Quantum Mechanics

Professor: Ehud Altman
Class: Physics 137b
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Contents

Administration

30% Homework, 30% Midterm (Tentative Midterm Oct. 18), 40% Final.
Quizzes in section (monday), don't count towards the final grade.
The syllabus will track basically as follows:

1. Stationary Perturbation Theory (time independent)
2. Variational Principle (not in townsend)
3. WKB (semicalssical) approximation (not in townsend, may skip)
4. Time Dependent Perturbation Theory

5. Coupling of Quantum Particles + Electromagnetic Fields (Aharonov-Bohm effect)
6. Quantize Light, Physics of Photons and Photon-Atom interaction.

1 Review

1.1 State Vector, Kets, Bras

$|\psi\rangle, \psi(x)$, difference between the two. State vector $|\psi\rangle$ can be constructed out of other vectors. I.e. $|\psi\rangle = \sum_i c_i |\psi_i\rangle$.
Our hilbert space is over $\mathbb{C}$.
Bra objects are the dual of their respective kets.

$$|\psi\rangle \in \mathcal{H} \qquad\qquad \langle\psi| \in \mathcal{H}^*$$

$\mathcal{H}^*$ is the space of linear operators

$$\langle\psi| : \qquad \mathcal{H} \to \mathbb{C}$$
$$\langle\psi|\psi\rangle = \langle\psi|\psi\rangle^* = ||\,|\psi\rangle\,||^2$$

We have to make a choice of basis in order to gain any useful information from this vector space.
A basis is any minimal collection of vectors whose span is the desired hilbert space.
Typically, we choose an orthonormal basis such that $\langle\psi_i|\psi_j\rangle = \delta_{ij}$
Under this expression, we have

$$|\psi\rangle = \sum_i \psi_i |\phi_i\rangle$$
$$\langle\psi|\psi\rangle \sum_i \sum_j \psi_i^* \psi_j \langle\phi_i|\phi_j\rangle = \sum_i |\phi_i|^2 = 1$$

Inner product is defined in the usual way.
We are allowed to have continuous bases. E.g. a particle on a 1-d line. We can attempt to measure a position of the particle on the line. We essentially use the same formalism, but with

$$\langle x|x'\rangle = \delta(x - x')$$

where δ is now the Dirac Delta function.
Similarly, we have

$$|\psi\rangle = \int dx \psi(x) |x\rangle \qquad\qquad \langle\psi| = \int dx \psi^*(x) \langle x|$$

Leading to the usual definition of the probability of $|\psi\rangle$ at a given x as

$$\langle x|\psi\rangle = \int dx' \psi(x') \langle x|x'\rangle = \psi(x)$$

and our other favorite

$$\langle\chi|\psi\rangle = \int dx \chi^*(x)\psi(x)$$

1.2 Operators→ observables

1.2.1 Operators, Bases, Linear Algebra

Observables include our old friends $\hat{x}, \hat{p}, \hat{H}, \hat{L}\,\hat{s}$.
What is an operator tho?

$$\hat{A} : \quad \mathcal{H} \to \mathcal{H}$$

also ∃ adjoint operator, $A^\dagger$ from $\mathcal{H}$ to itself.
We can construct projection operators by taking the outer product of two vectors.
Also lets us have some resolution of identity by summing over the projection operators in any orthonormal basis.
Also, matrix representations exist by arranging $A_{mn} = \langle\varphi_m| \hat{A} |\varphi_n\rangle$, for some particular basis φ_i
In other words

$$\hat{A} = \sum_{ij} |\varphi_i\rangle A_{ij} \langle\varphi_j|$$

Cute stuff with the momentum operator.

1.2.2 Observables↔Hermitian Operators

Hermitian operators are those operators that are self adjoint, e.g.

$$H = H^\dagger \qquad\qquad A_{ij} = A_{ji}^*$$

- Eigenvalues are real
- Eigenvectors form a complete orthonormal basis.

If we have degenerate eigenvalues, e.g. states $\{|a_1\rangle, \ldots, |a_g\rangle\}$ that are degenerate, then any superposition of those states will also be an eigenvector with the same eigenvalue (e.g. they lie along their own span).
e.g. spin has a degeneracy. Eigenvalues are always $a = s(s+1)$. It is degenerate $2s+1$ states. That's why we label by $|s, m\rangle$, because the operator corresponding to m is nondegenerate and commutes with S.
Went over an explanation of a pauli matrix for the S_z operator. We can do the same thing for S_x. This is an excercise
We then want the bloch sphere representation

$$|\psi\rangle = \alpha\,|{+z}\rangle + \beta\,|{-z}\rangle = \cos\frac{\theta}{2}\,|{+z}\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|{-z}\rangle$$

Operators need not commute with each other.[1]
Also, if we want to make the hamiltonian simpler, we cann just put it into a block structure and solve it.

commuting observables Sets of commuting observables have mutual eigenvectors. e.g.

$$\hat{B}\,|E, a, b, c\rangle = bE, a, b, c$$

called *quantum numbers*.

noncommuting observables We can also have noncommuting observables. Since we can't diagonalize them simultaneously, we cannot have complete symmetry because we collapse the wavefunction simultaneously.
We need to define the variance of an operator A as

$$\Delta A^2 = |\,\langle\psi|\,A^2\,|\psi\rangle\,| - |\,\langle psi|\,A\,|\psi\rangle\,|^2$$

Then, for two observables, we have

$$[A, B] = \hat{C}$$
$$\Delta A \Delta B = \frac{1}{2}\langle\hat{C}\rangle$$

1.2.3 Symmetries↔Unitary Operators

Read this on ur own.

1.3 Guest Discussion while Altman out of town (9/16/19)

1.3.1 System of Two Spin-1/2 Particles

Discussion of this motivated by desire to analyze hyperfine splitting in the hydrogen atom. We begin with discussion of the hamiltonian

$$\hat{H} = \frac{2A}{\hbar^2} S_1 \cdot S_2$$

Hilbert space is given by the tensor product of our two spin-1/2 systems. For two bases, $|\uparrow\rangle, |\downarrow\rangle$, we have our new space as $|\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle$.
We can also write our new hamiltonian as

$$2S_1 \cdot S_2 = S_1^+ S_2^- + S_1^- S_2^+ + 2S_1^z S_2^z$$

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[1] Q: Don't operators form a group under ×? How can we talk about commutation relations in a simpler way? Where does this relations $[A, B]$ come from?

where

$$S^{\pm}_{1,2} = S^{x}_{1,2} \pm iS^{y}_{1,2}$$

It can be checked explicitly that $\left|\uparrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle$ are still eigenstates of the hamiltonian, since.
We want to know then what

$$\left\langle\uparrow\downarrow\right| S^+_1 S^-_2 + S^-_1 S^+_2 + 2S^z_1 S^z_2 \left|\uparrow\downarrow\right\rangle$$

By symmetry arguments, a lot of these coefficients go to zero, so we get $\frac{-A}{2}$ for both oriientations on the diagonal, and A on the off. In total, the logic gives the following hamiltonian

$$\hat{H} = \begin{bmatrix} \frac{A}{2} & 0 & 0 & 0 \\ 0 & \frac{-A}{2} & A & 0 \\ 0 & A & \frac{-A}{2} & 0 \\ 0 & 0 & 0 & \frac{A}{2} \end{bmatrix}$$

We can get the eigenvalues, vectors of the central square matrix by taking

Spin Triplet	$\frac{1}{\sqrt{2}}(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle)$	$\frac{A}{2}$
Spin Singlet	$\frac{1}{\sqrt{2}}(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle)$	$\frac{-3A}{2}$

Now, we want to see if its possible to invent some symmetry that commutes with our hamiltonian.
It seems like it should be symmetric by rotation about $\hat{n}$ by an angle $\delta\theta$. We can write down $R(\delta\theta)$, which is generated by $\vec{S} \cdot \vec{n}$, which gives

$$R(\delta\theta) = e^{-i(\vec{S}\cdot\vec{n})\delta\theta}$$

We can show that $[S \cdot \hat{n}, H] = 0$.
What it means to take $S \cdot \hat{n}$ in our tensor product space is

$$S \cdot \hat{n} = S_1\hat{n} \otimes I + I \otimes S_2\hat{n}$$

[2] [3]

These all fulfill the basic requirements of the spin algebra,

$$[S_x, S_y] = iS_z$$

and cyclic permutations thereof.
Alternately,

$$[S_\alpha, S_\beta] = i\varepsilon_{\alpha\beta\gamma}S_\gamma$$

There's another operator

$$\hat{S}^2 = S_x^2 + S_y^2 + S_z^2 \qquad\qquad [\hat{S}^2, H] = 0$$

Theres another way to write this as

$$\begin{aligned} S^2 = (S_{1x} + S_{2x})^2 + (S_{1y} + S_{2y})^2 + (S_{1z} + S_{2z})^2 \\ = S_1^2 + S_2^2 + 2S_1 \cdot S_2 \end{aligned}$$

All of those individually commute with the hamiltonian, since $[S_1^2, S_1 \cdot S_2] = 0$, and same for S_2.
We call S^2 the *total spin operator*. With $S_{x,y,z}, S^2$ the total spin operators.
Now, check the eigenstates of the hamiltonian are eigenstates of the spin operators.

	$\hat{H}$	$\hat{S}^2$	$\hat{S}_z$
$\left|\uparrow\uparrow\right\rangle$	$A/2$	$2\hbar^2$	$\hbar$
$\frac{1}{\sqrt{2}}(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle)$	$-A/2$	$2\hbar^2$	0
$\left|\downarrow\downarrow\right\rangle$	$A/2$	$2\hbar^2$	$-\hbar$
$\frac{1}{\sqrt{2}}(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle)$	$-A/2$	0	0

We can see the first 3 are the spin-1 system, and the final system the spin-0.

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[2] Is this basically JCF?

[3] TODO: Write out spin operators for this state explicitly

1.3.2 Problems 11.16, 11.18 in Townsend

11.16 Considering $H_{\text{Hydrogen}} + \frac{\gamma}{r}$.

2 Stationary Perturbation Theory

2.1 Formalism for non-degenerate eigenstates

We can try to solve unsolveable problems by dividing the hamiltonian in two, taking

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$$

with $\hat{H}_0$ being some hamiltonian we can solve exactly, with

$$H_0 \left|\varphi_n^{(0)}\right\rangle = E_n^{(0)} \left|\varphi_n^{(0)}\right\rangle$$

2.1.1 First order energy correction

Let's take our first order expansion of $|n\rangle = \left|n^{(0)}\right\rangle + \lambda \left|n^{(0)}\right\rangle ...$

$$(H_0 + \lambda H_1) \sum_{i=0}^{\infty} \lambda^i \left|n^{(i)}\right\rangle = \sum_{i=0}^{\infty} \lambda^n E_n^{(0)} \sum_{i=0}^{\infty} \lambda^i \left|n^{(i)}\right\rangle$$

The first order correction comes out to be that the first order correction is $E_n^{(1)} = \left\langle n^{(0)}\right| H_1 \left|n^{(0)}\right\rangle$. Stated more consicely, it is

$$E_n^{(1)} = \langle H_1 \rangle_{(0)}$$

2.1.2 First order state correction

If we want to find the first order correction to our state $|n\rangle$, we should take some $\sum_m c_m \left|m^{(0)}\right\rangle$, where $|m\rangle$ is the "natural basis" given by solving the eigenvalue equation of the unperturbed case.
We can take

$$\left\langle m^{(0)}\right| H_0 \left|n^{(1)}\right\rangle + \left\langle m^{(0)}\right| H_1 \left|n^{(0)}\right\rangle = \left\langle m^{(0)}\middle|n^{(1)}\right\rangle E_n^{(0)}$$

Of course, $\left\langle m^{(0)}\middle|n^{(1)}\right\rangle$ is the c_1 correction we wanted from the sum above, so we can left multiply and get

$$E_0 \left\langle m^{(0)}\middle|n^{(1)}\right\rangle + \left\langle m^{(0)}\right| H_1 \left|n^{(0)}\right\rangle = \left\langle m^{(0)}\middle|n^{(1)}\right\rangle E_n^{(0)}$$

which gives

$$\left\langle m^{(0)}\middle|n^{(1)}\right\rangle E_n^{(0)} = \frac{\left\langle m^{(0)}\right| H_1 \left|n^0\right\rangle}{E_n^{(0)} - E_m^{(0)}}$$

We're still missing the $\left|n^{(0)}\right\rangle$ term, but if we use the fact that $|n\rangle$ is noramlized, we should have

$$\langle n|n\rangle = 1 = \left\langle n^{(0)}\middle|n^{(0)}\right\rangle + 2\lambda \operatorname{Re} \left\langle n^{(0)}\middle|n^{(1)}\right\rangle + O(\lambda^2)$$

This yields that $2\lambda \operatorname{Re} \left\langle n^{(0)}\middle|n^{(1)}\right\rangle \approx 0$ to order λ^2, which lets us write down

$$|n\rangle = \left|n^{(0)}\right\rangle + i\alpha \left|n^{(0)}\right\rangle + \lambda \sum_{m \neq n} \frac{\left\langle m^{(0)}\right| H_1 \left|n^0\right\rangle}{E_n^{(0)} - E_m^{(0)}}$$

If we want to correct the parallell component, we make a small angle approximation to write

$$|n\rangle = (1 + i\alpha) \left|n^{(0)}\right\rangle + ... = e^{i\alpha} \left|n^0\right\rangle + ...$$

which lets us simplify even further by writing

$$|n\rangle = \left|n^{(0)}\right\rangle + (1 - i\alpha)\lambda \sum_{m \neq n} \frac{\left\langle m^{(0)}\right| H_1 \left|n^0\right\rangle}{E_n^{(0)} - E_m^{(0)}}$$

and since α is of order λ, we can just drop it, since thier product is of order λ^2
Giving the final first order correction to the state is just (dropping λ by setting it equal to one, and letting H_1 be small compared to the energy difference)

$$|n\rangle = \left|n^{(0)}\right\rangle + \sum_{m\neq n}\left(\frac{\langle m^{(0)}|\, H_1\, |n^0\rangle}{E_n^{(0)} - E_m^{(0)}}\right)\left|m^{(0)}\right\rangle$$

2.1.3 Second Order Energy Correction

$$\langle n^0|\left(H_0\, |n^2\rangle + H_1\, |n^1\rangle\right) = \langle n^0|\left(E_n^{(0)}\, |n^2\rangle + E_n^{(1)}\, |n^1\rangle + E_n^{(2)}\, |n^0\rangle\right)$$

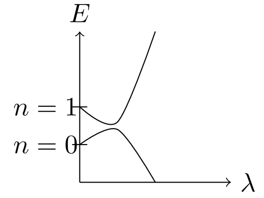
we get

$$E_n^0 \langle n^0|n^2\rangle + \langle n^0|\, H_1\, |n^1\rangle = E_n^{(0)} \langle n^0|n^2\rangle + E_n^{(1)} \langle n^0|n^1\rangle + E_n^{(2)} \langle n^0|n^0\rangle$$

We have cancellation, and also $E_n^{(1)} \langle n^0|n^1\rangle \sim 0 + \mathcal{O}(\lambda^2)$, so we get

$$E_n^{(2)} = \langle n^0|\, H_1\, |n^1\rangle = \sum_{m\neq n}\frac{\langle n^0|\, H_1\, |m^0\rangle \langle m^0|\, H_1\, |n^0\rangle}{E_n^{(0)} - E_m^{(0)}} = \sum_{m\neq n}\frac{|\langle m^0|\, H_1\, |n^0\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

An interesting property of this is level repulsion. Basically, higher order contributions cause repulsion.



