj})\cdots]$$

so the only non-zero term will be

$$\left\langle\hat{V}\right\rangle = \cos(\theta_q)\cos(\theta_{q'})\sin(\theta_q)\sin(\theta_{q'})V_{qq'}$$

so

$$E = \sum_q \frac{\hbar^2 q^2}{m}\sin^2(\theta_q) + \sum_{qq'} V_{qq'}\cos(\theta_q)\cos(\theta_{q'})\sin(\theta_q)\sin(\theta_{q'})$$

Now we want to find the θ_q which minimizes E.

$$\Omega = E - \mu N = E + \sum_q (-2\mu)\sin^2(\theta_q)$$

$$\frac{\partial\Omega}{\partial\theta_k} = \left[2\frac{\hbar^2 k^2}{m} - 4\mu\right]\sin(\theta_k)\cos(\theta_k) + \frac{1}{2}\cos(2\theta_k)\sum_{q'} V_{kq'}\sin(2\theta_q)$$

Let's introduce $\xi \equiv \frac{\hbar^2 k^2}{2m} - \mu$, so

$$\begin{aligned}\frac{\partial \Omega}{\partial \theta_k} &= 4\xi_k \sin(\theta_k)\cos(\theta_k) + \sum_{q'} V_{kq'}\cos(2\theta_k)\sin(2\theta_{q'}) = 0 \\ &= 2\xi_k \sin(2\theta_k) + \frac{1}{2}\cos(2\theta_k)\sum_{q'} V_{kq'}\sin(2\theta_{q'}) \\ &= 2\xi_k \tan(2\theta_k) + \frac{1}{2}\sum_{q'} V_{kq'}\sin(2\theta_{q'})\end{aligned}$$

Let's define $\tan(2\theta_k) \equiv -\frac{\Delta_k}{\xi_k}$, so $\sin(2\theta_k) = -\frac{\Delta_k}{\sqrt{\Delta_k^2+\xi_k^2}}$ and $\cos(2\theta_k) = \frac{\xi_k}{\sqrt{\Delta_k^2+\xi_k^2}}$:

$$\Delta_k = -\frac{1}{2}\sum_q \frac{V_{kq}\Delta_q}{\sqrt{\Delta_q^2+\xi_q^2}} \qquad \text{(Gap Equation)}$$

Let's think of the potential $V_{qk} = -V$ as long as the particles are within the Debye energy of the Fermi surface ($|\xi_{k,q}| < \hbar\omega_D$) and $V_{qk} = 0$ otherwise. With this simplification,

$$\Delta_k = \frac{V}{2}\sum_q \frac{\Delta_q}{\sqrt{\Delta_q^2+\xi_q^2}}$$

and

$$\Delta_0 = \frac{V}{2}\sum_q \frac{\Delta_0}{\sqrt{\Delta_0^2+\xi_q^2}}$$

because we have to eliminate momentum dependence from both sides.

$$\begin{aligned}1 &= \frac{V}{2}\int \frac{L^3\,\mathrm{d}^3 q}{(2\pi)^3}\frac{1}{\sqrt{\Delta_0^2+\xi_q^2}} \\ &= \frac{V}{2}\frac{L^3}{(2\pi)^3}(4\pi)\int \frac{\mathrm{d}q\, q^2}{\sqrt{\Delta_0^2+\xi_q^2}} \\ &= \frac{V}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\rho(\xi)\,\mathrm{d}\xi}{\sqrt{\Delta_0^2+\xi^2}}\end{aligned}$$

with $\rho(\xi) = \rho(0)$, we can solve this integral as

$$1 = V\rho(0)\sinh[-1]\left[\frac{\hbar\omega_D}{\Delta_0}\right]$$

so as $V \to 0$,

$$\Delta_0 = 2\hbar\omega_D e^{-\frac{1}{\rho(0)V}}$$

We can then use this to show that

$$2\sin^2(\theta) = \left[1 - \frac{\xi_q}{\sqrt{\xi_q^2+\Delta_0^2}}\right]$$

As $\xi_q \to \infty$ (large energy), $\theta_q \to 0$, and as $q \to 0$, $\xi \to -\mu$ and $\sin^2(\theta_q) = 1$. Therefore, we know that the probability of a Cooper pair at a particular q starts at 1 for small q and goes to 0 at high q with an inflection point at $\mu = \epsilon_F$. What does this mean physically? At low energy, the states above E_F don't even feel the potential, and we fill up all of the Cooper pairs below the surface. Near the Fermi surface, there will be some pairs above the trivial ground state and some gaps below the ground state. The gap function we found sets the scale for this splitting. But this means that only a tiny fraction of the electrons in a superconductor, the ones near the Fermi surface, contribute to this effect at all. Resistivity comes from scattering from one state into another. Deep inside the Fermi sea, the electrons have no place to

scatter because all of the states above and below are occupied. Therefore, all the resistivity is already coming from states near the Fermi surface. The first excited state has a gap of order $2\Delta_0$ (this is easy to show, but we don't have time). As a consequence, electrons without adequate energy can't get scatter to this excited state, and the gap scales inversely with the potential. As we increase the temperature, the thermal fluctuations of the electrons will give them enough energy to jump this gap, so there exists a T_C above which point superconductivity goes away, where $kT_C \sim \Delta_0$.

Conclusion

This concludes the lecture series taught by Dr. Ira Z. Rothstein during the Spring of 2020. I hope these notes will prove useful to current and future students of the course. Please note that by lecture number, I am missing lectures 31, 34, 35, and 39, but there might be a few more classes which I missed but for which I forgot to update the lecture number. These classes are mostly at the end of the course (and the missing dates will be clear from the headers of each lecture). I cannot guarantee the accuracy of these notes, since they were all typed (quickly) during class with minimal proofreading afterwards.
The textbook used for this class was "Modern Quantum Mechanics" by J. J. Sakurai and Jim Napolitano.