2.2 Example: Harmonic Oscillation + Perturbations

Take some hamiltonian for the simple harmonic oscillator, however, in the presence of an external electric field.

$$H = H_0 + H_1 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \mathcal{E}qx$$

2.2.1 First order

First, we attempt the first order correction

$$E_n^{(1)} = \left\langle n^{(0)}\right| /H_1 \left|n^{(0)}\right\rangle = -\mathcal{E}q\left\langle n^{(0)}\right| x \left|n^{(0)}\right\rangle = 0$$

where the final equality holds by the homework problem where we showed that x can only have non-vanishing matrix elements between states of opposite parity.

2.2.2 Second order

This means we have to go to second order

$$|n\rangle = \left|n^{(0)}\right\rangle - q\mathcal{E}\sum_{m\neq n}\left|m^{(0)}\right\rangle \frac{\langle m^{(0}|\, x\, |n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$$

rewriting $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$, we take

$$\begin{aligned}|n\rangle &= \left|n^{(0)}\right\rangle - q\mathcal{E}\left(\left|n^{(0)} + 1\right\rangle \frac{\sqrt{n+1}}{-\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}} + \left|n^{(0)} - 1\right\rangle \frac{\sqrt{n}}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}\right)\\ &= \left|n^{(0)}\right\rangle + \frac{q\mathcal{E}}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\left|n^{(0)} + 1\right\rangle - \sqrt{n}\left|n^{(0)} - 1\right\rangle\right)\end{aligned}$$

Then, we calculate the final energy correction as

$$E_n^{(2)} = \frac{\hbar q^2 \mathcal{E}^2}{2m\omega}\left(\frac{n+1}{-\hbar\omega} + \frac{n}{\hbar\omega}\right) = -\frac{q^2\mathcal{E}^2}{2m\omega^2}$$

2.2.3 Complete the Squares

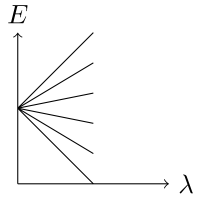
This is exactly the result that we get from completing the squares and writing

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)^2 - \frac{1}{2}\frac{q^2\mathcal{E}^2}{m\omega^2}$$

This gives us exactly the same result, which is a nice sanity check!

2.3 Degenerate Perturbation Theory

If we have some set of degenerate levels, and apply some perturbation, they might split, and be unique



Basically, we want to diagonalize our perturbation matrix within a basis where the degenerate states are no longer degenerate. We continue with gdegenerate perutrbation theroy, taking

$$\langle\varphi_{n,j}|\left(\hat{H}_0\left|\varphi_n^{(1)}\right\rangle + \hat{H}_1\sum_{i=1}^{N}c_i\left|\varphi_{n,i}^{(0)}\right\rangle = E_n^{(0)}\left|\varphi_n^{(1)}\right\rangle + E_n^{(1)}\sum_{i=1}^{N}c_i\left|\varphi_{n,i}^{(0)}\right\rangle\right)$$

which starts simplifying out to

$$\sum_{i=1}^{N}\left\langle\varphi_{n,j}^{(0)}\right|\hat{H}_1\left|\varphi_{n,i}^{(0)}\right\rangle c_i = E_n^{(1)}c_i$$

$$\sum_{i=1}^{N}\left[\hat{H}_1\right]_{ji}c_i = E_n^{(1)}c_i$$

where the final equality is just matrix multiplication of a vector.

2.4 More Examples!

2.4.1 Hydrogen Atom

Take

$$\begin{aligned} H_0 &= \frac{\hat{p}^2}{2m} - \frac{e^2}{|\hat{r}|} \\ H_1 &= -\mu_e\cdot\vec{E} = -e\hat{r}\cdot\vec{E} = eE\hat{z} \\ H &= H_0 + H_1 \end{aligned}$$

We're allowed to ignore spin here, since the electric field points along the spin axis.

Review: Spectrum of Hydrogen Atom Given by quantum numbers,

$$\left|\varphi_{n,\ell,m}^{(0)}\right\rangle = |n,\ell,m\rangle$$

where n is the principal quantum number, ℓ is related to L^2, and m is related to L^z.
For higher values of n, we have an increasing number of allowable values for ℓ, e.g. for $n=1$ only $\ell=0$ is allowed, but for $n=3, \ell\in\{0,1,2\}$.[4]

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[4] TODO: review this in townsend.

Nondegenerate $n = 1$ Now, we want to ask ourselevs what

$$E^{(1)}_{1,0,0} = \mathcal{E} \langle 1, 0, 0| \hat{z} |1, 0, 0\rangle = 0$$

Since we know its invariant under rotation, we have the last equality This means we need to go to second order in our energy correction, so we want

$$E^{(2)}_{1,0,0} = \mathcal{E}^2 \sum_{n=1}^{\infty} \sum_{\ell,m} \frac{| \langle n, \ell, m| \hat{z} |1, 0, 0\rangle |}{E^{(0}_1 - E^{(0)}_n}$$

This sum is really hard to evaluate, but we do know that it converges, and it's a challenge problem to show that it does.
We note that the state cannot ever mix different values of m, from symmetry arguments

Degenerate $n = 2$ This is cool for the nondegenerate case where $n = 1$, but what about the case where $n = 2$? It might be degenerate! This is something different.
Our basis can be written as

$$|2, 0, 0\rangle \qquad |2, 1, 0\rangle \qquad |2, 1, 1\rangle \qquad |2, 1, -1\rangle$$

If we didnt know any better, it is actually possible to write this matrix out in its full glory. Altman did it on the board, but was pretty clear that it's "boring to do", and unnecessary.
The question he poses is whether or not there's a simplification that can make this problem fun. For one thing, many matrix elements are actually 0 by symmetry arguments, so we can just eliminate those as contenders immediately. The way he keeps posing this argument is as a statement about integrating over functions that are odd under parity. The final form of the matrix he writes down is roughly

$$\hat{H} = -\mathcal{H} \begin{bmatrix} 0 & \langle 2, 0, 0| \hat{z} |2, 1, 0\rangle & 0 & 0 \\ \langle 2, 1, 0| \hat{z} |2, 0, 0\rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Recall quantum numbers, etc, from hydrogen atom. We care about the twofold degenerate case.
We noted that if we have the perturbation $H_1 = -e\varepsilon\hat{z}$, we have $[H_1, L_z] = 0$, so we get the matrix from the previous lecture.
We need to calculate this integral: $\langle 2, 1, 0| H_1 |2, 0, 0\rangle$. We can do this integral as, with R, Y as the radial component and spherical harmonic of the wavefunction.[5]

$$\int_0^\infty r^2 dr \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi R^*_{21}(r) Y^*_{1,0}(\theta, \varphi) r \cos\theta R_{2,0}(r) Y_{0,0}(\theta, \varphi) = -3e\varepsilon a_0$$

This gives splitting of degeneracies.
Perturbations we'd like to to include: spin-orbit coupling (omg!!!).

2.4.2 Relativistic Corrections to the Hamiltonian

Our normal hamiltonian is just $H = \frac{p^2}{2m}$. But, if we want the kinetic energy of a relativstic particle (classically), we have $K = \sqrt{p^2c^2 + (mc^2)^2} - mc^2$.
If we try in the limit where $\frac{v}{c} \ll 1$, we can expand the above kinetic energy

$$K \approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots = \frac{p^2}{2m} \left(1 - \frac{1}{4}\frac{v^2}{c^2}\right)$$

If we only account for this perturbation, we should have for some atom that

$$H_0 = \frac{p^2}{2m} - \frac{ze^2}{r} \qquad H_1 = -\frac{p^4}{8m^3c^2}$$

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[5] TODO: Go understand where Y comes from. Haeffner didn't have enough time to get through this. Maybe check during OH?

The first question we can ask is whether or not this still commutes with angular momentum? The answer is yes. We can ask whether this is invariant under rotation, and since it only depends on the magnitude of p, we find that $\langle n,\ell,m|\, p^4 \,|n,\ell,m\rangle$ can nonly be nonvanishing for matchin ℓ, m, so

$$\langle n,\ell,m|\, p^4 \,|n',\ell',m'\rangle = A(n,\ell,m)\delta_{\ell\ell'}\delta_{mm'}$$

We can compute this as

$$E^{(1)}_{n\ell} = -\langle n,\ell,m|\, \frac{p^4}{8m^3c^2} \,|n,\ell,m\rangle$$

Rather than integrate this expectation value explicitly, we will use one of altmans big trix, by writing

$$\frac{p^2}{8m^3c^2} = \frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2$$

Now, we take advantage of the fact that kinetic energy is just the unperturbed hamiltonian minus the potential energy, so we write

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

We put this into the expectation value to get

$$\begin{aligned} E^{(1)}_{n\ell} &= \frac{1}{2mc^2}\langle n,\ell,m|\left[H_0^2 + H_0\frac{e^2}{r} + \frac{e^2}{r}H_0 + \frac{e^4}{r^2}\right]|n,\ell,m\rangle \\ &\frac{1}{2mc^2}\left[(E_n^{(0)})^2 + 2E_n^{(0)}\langle\frac{e^2}{\hat{r}}\rangle_{n\ell m} + \langle\frac{e^4}{\hat{r}^2}\rangle_{n\ell m}\right] \end{aligned}$$

We then want to take advantage of the virial theorem for quantum mechanics. Specifically, for the hydrogen atom, we have

$$\langle K\rangle_{n\ell m} + \frac{1}{2}\langle V\rangle_{n\ell m} = 0$$

We take the above equaiton, along with

$$\langle K\rangle_{n\ell m} + \langle V\rangle_{n\ell m} = E_n^{(0)}$$

We have now two equations with two unknowns, so we get

$$\langle\frac{ze^2}{r}\rangle = -2E_n^{(0)}$$

We're out of time, but we can write down the first order correction as

$$\frac{-E_n^{(0)}}{2mc^2}\left(-3 + \frac{4n}{\ell+\frac{1}{2}}\right) = \frac{1}{2}mc^2z^4\alpha^4\left[-3 + \frac{4n}{\ell+\frac{1}{2}}\right]$$

where α is the fine structure constant.

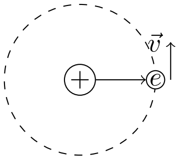
$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$$

2.4.3 Relativistic Corrections to the Atom (Guest: Prof. Mike Zaletel)

Hydrogen atom hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_k + \hat{H}_{s.o.} + \hat{H}_D$$

where H_0 is the usual hamiltonian, H_k contains corrections gained by inclusion of $\hat{p}^4$, $\hat{H}_{s.o.}$ is $\vec{L}\cdot\vec{S}$, or the spin orbit coupling term, and $\hat{H}_D$ is the "Darwin" component.



If we switch to the frame of our electron, the proton should move with velocity $-\vec{v}$. Let the charge of the proton be Z, so we get, in CGS units that our magnetic field should be

$$\vec{B} = \frac{-Ze\vec{v}\times\vec{r}}{cr^3}$$

Since the electron carries a spin, we want

$$\hat{H}_{so} = -\vec{mu}\cdot\vec{B}$$

We're gonna be off by a factor of 2, but that's because we aren't using the dirac equation to find solutions here. Moving on with that in mind, we write that

$$\vec{\mu} = g\mu_B\vec{S}$$

so the spin orbit coupling becomes

$$\frac{Ze^2}{m_e^2c^2r^3}\vec{S}\cdot\vec{L}$$

Remember, we have the factor of two though, so the actual result should be

$$\frac{Ze^2}{2m_e^2c^2r^3}\vec{S}\cdot\vec{L}$$

Our base hamiltonian has eigenspectra $H_0 : |n, \ell, m\rangle$. When we go to spin, we get $|n, \ell, m\rangle \otimes \left|Z = \pm\frac{1}{2}\right\rangle$. This is gonna yeet our $SO(3)$ symmetry in ℓ, Z, which is sad! But if we want to make this easier, we should take

$$\vec{J} = \vec{L} + \vec{S}$$

We should note the following properties

$$[\vec{L}^2, \hat{H}_{so}] = 0 \qquad\qquad [\vec{S}^2, \hat{H}_{so}] = 0$$

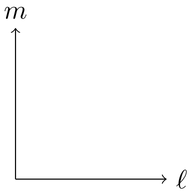
An easy way to show this is that

$$[J, J^2] = [J, (L+S)^2] = [L+S, L^2 + 2LS + S^2]$$

We have that $[L+S, L^2] = 0, [L+S, S^2] = 0$, o we have

$$2[J, LS] = 0$$

so $[J, LS] = 0$.
Let's just yEET n into obliviou for a moment, and think about the level diagram of our basis for ℓ, m.



We now have this general set of states

$$|n, \ell, m\rangle\,|\uparrow\rangle\,, |n, \ell, m+1\rangle\,|\downarrow\rangle$$

that have the same ℓ, J^2.
What we want to focus on is

$$H_{so} = \beta 2L\cdot S$$

Let's break $L \sim L_+, L_-, L_z$, andsame for $S \sim S_-, S_+, S_z$. If we go through these relations, we should just get that

$$2L\cdot S = L_+S_- + L_-S_+ + 2L_zS_z$$

WE can then try and write down the total contribution to the hamiltonian for each individual term

$$2L_zS_z = \hbar^2\begin{bmatrix} m & 0 \\ 0 & -(m+1)\end{bmatrix}$$

We can try and make out the second component, which is tedious apprantly, so he just reports the result, which has all those cancer tier off diagonal elements

$$L_+S_- + L_-S_+ = \hbar^2 \begin{bmatrix} 0 & \sqrt{\ell(\ell+1) - m(m+1)} \\ \sqrt{\ell(\ell+1) - m(m+1)} & 0 \end{bmatrix}$$

We compute the characteristic polynomial to be

$$\lambda^\lambda - \ell(\ell+1) = 0$$

which gives

$$\ell_+ = \ell \qquad\qquad \ell_- = -(\ell+1)$$

We can use this to work out the new energy spectrum

$$\hbar j(j+1) = \vec{J}^2 = L^2 + 2LS + S^2 = \hbar^2\left(\ell(\ell+1) + \frac{1}{2}\left(\frac{1}{2}+1\right) + 2LS\right)$$

or

$$\hbar^2 j(j+1) = \hbar^2\left(\ell(\ell+1) + \frac{1}{2}\left(\frac{1}{2}+1\right) + \begin{cases}\ell \\ -\ell-1\end{cases}\right)$$

We can hybridize then, to get

$$|n, \ell, j, m_j\rangle\,; m_j = \hbar J_z$$

Now, all that's left to do is actually compute the correction. We know the basis is diagonal, so we just put it in

$$\frac{Ze^2}{4m_e^2c^2}\langle n, \ell, j, m_j|\, 2\vec{L}\cdot\vec{S}\frac{1}{\hat{r}^3}\,|n, \ell, j, m_j\rangle$$

We dont know the expectation value $\langle\frac{1}{r^3}\rangle_{n,\ell}$, which townsend leaves as an excercise, and comes out to be

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

Then,

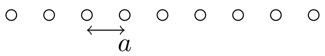
$$\langle 2LS\rangle = \begin{cases}\ell \\ -(\ell+1)\end{cases}$$

Finally, in it's full glory, we should have

$$\frac{Ze^2}{4m_e^2c^2}\langle n, \ell, j, m_j|\, 2\vec{L}\cdot\vec{S}\frac{1}{\hat{r}^3}\,|n, \ell, j, m_j\rangle = \frac{Z^3}{a_0^3 n^3 l\left(l+\frac{1}{2}\right)(l+1)}\begin{cases}\ell \\ -(\ell+1)\end{cases}$$

2.5 Electrons in metallic solids

Not really such a thing as a free electron. Mostly, we have atoms in a lattice.
Let's start with a 1-d situation



We can write down $|n\rangle$, the state of e^- sitting on an atom n, which gives $\langle n|m\rangle = \delta_{nm}$.
We can write down the hamiltonian as H_0, the usual, and some H_1 to account for the dynamics, where the electrons are only allowed to move between neighbors.

$$H_0 = E_0\sum_N |n\rangle\langle n| \qquad\qquad H_1 = -t\sum_N |n\rangle\langle n+1| + |n+1\rangle\langle n|$$

We just want to find eigenstates of this now, by putting this into Schroedingers equation and solving the eigenvalue equation, which gives us

$$E_0\sum_M \psi_m|m\rangle - t\sum_m \psi_{m+1}|m\rangle + \psi_m|m+1\rangle = E\sum_m \psi_m|m\rangle$$

Let's inner product on another state n, which gives us a set of equations for another state n, this gives us an equation

$$E_o\psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

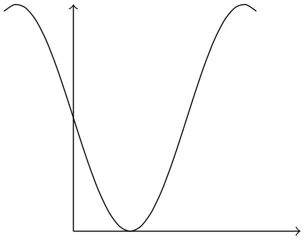
We can solve this to get

$$\psi_n = \frac{e^{ikna}}{\sqrt{N}}$$

If we take the symmetry $k \to k + \frac{2\pi}{a}$, then we only need to look at $k \in \left[\frac{-\pi}{a}, \frac{\pi}{a}\right]$. This is actually just the **Brilloun Zone** of the lattice. k comes in a discrete unit, $\frac{2\pi}{aN}$. This allows the counting of the basis. We can get this out by just enforcing periodic boundary conditions on k.
This spits out

$$E = E_0 - 2t\cos ka$$

We can plot this as



Remarks

1. For arbitrary small perturbations, the hopping wavefunction (pos space) completely delocalized.
2. All of original degeneracy has been lifted
3. For small $|k| \ll \frac{\pi}{a}$, we have $E_k \approx \frac{\hbar^2 k^2}{2m^*}$, with $m^* = \frac{\hbar^2}{2a^2 t}$.

This m^* can be tought of as a sort of renormalized mass that comes from the interaction with the lattice, but leaves our wavefunction completelet delocalized, as we expect.

2.5.1 More Realistic Treatment

Assume e^- can move anywhere along $\hat{x}$, but assume there's some weak periodic potential $V(x) = V(x+a)$. The hamiltonian is just

$$H = \frac{p^2}{2m} + V(x)$$

Bare energies of the problem can be obtained by taking the fourier transform, and getting

$$E_0(k) = \frac{\hbar^2 k^2}{2m}$$

We probably should do perturbation theory. Naively, it looks as if since for $\pm k$, $E_o(\pm k)$ is the same, we should do degenerate perurbation theory. We can just get a new basis expressed as linear combinations of $|\pm k\rangle$.
We should always check, however, that

$$\langle k| V |k'\rangle \neq 0$$

Since we know that V is periodic, we can re-expand our perturbation V in the fourier basis.
Let's expand V as

$$V(x) = \sum_n V_n e^{2\pi n x/a}$$

with

$$V_n = \frac{1}{a}\int_0^a dx V(x) e^{-2\pi i n x/a}$$

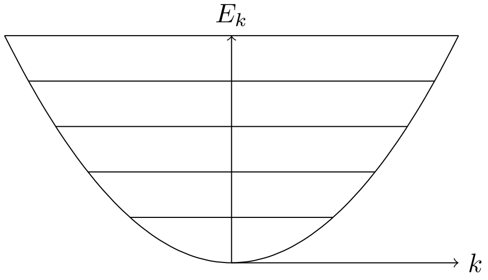
We can combine this all to get

$$\langle k| V |k'\rangle = \int dx \sum_n V_n e^{i\left(k-k'+\frac{2\pi n}{a}\right)x} = \sum_n V_n \delta\left(k' - k + \frac{2\pi n}{a}\right)$$

Momenta k, k' have to match $\frac{2\pi n}{a}$ in order for the V to have an effect. That is to say, that mixing occurs as

$$k = k' + \frac{2\pi n}{a}$$

Now, we apply the condition to our degenerate states



This is another way of thinking about the emergence of the Brillouin Zone. It's just the first place a periodic perturbation mixes a $|\pm k\rangle$ state.
We can consider some basic limits of this.

Case 1: Low momenta For low momenta, $|k| \ll \frac{\pi}{2a}$.

$$E(k) = \frac{\hbar^2 k^2}{2m} + \langle k| V |k\rangle + \sum_{k=k'} \frac{|\langle k| V |k'\rangle|^2}{E_0(k) - E_0(k')} + \dots$$

but the perturbation is small, so it should behave like a free particle.

Case 2: At Edge of Brillouin Zone We want to mix $|k\rangle, |-k\rangle$ at $\alpha |k\rangle + \beta |-k\rangle$, which comes down to solve the schroedinger equaltion in this degenerate subspace.
This gives

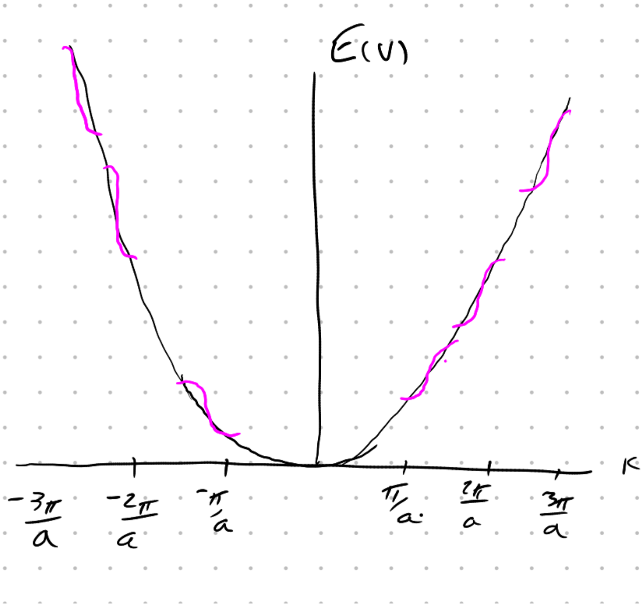
$$\begin{bmatrix} \langle k| H |k\rangle & \langle k| H |k'\rangle \\ \langle k'| H |k\rangle & \langle k'| H |k'\rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

This becomes

$$\begin{bmatrix} E_0(k) + V_0 & V_n \\ V_n^* & E_0(k') + V_0 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

We know that $E_0(k) = E_0(k' = -k) = \frac{n^2\hbar^2\pi^2}{2ma^2}$, with after a bit of algebra gives us mixing

$$E = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n|$$



Case 3: Close to edge of BZ We want to take a "continuous" approach to the edge at each band. We're gonna take $k = \frac{n\pi}{a} + \delta$, and $k' = -\frac{n\pi}{a} + \delta'$. This is going to give us some state where $\exists$ matrix elements, but the gap between energy levels no longer be zero.
Now, we want to solve the eigenvalue equaitons for

$$E_\pm = \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} \pm \delta^2\right) + V_0 \pm \sqrt{|V_n|^2 + \left(\frac{\hbar^2}{2m}\frac{2\pi n}{a}\delta\right)^2}$$

In the limit $\delta \to 0$, we justt get our original answer back, which is good. We can check out a few limits.
First, let $\delta \gg V_n$. To first order, it becomes

$$E_\pm = E_0\left(\frac{n\pi}{a} \pm \delta\right) + V_0 \pm \frac{|V_n|^2}{E\left(\frac{n\pi}{a} + \delta\right) - E\left(\frac{n\pi}{a} - \delta\right)}$$

Limit 2 is for $\delta \ll V_n$,

$$E_\pi = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n| + \frac{\hbar^2}{2m}\left(1 + \frac{1}{|V_n|}\frac{n^2\hbar^2\pi^2}{ma^2}\right)^2$$

There are some things we should take away from this

1. for $k \ll \frac{\pi}{a}$, we have basically a free electron
2. for $k = \frac{\pi n}{a}$, the spectrum splits as $2|V_n|$.

3 Variational Method

In most cases, it's basically impossible to solve schroedingers equation, because we can't diagonalize that "big ass matrix"[6].
The idea is to find the ground state of some hamiltonian H. Then, we make the staement

$$\forall \left|\psi\right\rangle ; E(\psi) = \frac{\left\langle\psi\right| H \left|\psi\right\rangle}{\left\langle\psi|\psi\right\rangle} \geq E_0$$

i.e. any state's energy will be larger than the ground state energy. We can find some trial wavefunctions parameterized by $\{\alpha, \beta, \gamma \ldots\}$. Then, the goal becoems to minimize $E(\psi)$ with respect to these variational parameters which results in **a rigorous bound on the ground state energy**.
In principle, we can always improve our bound by adding more variational parameters.

3.1 Ex: Free Particle

Let's take

$$H_0 = \frac{p^2}{2m} + \lambda x^4$$

The trial wavefunctions we are going to use are $\psi(x, \alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$.
We choose our functions to be "nice" based on the hamiltonian. Prof. Yao wrote this on the board

1. Gaussians are easy for this H
2. Symmetric Function w/ nodes

We then calculate the variational energy

$$E(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int dx e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda x^4\right) e^{-\frac{\alpha x^2}{2}} = \frac{\hbar^2}{2m}\alpha + \frac{3\lambda}{4\alpha^2}$$

The latter term means that we have $\alpha \to \infty$ wants localized wavefunction to be minimal, and the former is minimzed by $\alpha \to 0$, saying that low momentum minimizes that component of the wf.
We can solve this for

$$\alpha_0 = \left(\frac{6m\lambda}{\hbar^2}\right)^{1/3} \qquad E(\alpha_0) = \frac{3}{8}\left(\frac{6\hbar^4\lambda}{m^2}\right)^{1/3}$$

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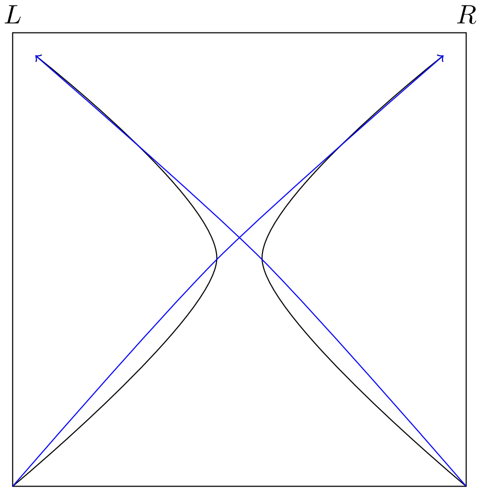
[6] Norman Yao, circa 2019.

4 Indistinguishabe Particles



In this diagram, we cannot tell the difference between the black and blue particles, which means $|L, R\rangle$, $|R, L\rangle$ can't be the right states. It must be some superposition of these two states that gives us indistinguishability.

Makes a lot of sense that it shouldl be eigensttates ofthe permutation operator. For the two particle system, these eigenstates are given by

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}}(|LR\rangle \pm |RL\rangle)$$

4.1 Bosons + Fermions

- Bosons: Wavefunction must be symmetric under permutation. (Photons, Higgs Boson, Composite particles (^{4}He, Mesons)
- Fermions: Wavefunction is antisymmetric under permutation (Most fundamental particles, electrons protons neutrons, neutrinos, quarks)

Consider the case with two fermions. The only legal state of these is then

$$\frac{1}{\sqrt{2}}(|\alpha_1, \alpha_2\rangle - |\alpha_2, \alpha_1\rangle)$$

if we let $\alpha_1 = \alpha_2$ exactly, we immediately get the probability of finding two fermions in the same state as 0, which is just the **pauli exclusion principle**.

4.2 Physical Effects of Particle Statistics

4.2.1 Effect on Spectrum

Take some example hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1) + V(x_2)$$

or $H = H_1 + H_2$. Naiveley, we could just solve the schrodinger equation by looking at wavefunctions that are products of eigenstates of H_1, H_2.

If we restrict to a square potential of finite magnitude, we have

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}nx\right)$$

or, we can let

$$E_n = Kn^2; n = \frac{\pi^2\hbar^2}{2ma^2}$$

In the distinguishable case, we get then that

$$E_0^D = E_1 + E_1 = \frac{\pi^2\hbar^2}{ma^2}$$

If we look at E_1^D, there's a double degeneracy. Maybe it's useful to put this in a table

Energy	Degeneracy	WF
$E_0 = 2K$	1	$\psi_1\psi_1$
$E_1 = 5K$	2	$\psi_2\psi_1; \psi_1\psi_2$

If we have two **bosons**, however, we're going to get indistinguishable particles
We're going to end up with

Energy	Degeneracy	WF
$E_0 = 2K$	1	$\psi_1\psi_1$
$E_1 = 5K$	1	$\frac{1}{\sqrt{2}}(\psi_1\psi_2 + \psi_2\psi_1)$

Fermions have yet a different spectrum. The lowest allowed energy level for a fermion is $5K$, since it must be antisymmetric. Wild stuff!

4.2.2 "Exchange Forces"

The effect of this statistics manifests itself as an inability of fermions to fill the same state, which causes them to space out more.
It's NOT a force.[7]
We want to check in on $\langle (x_1 - x_2)^2 \rangle_{(1,2)}$. Basically, we want to know what the expecation value of distinguishable particles, fermions, and bosons are when $E = 5K$.

Distinguishable Particles We can take

$$\langle 1,2| (x_1 - x_2)^2 |1,2\rangle = \langle 1| x_1^2 |1\rangle + \langle 2| x_2^2 |x\rangle - 2 \langle 1| x_1 |1\rangle \langle 2| x_2 |2\rangle$$

Since the final term contains the product of two odd integrals squared, it goes to zero, so we'll get

$$\langle 1,2| (x_1 - x_2)^2 |1,2\rangle = \langle 1| x_1^2 |1\rangle + \langle 2| x_2^2 |x\rangle$$

Bosons, Fermions This changes the calculation to be, collecting terms

$$\frac{1}{2} \left(\left(\langle 1,2| \pm \langle 2,1|\right) (x_1 - x_2)^2 \left(|1,2\rangle \pm |1,2\rangle\right)\right)$$
$$= \frac{1}{2} \left[\langle 1| x_1^2 |1\rangle + \langle 2| x_2^2 |2\rangle + \langle 2| x_1^2 |2\rangle + \langle 1| x_2^2 |1\rangle \pm \langle 1| x^2 |2\rangle \pm \langle 2| x_2^2 |1\rangle \mp \langle 1| x_1 |2\rangle \langle 2| x_2 |1\rangle \pm \langle 2| x_1^2 |1\rangle \pm\right]$$

Just a whole bunch of shit. Altman is going to write it down after cancelling, and what the heCK this is a lot of algebra.
Cancels to (after noting $x_1 - x_2$ is really just $\hat{x} \otimes I - I \otimes \hat{x}$, so that our integrals cancel out)

$$\frac{1}{2} \left(\left(\langle 1,2| \pm \langle 2,1|\right) (x_1 - x_2)^2 \left(|1,2\rangle \pm |1,2\rangle\right)\right) = I_1 + I_2 \mp |\langle 1| x |2\rangle|^2$$

where the minus corresponds to bosons.

4.3 Systems of N Particles

Consider a system of N particles. We can arrange this in terms of M single particle basis states. We need to count such systems using our 112 Memes.

- Distinguishable particles: M^N possible arrangements of states.

For fermions and bosons, things behave a bit differently.

Bosons The idea is that for our basis states $n_i = \{a, b, \dots,\}$, we need to hav $P_{ij}\psi(n_1, \dots, n_N) = \alpha\psi(n_1, \dots, n_N)$ where $\alpha = \pm 1$. We need to give our particle state some symmetry, so that

$$|n_1, \dots, n_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} |P(n_1, \dots, n_N)\rangle$$

where P_N is the action of taking all possible permutations of group N.

---

[7] TODO: Anyons are particles that have special statistics under the 2d operator called braiding. This sounds hella cool.

Fermions Again, we have to sum over all possible permutations, but then we need

$$|n_1, \dots, n_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} \chi(P) \, |P(n_1, \dots, n_N)\rangle$$

where $\chi(P)$ is the parity of the permutation, where parity is the number of single particle permutations necessary to achieve a given state.

This seems really complicated, but there's actually a trick. Let's try writing in the position basis

$$\begin{aligned} \langle x_1 x_2 x_3 | n_1 n_2 n_3 \rangle &= \psi_{n_1 n_2 n_3}(x_1, x_2, x_3) \\ \psi^B_{n_1 n_2 n_3}(x_1, x_2, x_3) &= \frac{1}{\sqrt{3!}} \sum_P \varphi_{P(n_1)}(x_1)\varphi_{P(n_2)}(x_2)\varphi_{P(n_3)}(x_3) \\ \psi^F_{n_1 n_2 n_3}(x_1, x_2, x_3) &= \frac{1}{\sqrt{3!}} \sum_P \chi_P \varphi_{P(n_1)}(x_1)\varphi_{P(n_2)}(x_2)\varphi_{P(n_3)}(x_3) \end{aligned}$$

The trick for fermions is to take the **slater determinant**,

$$= \frac{1}{\sqrt{3!}} = \det \left| \begin{bmatrix} \varphi_{n_1}(x_1) & \varphi_{n_2}(x_1) & \varphi_{n_3}(x_1) \\ \varphi_{n_1}(x_2) & \varphi_{n_2}(x_2) & \varphi_{n_3}(x_2) \\ \varphi_{n_1}(x_3) & \varphi_{n_2}(x_3) & \varphi_{n_3}(x_3) \end{bmatrix} \right|$$

The slater determinant actually spits out exactly the correct permutations and their signs for a fermion, because of the way signs work when taking the determinant.

This allows us to return to our original challenge: **counting of Bosonic/Fermionic States**. Consider M orbitals, with N particles.

For fermions, this is actually pretty easy. First off, there is no fermionic system with $N > M$. This should come out for $N < M$, there are $\binom{M}{N}$ states.

For bosons, we get a stars and bars problem, which gives there should be $\binom{M+N-1}{N-1}$ states.[8]

4.3.1 When does particle statistics matter?

Really only matters when we have a high probability of particle exchange.[9] The example Altman ggives is of a particle in a German lab, and in Haeffners lab. We probably don't need to apply a symmetrization requirement because they're unlikely to exchange.

Here's the mathy example.

Consider two particles, ψ_E the "earth" hydrogen atom, and ψ_M is the "moon" hydrogen atom.

Then, we apply the properly antisymmetric state

$$\psi_A(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_E(x_1)\psi_M(x_2) - \psi_E(x_2)\psi_M(x_1))$$

and the distinguishable state

$$\psi(x_1, x_2) \frac{1}{\sqrt{2}} \psi_E(x_1)\psi_M(x_2)$$

For the distinguishable case, what we find is

$$P(x) = \int dx_2 |\psi_E(x)|^2 |\psi_M(x_2)|^2 + \int dx_1 |\psi_E(x_1)|^2 |\psi_M(x)|^2 = |\psi_E(x)^2$$

because the integral over x_1 is just obscenely tiny.

For the antisymmetric case, we're going to find

$$P(x) = \int dx_2 |\psi_A|(x_1, x_2)|^2 + \int dx_1 |\psi_A(x_1, x_2)|^2 = \int dx_2 |\psi_E(x)\psi_M(x_2) - \psi_E(x_2)\psi_M(x)|^2$$

Basically, the exponentially decaying tails kind of disappear. It can be shown these come out to be the same.

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[8] THIS IS A GUESS, but im like 90% sure this is correct. Thank you math 55.

[9] is there a way to calculate the probability of exchange?

4.4 Identical Fermions with Spin

Consider $\psi(x_1, x_y, \sigma_1, \sigma_2)$. If no spin-orbit coupling, we just get $\psi(x_1, x_2)\chi(\sigma_1, \sigma_2)$. The product of the orbital DOF, and the spin DOF. Without tying ourselves to a basis we obtain $|\psi\rangle \otimes |\chi\rangle$, but this is kind of trivial.
The important thing is that our wf must be antisymmetric wrt exchange. There are two possibilities

- $\psi_A(x_1, x_2)\chi_S(\sigma_1, \sigma_2)$.
- $\psi_S(x_1, x_2)\chi_A(\sigma_1, \sigma_2)$.

When we're actually adding our spin multiplet, we get that (and you will recall)

- $s = 0$ corresponds to $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
- $s = 1$ corresponds to $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), |\uparrow\uparrow\rangle, |\downarrow, \downarrow\rangle$.

These correspond to the functions

$$\chi_S(\sigma_1, \sigma_2) = \begin{cases} \begin{array}{l|ll} \chi & \sigma_1 & \sigma_2 \\ \hline \frac{1}{\sqrt{2}} & \uparrow & \downarrow \\ \frac{1}{\sqrt{2}} & \downarrow & \uparrow \\ 0 & \uparrow & \uparrow \\ 0 & \downarrow & \downarrow \end{array} \end{cases} \qquad \chi_A(\sigma_1, \sigma_2) = \begin{cases} \begin{array}{l|ll} \chi & \sigma_1 & \sigma_2 \\ \hline \frac{1}{\sqrt{2}} & \uparrow & \downarrow \\ -\frac{1}{\sqrt{2}} & \downarrow & \uparrow \\ 0 & \uparrow & \uparrow \\ 0 & \downarrow & \downarrow \end{array} \end{cases}$$

This basically lets us index our χ_{S,S_z} by the additional S_z term when the spin state must be symmetric, and only by the spin-0 state when χ must be antisymmetric.

4.4.1 The Helium Atom

For helium, what is our hamiltonian? We have two particles orbiting a nucleus. We will approximate the mass of the proton to be roughly infinite (otherwise it's really hard), so we'll take

$$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{ze^2}{|\vec{r}_1|} - \frac{ze^2}{|\vec{r}_2|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

where $z = 2$. Our first attempt at this will utilize perturbation theory to solve it, by treating the interaction term as a perturbation.

Perturbative Approach In the perturbation scheme, we can think of

$$H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{ze^2}{r_1} - \frac{ze^2}{r_2} \qquad H_1 = \frac{e^2}{|r_1 - r_2|}$$

with

$$\hat{H} = H_0 + H_1$$

we now take the 0th order in perturbation theory, and basically think of it as the hydrogen atom, but coupled. We should note this is a pretty bad approach. Since we have that $z = 2$, $H_1 \sim H_0$, so we're going to get qualitatively correct but quantitatively incorrect results.
Note that to 0th order, we have

$$\psi_0^{(0)} = \tilde{\varphi}_{100}(r_1)\tilde{\varphi}_{100}(r_2)\chi_A(r_1, r_2)$$

In general to first order, we can write

$$\psi^{(0)} = [\varphi_{100}(r_1)\varphi_{n\ell m}(r_2) \pm \varphi_{100}(r_2)\varphi_{n\ell m}(r_1)]\, \chi_{A,S}(r_1, r_2)$$

Where the spin wavefunction is antisymmetric when the internal $\pm \mapsto +$, and symmetric when it's $-$. The names of this particle are $s = 0$: Parahelium. $s = 1$: Orthohelium.
Note that we also have degeneracies in energy, regardless of the sign. We have 1 state para, 3 states ortho. These four states are degenerate to first order, but we can lift this degeneracy with the interaction term. This happens because the spin component of the wavefunction is correlated with the orbital state. This turns out to be the source of basically all magnetism we see.

Let's do the ground state shift. Recall that for hydrogen (letting $a = \frac{a_0}{z}$, where a_0 is the bohr radius $a_0 = \frac{\hbar^2}{me^2}$)

$$\psi_{100}(r) = \sqrt{\frac{1}{\pi a^3}} e^{-r/a}$$

We compute (assuming resolution of identity, etc for position repr)

$$\Delta E_0 = \left\langle \psi^{(0)} \middle| H_1 \middle| \psi^{(0)} \right\rangle = \int d^3r_1 d^3r_2 |\varphi_{100}(r_1)|^2 |\varphi_{100}(r_2)|^2 \frac{e^2}{|r_1 - r_2|}$$

Since the square of the wavefunction is really just the probability of finding it at r, we can bring an e inside both of them, and reexpress this as what is essentially an electrostatic calculation, letting ρ be charge density

$$\int d^3r_1 d^3r_2 \frac{\rho(r_1)\rho(r_2)}{|r_1 - r_2|}$$

We skipped the actual computation of this in lecture, but we can continue, skipping steps to get

$$\frac{ze^2}{2a_0(4\pi)^2} \int d^3x_1 d^3x_2 \frac{e^{-(x_1+x_2)}}{|x_1 - x_2|}$$

Where

$$\frac{1}{(4\pi)^2} \int d^3x_1 d^3x_2 \frac{e^{-(x_1+x_2)}}{|x_1 - x_2|} = \frac{5}{4}$$

And, we take that one Rydberg= $\frac{e^2}{2a_0}$, we get

$$\int d^3r_1 d^3r_2 |\varphi_{100}(r_1)|^2 |\varphi_{100}(r_2)|^2 \frac{e^2}{|r_1 - r_2|} = z\frac{5}{4}\text{Ry}$$

Yielding a full energy correction

$$E_0^{(1)} = \left(-2z^2 + \frac{5}{4}\right)\text{Ry} = -5.5\text{Ry} = -74.8\text{eV}$$

So, we have now $\psi^{(0)}_{n\ell m\alpha}$, where α is either ortho or para. We also have $E^{(0)}_{n\ell m} = E^{(0)}_{100} + E^{(0)}_{n\ell m}$.
Our goal now is to forget about degenerate perturbation theory, and pick some nice basis (which I think we can, since we're nondegenerate on H_1?) We computed

$$\Delta E_{n\ell m\alpha} = \left\langle \psi^{(0)}_{n\ell m\alpha} \middle| \frac{e^2}{|r_1 - r_2|} \middle| \psi^{(0)}_{n\ell m\alpha} \right\rangle = \frac{e^2}{2} \int d^3r_1 d^3r_2 \frac{|\tilde{\varphi}100(r_1)\tilde{\varphi}_{n\ell m}(r_2) \pm \tilde{\varphi}_{100}(r_2)\tilde{\varphi}_{n\ell m}(r_1)|^2}{|r_1 - r_2|} = J_{n\ell} \pm K_{n\ell}$$

where

$$J_{n\ell} = e^2 \int d^3r_2 d^3r_2 \frac{|\tilde{\varphi}_{100}(r_1)|^2 |\tilde{\varphi}_{100}(r_2)|^2}{|r_1 - r_2|}$$
$$K_{n\ell} = e^2 \int d^3r_1 d^3r_2 \frac{\text{Re}[\varphi^*_{100}(r_1)\tilde{\varphi}_{100}(r_2)\tilde{\varphi}_{n\ell m}(r_2)^* \tilde{\varphi}_{n\ell m}(r_1)]}{|r_1 - r_2|}$$

Altman does not want to compute these integrals. They look yucky, so I don't blame him.
Basically, since we have two indistinguishable fermions, we can't ever find them in exactly the same state. So, if we think of exchange in orbital space, for the antisymmetric spin state, we will have a symmetric wave function, and vice versa.
[10]

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[10] Homework Toy Model Basically, we are going to take some toy helium atom and solve it completeley with perturbation theory and the variational approach. We're going to take $H = H_1 + H_2 + u\delta(x_1 - x_2)$ Bonus points to the person who finds the nicest variational function.

Variational Approach WTS we can do way better than perturbation theory. Let's go back to our hamiltonian.

$$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{2e^2}{|\vec{r}_1|} - \frac{2e^2}{|\vec{r}_2|} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

Let's consider the ground state representation in the position basis as a variational function, with z a variational parameter.

$$\tilde{\varphi}_{100}(r_1) = \sqrt{\frac{z^3}{\pi a_0^3}} e^{-zr/a_0}$$

We're going to write the hamiltonian now as

$$H = \frac{p_1^2}{2m} - \frac{ze^2}{r_1} + \frac{p_2^2}{2m} - \frac{ze^2}{r_2} + \frac{(z-2)e^2}{r_1} + \frac{(z-2)e^2}{r_2} + \frac{e^2}{|r_1 - r_2|}$$

We consider that $\psi_z(r_1, r_2) = \varphi_{100,z}(r_1)\varphi_{100,z}(r_2)$. Then, we compute

$$\langle\psi_z| H |\psi_z\rangle = -2z^2\text{Ry} + 2I_1 + \frac{e^2z^3}{\pi a_0^3}\int d^3r_1 d^3r_2 \frac{e^{-z(r_1+r_2)}}{|r_1 - r_2|} = -8z + 2z^2 + \frac{5}{4}z$$

I_1 is a pretty simple integral apparently.

$$I_1 = \langle\psi_z| \frac{(z-2)e^2}{|r_1|} |\psi_z\rangle = \frac{e^2z^3}{\pi a_0^3}\int d^3r_1 \frac{(z-2)}{r_1} e^{-zr_1/a_0} = \frac{e^2z^3}{\pi a_0^3} 4\pi \int dr_1 r_1 e^{-zr_1/a_0}(z-2)$$

or something along those lines, it works out though. Altman wasn't really sure his normalization was right, but we have something close and could probably figure it out Either way, we end up with

$$\frac{\partial E}{\partial z} = -8 + 4z + \frac{5}{4} \Rightarrow z_* = 2 - \frac{5}{16}$$

z_* minimizes the energy. Then, we can plug this back into the energy, and we end up with

$$E_0 = -77.5\text{eV}$$

We got a 1% approximation, whereas perturbation theory gave us an answer within roughly 10%.

4.5 Multi-Electron Atoms

What we expect from perturbation theory from the non-interacting model of these energy shells is

n	ℓ	Degeneracy	N
1	0	2	2
2	0,1	2(1+3)=8	2+8=10
3	0,1,2	2(1+3+5)=18	2+10+18=28
4	0,1,2,3	2(1+3+5+7)=32	2+8+18+32=60

What is the origin of this degeneracy though? in m, it's clear that this comes from rotational invariance of the hydrgoen atom, but for ℓ, it's much less clear. Turns out there's an $SO(4)$ symmetry in the hydrogen atom.[11]

It's no bueno in experiment. It holds for $n = 1, 2$ for hydrogen and neon, but for argon, it sucks! We get $n = 3, N = 18$. No Bueno!

Brief overview of s, p, d, f notation.

We can take the next row of the PTE

Z	3	4	5	6	7	8	9	10
	Li	Be	B	C	N	O	F	Ne
He	$2s^1$	$2s^2$	$2s^2 2p^1$	$2s^2 2p^2$	$2s^2 2p^3$	$2s^2 2p^4$	$2s^2 2p^5$	$2s^2 2p^6$

But why the heck is, for instance, in Argon, and it's rows, is the $4s$ orbital filled before the $3d$ orbital? An electron in a MEA feels an effective potential of

$$U(r) = \begin{cases} -\frac{e^2}{r} & r \to \infty \\ -\frac{Ze^2}{r} & r \to 0 \end{cases}$$

The self-consistent approach to solving this problem is to iteratively solve for better and better approximations of this, using some interpolating function to get $U(r)$ to exhibit this behavior.[12]

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[11] TODO: for fun, read weinberg paper

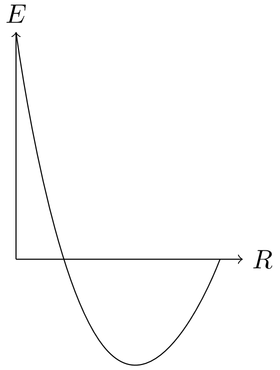
[12] TODO: Look up Hartree-Fock approximation/Self-consistent field method.

4.6 H_2

This has some hamiltonian

$$H = \frac{p^2}{2m} - \frac{e^2}{\left|r - \frac{R}{2}\right|} - \frac{e^2}{\left|r + \frac{R}{2}\right|} + \frac{e^2}{|R|}$$

What we want to find is some ground state energy of this H.
We think it's probably going to look something like



The full wavefunction is going to be

$$|\psi(R)\rangle = |\psi_e\rangle \otimes |R/2\rangle \otimes |{-R/2}\rangle$$

We can pick some non-orthogonal set of states $|1\rangle$, $|2\rangle$, which are the states where we ignore the existence of proton 1, 2 antirespectively, and compute the behavior of the electron about each remaining proton.
We can express this as

$$\left|\varphi_e^{\pm}\right\rangle = |1\rangle \pm |2\rangle$$

where

$$\langle x|1\rangle = \varphi_{100}\left(x - \frac{R}{2}\right)$$
$$\langle x|2\rangle = \varphi_{100}\left(x + \frac{R}{2}\right)$$

We like this, because it's symmetric under permutation. We're going to treate R as our variational parameter. Since we haven't actually normalized our state, we need to divide through by the normalization in perturbation theory, so we get

$$E_{\pm}(R) = \frac{\langle\psi^{\pm}|\,H\,|\psi^{\pm}\rangle}{\langle\psi^{\pm}|\psi^{\pm}\rangle} = \frac{1}{\langle\psi^{\pm}|\psi^{\pm}\rangle}\left(\langle 1|\,H\,|1\rangle + \langle 2|\,H\,|2\rangle \pm (\langle 1|\,H\,|2\rangle + \langle 2|\,H\,|1\rangle)\right)$$

Recall, we chose some variational wavefunction[13]

$$|\psi_{\pm}\rangle = (|1\rangle \pm |2\rangle) \otimes \left|\frac{R}{2}\right\rangle \otimes \left|-\frac{R}{2}\right\rangle$$

Now, we're going to find this variation as a function of distance between the protons, which gives

$$E_{\pm}(R) = \frac{\langle\psi_{\pm}|\,H\,|\psi_{\pm}\rangle}{\langle\psi_{\pm}|\psi_{\pm}\rangle}$$

This really corresponds to a bunch of integrals we have to do,

$$\langle\psi_{\pm}|\psi_{\pm}\rangle = \langle 1|1\rangle + \langle 2|2\rangle \pm 2\,\mathrm{Re}(\langle 1|2\rangle)$$

---

[13] NOTE: that the hamiltonian is mirror symmetric about the origin, which is why $|1\rangle \pm |2\rangle$ doesn't have multiplicative constants like $a\,|1\rangle \pm b\,|2\rangle$. Such a mirror symmetry is like decomposing the hamiltonian in to block-diagonal form.

Since $\langle 1|1\rangle$ is the ground state of hydrogen (same for $\langle 2|2\rangle$), they're automatically normalized, and thus equal to 1. For large R, $\langle 1|2\rangle$ will be very small, since our WF is exponentially decaying, so we expect $\langle 1|2\rangle \sim e^{-R/a_0}$. Let's call $\langle 1|2\rangle = I$.
We can compute

$$I(r) = \int d^3r\varphi^*\left(\vec{r}+\frac{R}{2}\right)\varphi\left(\vec{r}-\frac{R}{2}\right) = e^{-R/a_0}\left[1+\frac{R}{a_0}+\frac{1}{3}\left(\frac{R}{a_0}\right)^2\right]$$

where the derivation, if not in townsend is in griffiths.
Let's call $D_n := \langle n| H |n\rangle$, where D stands for *direct*.
We will call $X_{ab} := \langle a| H |b\rangle$, the *eXchange* operator.

$$\langle 1| H |1\rangle = \langle 1| \frac{p^2}{2m} - \frac{e^2}{\left|r-\frac{R}{2}\right|} |1\rangle - \langle 1| \frac{e^2}{\left(r+\frac{R}{2}\right)} |1\rangle + \langle 1| \frac{e^2}{|R|} |1\rangle = -\frac{e^2}{a_0} - D(R) - \frac{e^2}{R}$$

but, because 1 is the eigenstate of this first operator, we are just going to get the energy of this state, $-1\text{Ry} = \frac{e^2}{a_0}$. This gives that

$$D(R) = \int d^3r\left|\varphi\left(r-\frac{R}{2}\right)\right|^2\frac{e^2}{\left|r+\frac{R}{2}\right|} = \frac{e^2}{a_0}\left[\frac{a_0}{R}-(1+\frac{a_0}{R})e^{-2R/a_0}\right]$$

For the numerator, we have

$$\langle\psi_\pm| H |\psi_\pm\rangle = \langle 1| H |1\rangle + \langle 2| H |2\rangle \pm \langle 1| H |2\rangle \pm \langle 2| H |1\rangle$$

Altman kind of fucked the notation for X, D so just bear with it. The later stuff uses the correct notation.

$$\langle 2| H |1\rangle = \langle 2|\left(\frac{p^2}{2m} - \frac{e^2}{\left|r-\frac{R}{2}\right|}\right)|1\rangle + \langle 2| \frac{e^2}{\left|r+\frac{R}{2}\right|} |1\rangle + \langle 2| \frac{e^2}{|R|} |1\rangle = \frac{-e^2}{a_0}\langle 2|1\rangle + X(R) + \frac{e^2}{R}\langle 2|1\rangle$$

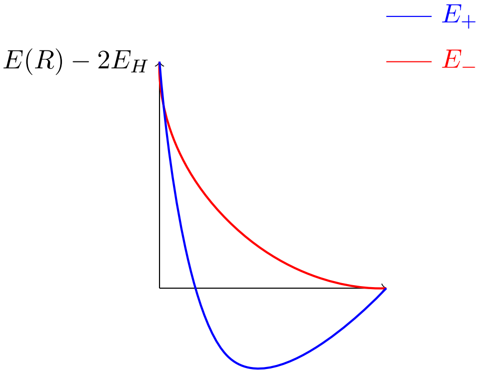
where $X(R)$ can be calculated by taking

$$X(R) = \int d^3r\varphi^*\left(r+\frac{R}{2}\right)\varphi\left(r-\frac{R}{2}\right)\frac{e^2}{\left|r+\frac{R}{2}\right|} = \left(1+\frac{R}{a_0}\right)e^{-R/a_0}$$

So, if we plug all of this back into our expression for energy, we obtain, letting $X = \frac{\tilde{X}e^2}{a_0}$, and likewise for D so that $\tilde{X}, \tilde{D}$ are dimensionless

$$E_\pm(R) = \frac{e^2}{a_0}\frac{1 \pm I + 2(\tilde{D} \pm \tilde{X}) + 2\frac{a_0}{R}(1 \pm I)}{2(1 \pm I)}$$

Altman then suggests we put this into mathematica and plot it, which gives us some really nice function



Where the negative potential is what essentially acts as a bonding state between the hydrogen atoms.
We can optimize these wavefunctions in mathematica (lol) to gget some numbers, with the binding energy of H_2 coming out as roughly 4.7eV.
We're probably gonna start scattering wendesday!

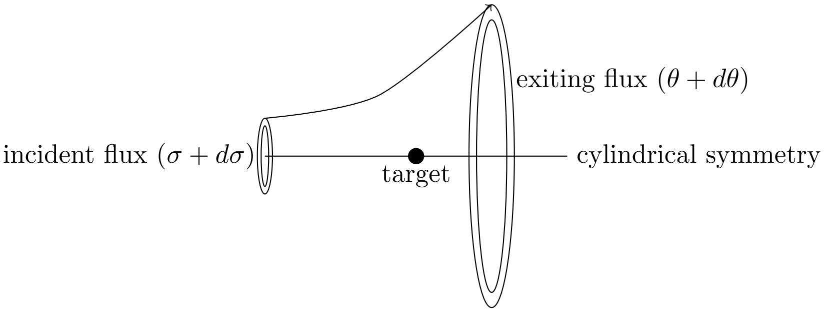
5 Quantum Scattering

5.1 Classical Scattering

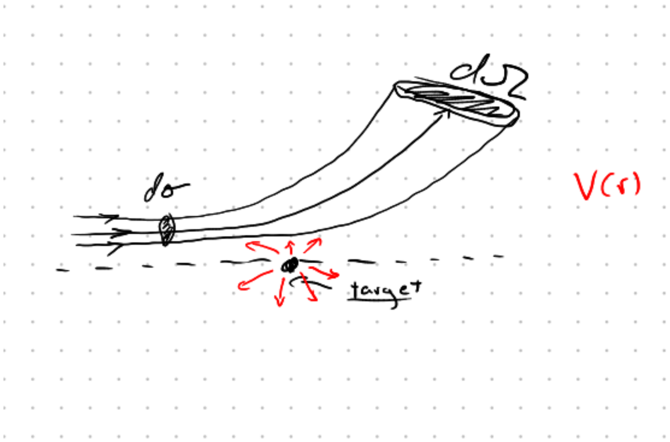
We want first to compare quantum with classical scattering. Consider the following setup, with some flux of particles coming into a sheet at a flux $j_{\text{in}} = \frac{\partial I}{\partial A}$. We have the outgoing flux per steradian, $\frac{\partial I}{\partial \Omega}$, and want t ocompute the ratio

$$\frac{\partial \sigma}{\partial \Omega} = \frac{\frac{\partial I}{\partial \Omega}}{\frac{\partial I}{\partial A}}$$

We will consier our target to exhibit some central potential $V(r)$. The classical model should project that it will behave as follows[14]



We're going to consider



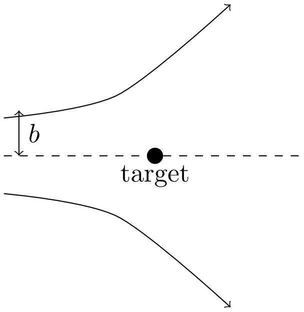
which has

$$dI = \frac{\partial n}{\partial t} = j_{\text{in}} d\sigma = j_{\text{in}} \frac{\partial \sigma}{\partial \Omega} d\Omega$$

where

$$\frac{\partial \sigma}{\partial \Omega} = \frac{\partial I / \partial \Omega}{j_{\text{in}}}$$

which gives our previous result!
We can attempt to characterise this differential cross section by the distance b from the axis of symmetry of the incoming particle.



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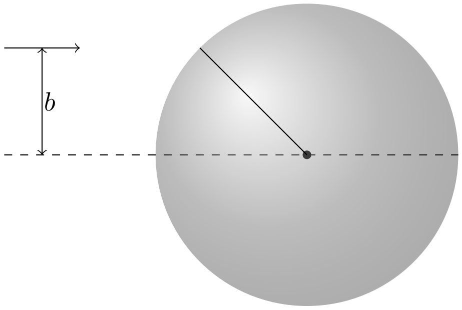
[14] this is just copy-pasted from my 105 notes, so the notation might not be exactly the same.

We can consider $d\sigma$ to be a small piece of area, $d\sigma = bdbd\phi$. This gives that $dI = jd\sigma = jdbd\phi = j\frac{\partial\sigma}{\partial\Omega}d\Omega$, which gives (after cancelling the $d\phi$ from $d\Omega = sin\theta d\phi d\theta$), so we have

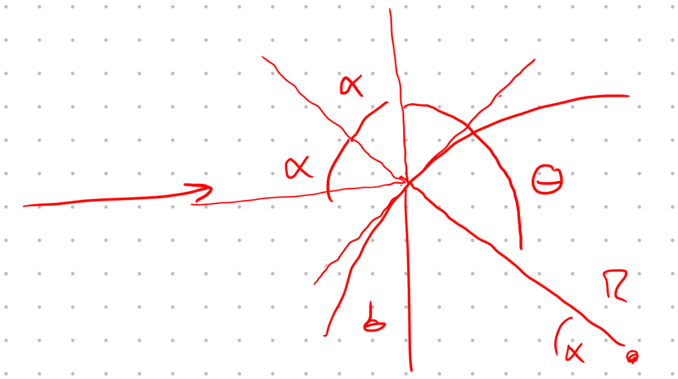
$$\frac{\partial\sigma}{\partial\Omega} = \frac{b}{\sin\theta}\frac{\partial b}{\partial\theta}$$

This is a pretty niche equation though. We have it in terms of b, the impact parameter, E, the precise energy that we shoot it at. We want a more general quantity, which we call σ_T, the total cross section. We're going to integrate over a sphere surrounding the target. We take

$$\sigma_T = \iint_V d\Omega\frac{\partial\sigma}{\partial\Omega}$$



I'll try and finish the pretty drawing later.



We can compute

$$\sigma_T = \int\frac{\partial\sigma}{\partial\Omega}d\Omega = \frac{R^2}{4}\int d\Omega = \frac{4\pi R^2}{4} = \pi R^2$$

For more on this topic, check out Chapter 14 of Taylor[15]. Altman is going to move on to quantum though.

5.2 Beginning Quantum Scattering

We're going to look for eigenvalues of the schroedinger equation, where we have

$$\left[\frac{-\hbar}{2m}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$$

We're going to begin by looking for solutions of the form

$$\psi(r) = \psi_{\text{inc}}(r) + \psi_{\text{sc}}(r)$$

where ψ_{inc} is an incident plane wave, and ψ_{sc} is the scattered component, where

$$\psi_{\text{inc}} = e^{ikz} \qquad\qquad \psi_{\text{sc}} = f(\theta,\phi)\frac{e^{ikr}}{r}$$

---

[15] Not reccomended by altman, I just like the book lol. He said he would post a summary.

We make the switch to spherical coordinates, in the following manner

$$\vec{r} = (\sin\theta\cos\phi|r|, \sin\theta\sin\phi|r|, \cos\theta|r|)$$

Eventually, we're going to find for various cylindrical symmetries that ϕ will drop out of our function f.
We first define the **scattering amplitude** $f(\theta, \phi)$, and connect it to the physical quantity $\frac{\partial\sigma}{\partial\Omega}$, the **differential cross section**.
We need some spherically symmetric $V(r)$ with what Altman referred to as "finite support", which means it is nonzero in a finite region of space, and decays as $\frac{1}{r^{2+\varepsilon}} \sim V(r)$.

5.2.1 Solving the Schroedinger in Spherical Coordinates

I'm pretty sure we did this in 137A, but basically, these bad boys separate out to

$$\psi_{\ell,m}(\vec{r}) = R_\ell(r)Y_{\ell,m}(\theta,\phi)$$

We then get a radial equation, where $u_\ell = R_\ell(r)r$,

$$Eu_\ell = \frac{-\hbar^2}{2m}\frac{\partial^2 u_\ell}{\partial r^2} + \frac{\ell(\ell+1)}{2mr^2}u_\ell$$

In the limit where $r \to \infty$, we get that our solutions are

	Outgoing	Incoming
$R_\ell(r)$	e^{ikr}/r	$e^{-i(kr+Et)}/r$

We also have the current density

$$\frac{j_{sc} d\vec{A}}{j_{inc}} = d\sigma = \frac{d\sigma}{d\Omega}d\Omega = \frac{\text{current scattered into } d\Omega}{\text{incident current per unit area}}$$

we should also note $dA = r^2 d\Omega\hat{r}$.

5.2.2 Probability Current

We can recall the probability current from 137A, where we have $p(r) = |\psi(r)|^2$, and then apply some continuity equation so that

$$\partial_t p(r) = -\nabla j$$

Now, we have

$$\partial_t(\psi^*\psi) = \psi^*\partial_t\psi + \psi\partial_t\psi^*$$

We also have

$$j = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \frac{\hbar}{m}\text{Re}[\psi^*\hat{p}\psi]$$

So, for the incident wave, we have

$$j_{\text{inc}} = \frac{\hbar k}{m}$$

Now, we take j_{sc}.

$$j_{\text{sc}} = \frac{\hbar k}{mr^2}|f(\theta,\phi)|^2\hat{r}$$

So, we have

$$\frac{\partial\sigma}{\partial\Omega}d\Omega = \frac{j_{\text{sc}}\hat{r}r^2 d\Omega}{j_{\text{inc}}} = |f(\theta)|^2 d\Omega$$

which all yields that

$$\frac{\partial\sigma}{\partial\Omega} = |f(\theta)|^2$$

where we have made the approximation that $r \to \infty$ for the scattered component of the wavefunction.

5.3 Born Approximation

We're going to take $E = \frac{\hbar^2 k^2}{2m}$, with

$$(\nabla^2 + k^2)\psi(r) = \frac{2m}{\hbar^2} V(r)\psi(r)$$

We're going to use Green's functions to solve this, which gives

$$\psi(r) = e^{ikz} + \int d^3r' G_0(k, r, r') \frac{2m}{\hbar^2} V(r')\psi(r')$$

We need $(\nabla^2 + k^2)G(k^2, r, r') = \delta^3(r - r')$, where G is still the greens function. If we apply our operator to the above equation, we get

$$(\nabla^2 + k^2)\psi(r) = (\nabla^2 + k^2)\left(e^{ikz} + \int d^3r' G_0(k, r, r') \frac{2m}{\hbar^2} V(r')\psi(r')\right)$$

As an aside, we can think of greens function as being the inverse of the operator $\nabla^2 + k^2$ so that $\hat{G}_0 = (\nabla^2 + k^2)^{-1}$

5.3.1 Deriving Green's Function

We express greens function as the function which obeys $(\nabla^2 + k^2)G_0(r, r') = \delta^3(r - r')$. Since the hamiltonian is translationally invariant, we have that G_0 must be a function of $G_0(r - r')$, whch we can write as a function of a single r, so that

$$(\nabla^2 + k^2)G_0(r) = \delta^3(r)$$

We can do this using a contour integral.[16]
Altman starts wth the townsend integral first. We think that $G_0(r, 0) = c\frac{e^{ikr}}{r}$,so we can carry out some derivative

$$\nabla^2 \frac{e^{ikr}}{r} = \nabla\left(\nabla \frac{e^{ikr}}{r}\right) = \frac{\nabla^2(e^{ikr})}{r} + ...$$

it's a bunch of stupid crap and really simple derivatives. The one thing that we need to note is that $\nabla^2 \frac{1}{r} = -4\pi\delta(r)$
This gives us

$$-k^2 \frac{e^{ikr}}{r} - 4\pi\delta^3(r)e^{ikr} = \nabla^2 \frac{e^{ikr}}{r}$$

If we plug this back in, we get

$$G(r) = \frac{-e^{ikr}}{4\pi r}$$

Thus,

$$G(r, r') = \frac{-e^{ik|r-r'|}}{4\pi|r - r'|}$$

When $r \gg r'$, we should have $\sqrt{(r - r')^2} \sim r - \frac{2r\cdot r'}{r}$.

5.3.2 First Born Apprixmation

What we end up ggetting is substitution of $e^{ikz} = \psi^{(0)}$ into our equation, which gives

$$\psi^{(1)}(r) = e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int dr' e^{-ik_f r'} V(r') e^{ik_i r'} = e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int dr' V(r) e^{i(k_i - k_f)r'} = e^{ikz} - \frac{m}{2\pi\hbar^2} V(\vec{q})\frac{e^{ikr}}{r}$$

So the scattering amplitude is just the fourier transform of the potential amplitude!!! That's kind of fun!

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[16] Math 185.

5.4 Method of Partial Waves (Guest Lecturer N. Yao)

Idea is we want to learn about scatter-er by takoing $\varphi(r) = \varphi_{\text{inc}}(r) + \varphi_{\text{sc}}(r)$.
Partial waves is distinct from born approximation. We want to calculate phase shifts in low energies relative to the potential. We're going to assume a radial potential $V(r)$, will give us that angular momentum is a good basis. We can break this down into $\ell = 0, 1, 2 \dots$, and get that for each ℓ we have an individual scattering problem.

$$g(\theta, \varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_{\ell m} Y_{\ell m}(\theta, \varphi)$$

since f independent of φ, we really have some $f_k(\theta)$, where

$$f_k(\theta) = \sum_{\ell=0}^{\infty} f_{\ell 0} Y_{\ell 0}(\theta)$$

Now, we're going to change into the *Legendre Basis*, where

$$f_k(\theta) = \sum_{\ell=0}^{\infty} f_{\ell 0} Y_{\ell 0}(\theta) = \sum \frac{2\ell+1}{k} f_\ell P_\ell(\cos\theta)$$

where now, our f_ℓ are known as the **partial wave scattering amplitudes** $f_\ell(k)$.
So now, if we have

$$\varphi_{\text{inc}}(r, \theta) = e^{ikr\cos\theta} = \sum_\ell (2\ell+1) u_\ell(kr) P_\ell(\cos\theta)$$

The Legendre polynomials have a nice property

$$\int_{-1}^{1} \omega P_\ell(\omega) P_\varpi(\omega) = \frac{2}{2\ell+1} \delta_{\ell\varpi}$$

Now, we're going to solve for $u_\ell(kr)$. Let's multipy φ_{inc} by $P_\ell(\cos\theta)$ and integrate[17]

$$u_\ell(kr) = \frac{1}{2} \int_{-1}^{1} d\omega e^{ikr\omega} P_\ell(\omega)$$

If we integrate this by parts, we have

$$u_\ell(kr) = -\frac{i}{2kr} \left[e^{ikr\omega} P_\ell(\omega) \right]_{-1}^{1} + \frac{1}{2ikr} \int_{-1}^{1} d\omega e^{ikr\omega} \frac{\partial P_\ell}{\partial \omega}$$

where

$$\frac{1}{2ikr} \int_{-1}^{1} d\omega e^{ikr\omega} \frac{\partial P_\ell}{\partial \omega} \sim \frac{1}{r^2}$$

The fina answer ends up being

$$\varphi_{\text{inc}}(r) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2ik} \left[(-1)^{\ell+1} \frac{e^{-ikr}}{r} + \frac{e^{ikr}}{r} \right] P_\ell(\cos\theta)$$

If we put this togehter with the scattered component, we get the full wavefunction

$$\sum_\ell \frac{2\ell+1}{k} \left[(-1)^{\ell+1} \frac{e^{-ikr}}{r} + (1 + 2if_\ell(k)) \frac{e^{ikr}}{r} \right] P_\ell(\cos\theta)$$

So we want a unitarity property, i.e. conservation of probability density.

$$|(-1)^{\ell+1}| = |1 + 2if_\ell(k)|$$

and

$$1 + 2if_\ell(k) = e^{2i\delta_\ell(k)}$$

---

[17] check out david Tong's lectures

where $\delta_\ell(k)$ is known as the **Partial Wave Scattering Phase Shift**.
This all gives that

$$f(\theta) = \frac{1}{k}\sum_\ell (2\ell+1)\sin(\delta_\ell(k))e^{i\delta_\ell(k)}P_\ell(\cos\theta)$$

Intuitively, we should have that the net effect of the potential on the wavefunction will be a phase shift. This is because we have reduced the equation in $f(k,\theta)$ in two variables to an infinite series of $f_\ell(k)$, where for small potentials we can consider finitely many ℓ to a good approximation. For future reference, we have the scattering length $a_\ell = \frac{\delta_\ell}{k}$.

5.4.1 Optical Theorem (Guest Lecturer: M. Zaletel)

We have the differential cross section

$$\frac{\partial\sigma}{\partial\Omega} = |f(\theta)|^2 = \frac{1}{k^2}\sum_{\ell,\ell'}(2l+1)(2\ell'+1)f_\ell f_{\ell'}^* P_\ell(\cos\theta)P_{\ell'}(\cos\theta)$$

Legendre polynomials are orthonormal, so we can take

$$\sigma_T = 2\pi\int_{-1}^{1} d\cos\theta |f^2(\theta)|^2 = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2(\delta_\ell)$$

There's also a unitarity bound. He erased before I was able to write this down so TODO: GO to the Tong lecture.

5.4.2 Hard-Sphere Scattering

Let's consider the following hard-sphere scattering.

$$\psi(r,\theta) = \sum_\ell R_\ell(r)P_\ell(\cos\theta)$$

Then, for $r > a$,

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right](rR_\ell(r))$$

Basically, we write it down in terms of the bessell functions

$$\rho \gg 1 \Rightarrow \begin{cases} j_\ell(\rho) = \frac{1}{\rho}\sin(\rho - \ell\pi/2) \\ n_\ell(\rho) = \frac{1}{\rho}\sin(\rho - \ell\pi/2) \end{cases} \qquad \rho \ll 1 \Rightarrow \begin{cases} j_\ell(\rho) = \frac{\rho^\ell}{(2\ell+1)!!} \\ n_\ell(\rho) = (2\ell-1)!!\rho^{-(2\ell+1)} \end{cases}$$

Taking asymtotics then, we take

$$\lim_{\rho\to\infty} R_\ell(\rho) \propto \left[(-1)^{\ell+1}\frac{e^{-i\rho}}{\rho} + e^{2i\delta_\ell}\frac{e^{i\rho}}{\rho}\right] = \frac{e^{i\delta\ell}e^{i\pi\ell/2}}{\rho}\left[-e^{i(\rho+\delta_\ell-\pi\ell/2)} + e^{i(\rho+\delta_\ell-\pi\ell/2)}\right]$$

We can solve for various ℓ by substituting in the asymptotics for ℓ. For instance, in the limit where $\rho \ll 1$, $\tan(\alpha_\ell = \delta_\ell) = \frac{j_\ell(ka)}{n_\ell(ka)}$, which gives

$$\lim_{\rho\ll 1}\tan(\delta_\ell) = \frac{(ka)^{2\ell+1}}{(2\ell+1)!!(2\ell-1)!!}$$

Now, we can take the total contribution from all sections

$$\sigma_T = \sum_{\ell=0}^{\infty}\sigma_\ell = \frac{4\pi}{k^2}(ka)^2 + \dots = 4\pi a^2 + \dots$$

We can also always define $a_\ell = \lim_{k\to 0}\frac{\tan(\delta_\ell)}{k}$

5.4.3 Ex: Soft Sphere Scattering (Altman Returns)

We have some radial potential

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & r \geq R \end{cases}$$

where

$$U(r) = \frac{2mV(r)}{\hbar^2}$$

What's going to happen when we send a low-energy wavevector into this spherical potential? We can write down the radial equation for $\ell = 0$ (an s-wave).

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - U(r) + k^2\right)\psi$$

Take ξ such that

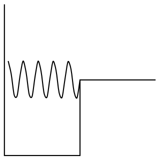
$$\xi(r) = r\psi(r)$$

where the new wave equation becomes

$$\left(\frac{\partial^2}{\partial r^2} - U(r) + k^2\right)\xi(r) = 0$$

This is going to give us a plane wave solution to the schroedinger equation, so we're going to get

$$\xi(r) = \begin{cases} c\sin(kr + \delta_0) & r > R \\ A\sin(Qr) & r < R \end{cases}$$



We then apply continuity at $R = r$, where $Q = \sqrt{k^2 + r^2}$, to get[18]

$$A\sin Qr = c\sin(kR + \delta_0) \qquad\qquad AQ\cos Qr = ck\cos(kR + \delta_0)$$

From this, we're going to end up dividing the two equations by each other to find that

$$\tan(kR + \delta_0) = \frac{kR}{QR}\tan(QR)$$

Tangent has a lot of divergences though, which makes this equation somewhat challenging to solve. If we assume the argument of tan is small however, we can taylor expand this to find a close solution to our problem.
We'll take $\tan(QR) \sim 1 \Rightarrow kR + \delta_0 \cong \frac{kR}{QR}\tan(QR)$, so

$$\delta_0 \cong kR\left(\frac{\tan(QR)}{QR}01\right)$$

We can find our scattering length as

$$a_s = -\lim_{k\to 0}\frac{\tan(\delta_0)}{k} = -R(\frac{\tan(\gamma R)}{\gamma R} - 1)$$

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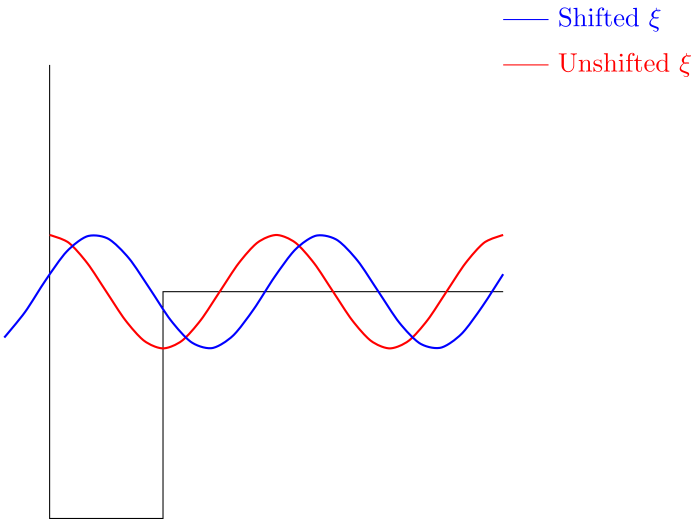
[18] note that on the homework, we have a δ function potential which has different discontinuous boundary conditions at the boundary



Scattering Resonances When $\tan(QR)$ diverges, we're going to have

$$\tan(kR + \delta_0) = \frac{k}{\gamma}\tan(\gamma R)$$

where $\gamma R \approx \frac{\pi}{2}$. We then have the limit where $k \to 0$, we have that $\delta_0 = \pi/2$, so we have a condition. We end up with

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2}$$

Now, if we want to tune across the resonances, we assume phase shift goes through $\pi/2$ at a certain energy.[19] Recall that we have

$$\tan(kR + \delta_0) = \frac{k}{\gamma}\tan(\gamma R)$$

Let's take some δ_ℓ, and find the scattering amplitude

$$f_\ell = \frac{e^{i\delta_\ell(E)}}{k}\sin\delta_\ell(E) = \frac{1}{k}\frac{1}{\cot(\delta_\ell(E)) - i}$$

So, we'll expand $\delta(E_0) = \frac{\pi}{2}$, which gives out

$$\cot(\delta_\ell(E)) = \cot(\delta(E_0)) + \left(\frac{\partial \cot\delta}{\partial E}\right)_{E=E_0}(E - E_0) + \dots$$

We're going to let

$$\frac{\partial\delta}{\partial E} = \frac{2}{\gamma}$$

and after the full taylor expansion, we're going to end up with

$$\cot(\delta(E_0)) + \left(\frac{\partial \cot\delta}{\partial E}\right)_{E=E_0}(E - E_0) + \dots = -\frac{1}{k}\frac{\Gamma/2}{(E - E_0) + i\frac{\Gamma}{2}}$$

this gives out a scattering cross setion

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell + 1)\frac{\Gamma^2/4}{(E - E_0)^2 + \Gamma^2/4}$$

So, here's the new cross sectoin

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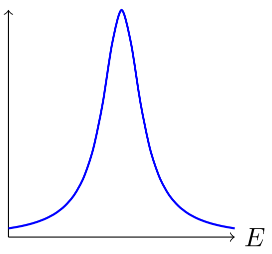
[19] We started discussion here



We see the typical sort of resonance shape we expect. Also,

$$a_s = -\lim \frac{\tan \delta}{k}$$

6 Time Dependent Perturbation Theory

6.1 Introduction

A good example is to think of the way light changes the energy level of electrons orbiting a hydrogen atom. We can roughly consider light as a weak oscillatory potential, which is where this becomes super relevant. The broad situation we are considering is

$$H = H_0 + H_1(t)$$

What we essentially want is the probability of a transition into any other state as a function of time, $|\left\langle m^{(0)} \middle| \psi(t) \right\rangle|^2$.

6.2 Formalism: First Order

We should take the schroedinger equation

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

where $H(t) = H_0 + H_1(t)$. What we will assume for the most part is that $|\psi(t=0)\rangle = \left|n^{(0)}\right\rangle$, that the system is in an eigenstate of H_0 at time $t = 0$. We then ask what the probability is $P_m(t)$ that we end up in another state at time t.

$$P_m(t) = |\left\langle m^{(0)} \middle| \psi(t) \right\rangle|^2$$

In the presence of only the unperturbed hamiltonian, we have a phase dependence

$$\left|n^{(0)}\right\rangle = e^{iE_n^{(0)}t} \left|n^{(0)}\right\rangle$$

Before starting the perturbation, we can try to solve exactly, by taking

$$|\psi(t)\rangle = \sum_n c_n(t) \left|n^{(0)}\right\rangle$$

Given $c_n(0)$, we want $c_n(t)$, which will give

$$c_n(t) = e^{-iE_n^{(0)}t} c_n(0)$$

We'll define something with no time dependence, $d_n(t)$ as the thing with no time dependence,

$$d_n(t) = e^{iE_n^{(0)}t} c_n(t) = c_n(0)$$

If we define such a d, if the perturbation is small, the time dependence will be only due to the perturbation, and if the perturbation is small, the time dependence will be very slow.
Rewriting everything in terms of $d_n(t)$, we get

$$|\psi(t)\rangle = \sum_n d_n(t) e^{-iE_n^{(0)}t} \left|n^{(0)}\right\rangle$$

Now, we operate on both sides by

$$\left[i\hbar \frac{\partial}{\partial t} - H\right] (|\psi(t)\rangle) = \left[i\hbar \frac{\partial}{\partial t} - H\right] \left(\sum_n d_n(t) e^{-iE_n^{(0)}t} \left|n^{(0)}\right\rangle\right)$$

we get that the lhs is 0, since it satisfies the schroedinger equation, we get

$$0 = \sum_n \left(i\hbar \dot{d}_n - H_1 d_n \right) e^{-iE_n^{(0)}t/\hbar} \left| n^{(0)} \right\rangle$$

We're going to bra it with the state

$$\left\langle f^{(0)} \right| e^{iE_f^{(0)}t/\hbar}$$

which gives out

$$0 = i\hbar \dot{d}_f - \sum_n \left\langle f^{(0)} \right| H_1 \left| n^{(0)} \right\rangle d_n(t) e^{i(E_f - E_n)t/\hbar}$$

simplifying this, we find

$$i\hbar \dot{d}_f = \sum_n \left\langle f^{(0)} \right| H_1 \left| n^{(0)} \right\rangle d_n(t) e^{i\omega_{fn}t}$$

where $\omega_{fn} = \frac{E_f - E_n}{\hbar}$.
We've eliminated H_0 from our expansion! this is very exciting. We're going to make the assumption that to lowest order $d_n(t) = \delta_{in}$, since any dependence on H_1 will induce linear dependence in d, so we end up with

$$i\hbar \dot{d}_f = \left\langle f^{(0)} \right| H_1(t) \left| i^{(0)} \right\rangle e^{i\omega_{fi}t}$$

This will give us that

$$d_f(t) = \delta_{if} - \frac{i}{\hbar} \int_{t_0}^{t_f} \left\langle f^{(0)} \right| H_1(t') \left| i^{(0)} \right\rangle e^{i\omega_{fi}t'} dt'$$

and $p_{if}(t) = |d_f(t)|^2$.

6.2.1 Infinite Time Perturbation

Recall we have some $H = H_0 + H_1(t)$ where $H_1 = g(t)\hat{V}$. We defined $d_f(t) = c_f(t)e^{iE_f^{(0)}t}$, in order to undo the time dependence of c_f in an eigenstate, where we just shift the phase oscillation in the other direction. We computed such $d_f(t)$ to be as follows:

$$d_f(t) = \delta_{if} - \frac{i}{\hbar} \int_{t_0}^{t_f} \left\langle f^{(0)} \right| H_1(t') \left| i^{(0)} \right\rangle e^{i\omega_{fi}t'} dt' = \delta_{if} - \frac{i}{\hbar} \left\langle f^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle \int_{t_0}^{t} dt' g(t') e^{i\omega_{if}t'}$$

In the limit where $t_0 \to -\infty$, $t \to \infty$, we have that this expression is just a fourier transform of $g(t)$, and can reexpress this as

$$d_f(t) = \delta_{if} - \frac{i\tilde{g}(t)}{\hbar} \left\langle f^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle$$

where $\tilde{g}$ represents the fourier transform of g.

6.2.2 Sudden Perturbation

If we have

$$H_1(t) = \Theta(t)\hat{V}$$

It sets our lower limit of integration to 0, and so we're left with

$$d_f^{(1)}(t) = -\frac{i}{\hbar} \left\langle f^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle \int_0^t dt' e^{i\omega_{fi}t} = \begin{cases} -\frac{2i\langle f|\hat{V}|i\rangle}{\hbar\omega_{fi}} \sin\left(\frac{\omega_{fi}t}{2}\right) e^{i\omega_{fi}t/2} & f \neq i \\ -\frac{i}{\hbar} \langle i| \hat{V} |i\rangle & f = i \end{cases}$$

This is actually a really nice sanity check, since $\left\langle i^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle$ is the energy we'd expect from first order perturbation theory without time dependence! So our phase shift is nicely consistent with our previous results.
If we want the transition probability, we can just take

$$p_{i\to f} = \frac{2}{\hbar^2} \left| \left\langle f^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle \right|^2 \frac{2\sin^2(\omega_{fi}t/2)}{\omega_f it} t$$

where we call $F(\omega_{fi}, t)$, so we have

$$p_{i\to f} = \frac{2}{\hbar^2} \left| \left\langle f^{(0)} \right| \hat{V} \left| i^{(0)} \right\rangle \right|^2 \frac{2\sin^2(\omega_{fi}t/2)}{F(\omega_{if}, t)} t$$

6.3 Examples

6.3.1 Harmonic Oscillator (infinite time)

Consider

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$
$$H_1(t) = -e\varepsilon\hat{x}e^{-t^2/\tau^2}$$

We want to know what the amplitude $d_n(\infty)$ is, the probability to find the oscillator in state n after finite time, assuming that we start in the ground state? We just put it in to the formula,

$$d_n(t) = -\frac{i}{\hbar} - e\varepsilon \langle n| \hat{x} |0\rangle \int dte^{-t^2/\tau^2}e^{in\omega t}$$

We can just take

$$d_n(t) = \frac{ie\varepsilon}{\hbar}\sqrt{\frac{\hbar}{2m\omega}} \langle n| (a_- + a_+) |0\rangle \int dte^{-t^2/\tau^2 - in\omega t} = \delta_{n1}\frac{ie\varepsilon}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\pi\tau^2}e^{-\omega^2\tau^2/4}$$

which gives

$$|d_n|^2 = \delta_{10}\frac{e^2\varepsilon^2\pi\tau^2}{2m\omega\hbar}e^{-(\omega\tau)^2/2}$$

6.4 Validity Criterion

This was an aside on the date 11-4-19. We ended up getting a sinc function from the last time. I made an error, last time. WE should actually have

$$F(t,\omega) = \frac{2\sin^2(\omega_{fi}t/2)}{\omega_{fi}^2 t}$$

where in the limit of very large times, $F(t,\omega) \to \pi\delta(\omega)$.
From this[20], we can get the maximum probability

$$P_{fi}^{\max} = \frac{2|\langle f| H_1 |i\rangle|^2}{E_f^{(0)} - E_i^{(0)}}$$

The validity criterion here is the same roughly as it was previously, where the energy difference should be small. Also, resonant transitions are going to give a really weird case that we need to be extra mindful of.
Even if one transition is resonant, it breaks validity of perturbation theory, the true criterion is

$$\sum_f P_{fi}^{\max} = \sum_f \frac{2|\langle f| H_1 |i\rangle|^2}{E_f^{(0)} - E_i^{(0)}} \ll 1$$

We're going to move on, we want to take

- Static Perturbations → Oscillatory Perturbation
- Transition into a Continuum of Levels

We're going to discuss this through the lense of **Fermi's Golden Rule**.

6.5 Periodic Perturbations

Consider

$$H_1(t) = \Theta(t)\left[\hat{V}e^{-i\omega t} + \hat{V}^\dagger e^{i\omega t}\right]$$

As an example of ramping up a perturbation suddenly. Or,

$$\bar{H}_1(t) = e^{\varepsilon t}\left[\hat{V}e^{-i\omega t} + \hat{V}^\dagger e^{i\omega t}\right]$$

here $t < 0, \varepsilon \ll \frac{2\pi}{t}$ as an example of ramping up slowly.

---

[20] todo: wtf

6.5.1 Sudden Step Into Periodicity

We can just use the first order formalism to get

$$d_f^{(1)}(t) = -\frac{i}{\hbar}\langle f|\,\hbar V\,|i\rangle \int_0^t e^{i(\omega_{fi}-\omega)t'}dt' - \frac{i}{\hbar}\langle f|\,\hat{V}^\dagger\,|i\rangle \int_0^t e^{i(\omega_{fi}+\omega)t'}dt'$$

if we let $V_{fi} = \langle f|\,\hat{V}\,|i\rangle$, we have

$$d_f^{(1)}(t) = V_{fi}\frac{1-\exp(i(\omega_{fi}-\omega)t)}{\hbar(\omega_{fi}-\omega)} + V_{fi}^\dagger\frac{1-\exp(i(\omega_{fi}+\omega)t)}{\hbar(\omega_{fi}+\omega)}$$

which gives

$$P_{fi} = \left|V_{fi}\frac{1-\exp(i(\omega_{fi}-\omega)t)}{\hbar(\omega_{fi}-\omega)} + V_{fi}^\dagger\frac{1-\exp(i(\omega_{fi}+\omega)t)}{\hbar(\omega_{fi}+\omega)}\right|^2$$

We have really strong resonances at $\omega = \omega_{fi}$, and decay over time otherwise. This gives us that it's a reasonable approximation to use

$$P_{fi} = \begin{cases} \frac{2}{\hbar^2}(V_{fi})^2F(t,\omega_{fi}-\omega)t & \omega_{fi}\approx\omega \\ \frac{2}{\hbar^2}(V_{fi}^\dagger)^2F(t,\omega_{fi}+\omega)t & \omega_{fi}\approx-\omega \end{cases} \underset{t\to\infty}{\longmapsto} \begin{cases} \pi\delta(\omega_{fi}-\omega) & \omega_{fi}\approx\omega \\ \pi\delta(\omega_{fi}+\omega) & \omega_{fi}\approx-\omega \end{cases}$$

6.5.2 Slowly Ramped Perturbation

Let's consider as an example, the case where we are nearly resonant with the first term of our perturbation $\bar{H}$.

$$V(t) = \hat{V}e^{\varepsilon t}e^{-i\omega t}$$

Then we have

$$d_f^{(1)}(t) = -\frac{i}{\hbar}\int_{-\infty}^t \hat{V}_{fi}e^{i(\omega_{fi}-\omega-i\varepsilon)t'}dt' = -\frac{1}{\hbar}\frac{e^{i(\omega_{fi}-\omega-i\varepsilon)t}}{\omega_{fi}-\omega-i\varepsilon}$$

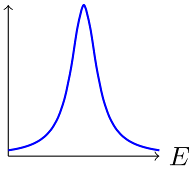
If we consider the probability, we're going to get

$$P_{fi}(t) = \frac{1}{\hbar^2}\frac{e^{2\varepsilon t}}{(\omega_{fi}-\omega)^2+\varepsilon^2}|V_{fi}|^2$$

we can ask what is the rate of transitions we make at long times,

$$W_{fi} = \frac{\partial P_{fi}}{\partial t} = \frac{2}{\hbar^2}\frac{\varepsilon}{(\omega_{fi}-\omega)^2+\varepsilon^2}|V_{fi}|^2$$

this is a a Lorenztian! We have some peaked function



6.6 Density of States

Recall, we have this weird transition rate in first order perturbation theory,

$$\omega_{fi-} = \frac{2}{\hbar^2}\left[|V_{fi}|^2\delta(\omega_{fi}-\omega) + |V_{fi}^\dagger|^2\delta(\omega_{fi}+\omega)\right]$$

Now, we want to rewrite this in terms of a transition into a continuum of levels, i.e.

$$W(\omega) = \sum_f W_{fi}(\omega) \mapsto \int dE\rho(E)W(E,\omega)$$

In the continuum limit, we have that the sum over final states is going to map to an integral.[21] We can think of this as a change of variables, where the density of states is the jacobian which transforms $\int dn \mapsto \int dE\left|\frac{\partial n}{\partial E}\right|$.

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[21] This shows up a lot in 112 and 141A (Statistical Mechanics and Solid State Physics). Worth Checking out maybe Ashcroft & Mermin and Kittel Solid State.

6.6.1 Ex: Free particles in one dimension

We have $E = \frac{\hbar^2 k^2}{2m}$ with $\hbar k = p$. Consider a finite 1d system of size L with periodic boundary conditions, i.e. $\varphi_k(x) = \varphi_k(x+L) = \langle x|k\rangle = \frac{1}{\sqrt{L}}e^{ikx} = \frac{1}{\sqrt{L}}e^{ix\frac{2\pi}{L}}$ Integrating over the number of states then becomes

$$\int_{-\infty}^{\infty} dn = \frac{L}{2\pi}\int_{-\infty}^{\infty} dk$$

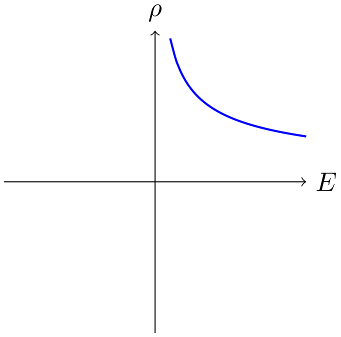
Now, we need to change variables to energy to get

$$\frac{\partial k}{\partial E} = \frac{1}{\hbar}\sqrt{\frac{m}{2E}}$$

So, after our requsite change of variables, we should get

$$\int_{-\infty}^{\infty} dn = \frac{L}{2\pi\hbar}\int_{-\infty}^{\infty} dE\sqrt{\frac{m}{2E}}$$

which is interesting, since in 1-d the density of states diverges as $\frac{1}{\sqrt{E}}$. We can plot it as



6.6.2 Ex: Free Particles in 2 Dimensions

We have, with the same periodicity requirements

$$\int dn = \frac{L^2}{(2\pi)^2}\int d^2k = \frac{L^2}{(2\pi)^2}\int dk 2\pi k = \frac{L^2}{(2\pi^2)\hbar}\int dE\sqrt{\frac{m}{2E}}2\pi\frac{1}{\hbar}\sqrt{2mE}$$

which gives density of states in 2-dimensions is constant, i.e. independent of energy

$$\rho_{2d} = \frac{L^2 m}{2\pi\hbar^2}$$

3-d is probably gonna be a homework problem. Freakin statistical mechanics man!!

6.7 Fermi's Golden Rule

If we stick the density of states into our equation from before, we should find (with the $\hbar^2$ in the denominator dissapearing from our change of variables from $\omega \mapsto E$)

$$\begin{aligned} W_i(\omega) &= \frac{2}{\hbar}\int dE\rho(E)\left[|V_i(E)|^2\delta(E-E_i-\hbar\omega) + |V_i(E)|^2\delta(E-E_i+\hbar\omega)\right] \\ &= \frac{2}{\hbar}\left[\rho(E_i+\hbar\omega)|V_i(\omega)|^2 + \rho(E_i-\hbar\omega)|V_i(-\omega)|^2\right] \end{aligned}$$

Your intuition for this should go that we have the rate of transition will be the density of states at your current energy plus $\hbar\omega$, times the matrix element of transitioning to this probability. The crucial assumption that we've made here is that the matrix elements themselves are smooth functions on ω. This might not always be the case, which means (probably not in our class) there are instances where it is worthwhile to check the matrix element of transition case by case.

6.8 Higher Order Time Dependent Perturbation Theory

Here, we're going to discuss a nicer framework for deriving time dependent perturbation theory, and use it to see how we might be able to go to higher orders. Specifically, we're going to highlight it in the **interaction picture**.

6.8.1 Different Interpretations of Quantum Mechanics

Schroedinger Picture The schroedinger equation is one picture of quantum mechanics. It stems from the fundamental equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi_s\right\rangle = H_s\left|\psi_s\right\rangle$$

where the subscript s denotes that we are working with the schroedinger picture.
We have time dependent wavefunctions $\left|\psi_s(t)\right\rangle = U_s(t,t_0)\left|\psi_s(t_0)\right\rangle$, where U_s is some unitary time translation operator. In the simplest case of a time independent hamiltonian, we have $U_s(t,t_0) = e^{-iH(t-t_0)/\hbar}$. In general though, we can solve our differential equation to find such a U.
Also, observables exist and are time independent, and hermitian.

Heisenberg Picture We basically fix the states as time independent, and apply some unitary transformation to the operators which gives them the requisite time dependence. I.e.

$$\left\langle\psi_s(t_0)\right| U^\dagger(t,t_0)\hat{O}U(t,t_0)\left|\psi_s(t_0)\right\rangle$$

and we just call

$$\tilde{O} = U^\dagger(t,t_0)\hat{O}U(t,t_0)$$

where we now have

$$\left|\psi_H\right\rangle = U^\dagger(t,t_0)\left|\psi_s(t)\right\rangle$$

Our new equation to find the operator becomes

$$\frac{\partial\hat{O}_H}{\partial t} = \frac{i}{\hbar}[H,\hat{O}_H]$$

which we call the **Heisenberg Equation of Motion**. This is basically a meme'd poisson bracket.[22]

Interaction Picture We want to consider our hamiltonian as some $H = H_0 + \hat{V}$, where $\hat{V}$ is some interaction, and H_0 is something that we can solve analytically. Now, we want to only yeet the "rotation" due to time evolution of H_0, but not the time evolution of the interaction, so that we can consider the slow evolution due to $\hat{V}$.
We can write down an interaction wavefunction (lack of subscript denotes the schroedinger picture)

$$\left|\psi_i(t)\right\rangle = U_0^\dagger(t,t_0)\left|\psi(t)\right\rangle = U_0^\dagger(t,t_0)U(t,t_0)\left|\psi(t_0)\right\rangle$$

We define the new operator

$$U_I(t,t_0) = U_0(t,t_0)U(t,t_0)$$

We can try to find a schroedinger-adjoint equation for ψ_I, which comes out to

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle &= i\hbar\left(\frac{\partial}{\partial t}U_0^\dagger\right)\left|\psi\right\rangle + i\hbar U_0^\dagger\left(\frac{\partial}{\partial t}\left|\psi\right\rangle\right) \\ &= -U_0^\dagger H_0\left|\psi\right\rangle + U_0^\dagger\left(H_0+V\right)\left|\psi\right\rangle = U_0^\dagger\hat{V}\left|\psi\right\rangle \\ &= U_0^\dagger V U_0 U_0^\dagger\left|\psi\right\rangle \end{aligned}$$

where we let $V_I = U_0^\dagger V U_0$ and $\left|\psi_I\right\rangle = U_0^\dagger\left|\psi\right\rangle$. So, we have the final result

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle$$

where operators evolve very quickly $O_I(t) = U_0^\dagger\hat{O}U_0$.

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[22] OMG THAT IS SO COOL THOUGH.

6.8.2 Higher Order Perturbations

Our goal now becomes to find $U_I(t,t_0)$. If we have $i\hbar\frac{\partial U_I}{\partial t} = V_I(t)U_I$, then we want

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')U_I(t',t_0)dt'$$

To first order, we have that $U_I(t',t_0) = \mathbb{I}$, so so

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')dt'$$

if we want to go to arbitrarily higher orders, we should have

$$U_I(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)\ldots V_I(t_n)$$

which is a time ordered product. We can write this compactly by saying

$$U_I(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)\ldots V_I(t_n) = \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt' V_I(t')\right)$$

where the $\mathbb{T}$ means we should time order our products.

6.8.3 Deriving Higher Order Corrections

Now, lets say we have some initial state $|\psi_i(0)\rangle = |i\rangle$, and we want to transition it into some other state. We should have in the schroedinger picture

$$|\psi_i(t)\rangle = U(t,0)\,|i\rangle$$

or, in the interaction picture

$$|\psi_i(t)\rangle = U_0(t,t_0)U_I(t,t_0)\,|i\rangle$$

Now, recall our $d_f(t) = e^{\frac{i}{\hbar}E_f t}\langle f|\psi_i(t)\rangle$, so we can write

$$\begin{aligned} d_f(t) &= e^{\frac{i}{\hbar}E_f t}\langle f|\psi_i(t)\rangle \\ &= e^{\frac{i}{\hbar}E_f t}\langle f|\, U_0(t,t_0)U_I(t,t_0))\,|i\rangle \\ &= \langle f|\, U_i(t,t_0)\,|i\rangle \end{aligned}$$

This gives us a formula for d_f.

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\langle f|\, V_I(t_1)\,|i\rangle\, dt_1$$

and, if we want to go to second order,

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\langle f|\, V_I(t_1)\,|i\rangle\, dt_1 - \frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \,\langle f|\, V_I(t_1)V_I(t_2)\,|i\rangle$$

in the second term, we're going to insert a unit matrix, resolution of identity, so that we have

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\langle f|\, V_I(t_1)\,|i\rangle\, dt_1 - \frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \sum_m \langle f|\, V_I(t_1)\,|m\rangle\,\langle m|\, V_I(t_2)\,|i\rangle$$

if we now insert the form for V_I we derived earlier, we should have, letting $V_{fi}(t) = \langle f|\, V\,|i\rangle$,

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 e^{i\omega_{fi}t_1}V_{fi} - \sum_m \frac{1}{\hbar^2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 e^{i\omega_{fm}t_1}e^{i\omega_{mi}t_2}V_{fm}(t_1)V_{mi}(t_2)$$

This is really hinting at the path integral formulation of quantum mechancis, but we're gonna yeet that now.

6.9 Ex: Harmonic Perturbation

Consider our perturbation to be

$$V(t) = \hat{V}e^{-i\omega t+\varepsilon t}$$

If we assume that $\langle f|\, \hat{V}\, |i\rangle = 0$, we can immediately compute that

$$d_f^{(2)} = -\frac{1}{\hbar^2}\sum_m \langle f|\, \hat{V}\, |m\rangle \langle m|\, \hat{V}\, |i\rangle \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 e^{i(\omega_{fm}-\omega-i\varepsilon)t_1} e^{i(\omega_{mi}-\omega-i\varepsilon)t_2}$$

This is kind of a nasty integral, but we can get it by taking

$$d_f^{(2)} = \frac{1}{\hbar} e^{i(\omega_{fi}-2\omega)} \frac{e^{2\varepsilon t}}{\omega_{fi}-2\omega-2i\varepsilon} \sum_m \frac{\langle f|\, V\, |m\rangle \langle m|\, V\, |i\rangle}{\omega_{mi}-\omega-i\varepsilon}$$

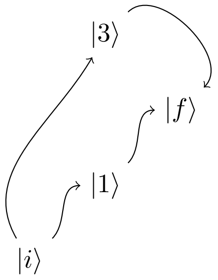
Then, we want the transition rate, which we find by taking the time derivative of the modulus as $\varepsilon \to 0$, which gives

$$\lim_{\varepsilon\to 0} W_{fi} = \lim_{\varepsilon\to 0} \frac{\mathrm{d}}{\mathrm{dt}} |d_f^{(2)}|^2 = \frac{2\pi}{\hbar^4} \left| \sum_m \frac{V_{fm}V_{mi}}{\omega_{mi}-\omega-i\varepsilon} \right|^2 \delta(\omega_{fi}-2\omega)$$

where the δ appears since there is a lorenzian term in there. It's not super necessary to keep the ε in the denominator of the sum, but he's about to explain why we did.

$$W_{fi} = \frac{2\pi}{\hbar^4} \left| \sum_m \frac{V_{fm}V_{mi}}{\omega_{mi}-\omega} \right|^2 \delta(\omega_{fi}-2\omega)$$

Basically, just watch out for resonances. Our interpretation of the intermediate terms should be in terms of paths,



6.10 Fermi's Golden Rule: Redux

FGR is a simple formula that we really don't need to rederive.

$$W_i(\omega) = \frac{2\pi}{\hbar}\left(|V_i(\omega)|^2 \rho(E_i+\hbar\omega) + |V_i(-\omega)|^2 \rho(E_i-\omega) \right)$$

where

$$|V_i(\omega)|^2 = |\langle f|\, V\, |i\rangle|^2$$

which we have to evaluate with resolution of identity to get

$$\int dx dx' \langle f|x\rangle \langle x|\, V\, |x'\rangle \langle x'|i\rangle$$

Also, in the fourth problem on the last set, where we have

$$V(t) = V\cos(\omega t)\mathbb{I}\otimes\sigma^x$$

which acts on the wavefunction $|\psi\rangle \otimes |\sigma\rangle$. This is going to make our function

$$\langle \psi_f|\, \mathbb{I}\otimes\sigma^x\, |\psi_i\rangle = \int d^3x \varphi_{f\uparrow}^* \varphi_{i\downarrow}$$

which, we can use plane waves as the basis

$$\psi_\downarrow = \frac{1}{(2\pi x_0)^{1/4}} e^{r^2/4x_0^2}$$

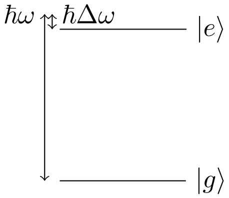
and

$$\psi_\uparrow = \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{x}}$$

This is going to fall off as an exponential, after some initial rise. It'll be a peaked function.

6.11 Nearly Resonant Perturbation

We'll consider the following



We're going to end up with

$$\begin{aligned} P_{ge}^{(1)}(t) &= \frac{2}{\hbar^2}|A_{ge}^\dagger|^2 F(t, \Delta\omega) t \\ &= \frac{4|A_{ge}^\dagger|^2}{(\hbar\Delta\omega)^2}\sin^2(\Delta\omega t/2) \end{aligned}$$

and where $\Delta\omega \to 0$ we should have some divergence where this goes to

$$\frac{1}{\hbar^2}|A_{eg}|^2 t^2$$

which can be larger than one. This is bad. So, we need to step back and rewrite the hamiltonain, solving the schroedinger equation

$$H = H_0 + H_1(t)$$

where

$$G_1(t) = \left(\hat{A}e^{-i\omega t} + \hat{A}^\dagger e^{i\omega t}\right)\mathcal{V}(t)$$

We take our usual

$$d_n(t) = e^{-iE_n t} c_n(t)$$

so the schroedinger equaiton has to become

$$i\hbar \dot{d}_m = \sum_n \left[A_{mn} e^{-i(\omega_{mn} - \omega)t} + A_{mn}^\dagger e^{-i(\omega_{mn} + \omega)t}\right] d_n(t)$$

If we think about the exactly resonant term, our first exponent becomes non-oscillating.
On strongly oscillating terms. on reaosnable time scales this is going to average out to becomes zero. So we can ignore non-resonant terms, but we need to leave terms which don't oscillate. So, our schroedinger equation now becomes in terms of

$$\begin{aligned} i\hbar\dot{d}_e &= A_{ge} e^{i\Delta\omega t} d_g \qquad\qquad \downarrow = e \\ i\hbar\dot{d}_g &= A_{ge}^\dagger e^{-i\Delta\omega t} d_e \qquad\qquad \uparrow = g \end{aligned}$$

So, we have

$$i\hbar \begin{bmatrix} \dot{d}_g \\ \dot{d}_e \end{bmatrix} = \begin{bmatrix} 0 & -\frac{B}{2}e^{-i\varphi}e^{-i\Delta\omega t} \\ -\frac{B}{2}e^{i\varphi}e^{i\Delta\omega t} & 0 \end{bmatrix} \begin{bmatrix} d_g \\ d_e \end{bmatrix}$$

we can think about making this into a spin-$\frac{1}{2}$ system

$$i\hbar|\chi\rangle = \hat{H}|\chi\rangle$$

where

$$\hat{H} = -\frac{B}{2}\cos(\Delta\omega t + \varphi)\sigma^x - \frac{B}{2}\sin(\Delta\omega t + \varphi)\sigma^y$$

This looks like a spin-1/2 rotating magnetic field

6.11.1 Exact Resonance $\Delta\omega = 0$ (Rabi Oscillations)

We now have a perfect spin$\frac{1}{2}$ system in a static field

$$H = -\frac{1}{2}\vec{B}\cdot\vec{\sigma}$$

which gives

$$|\psi(t)\rangle\, e^{-iHt}\,|\psi(0)\rangle = e^{-\frac{i}{2}B\cdot\sigma t}\,|\uparrow\rangle$$

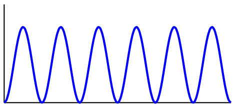
So, the rotation goes as $\theta = Bt$, with frequency $\Omega = B$. If we pick $\varphi = 0$, then we have

$$|\psi(t)\rangle = \cos\left(\frac{1}{2}\Omega t\right)|\uparrow\rangle - i\sin\left(\frac{1}{2}\Omega t\right)|\downarrow\rangle$$

with

$$P_e(t) = \sin^2\left(\frac{\Omega}{2}t\right)$$

which gives



6.11.2 Off Resonant Case

We're going to pick an axis to remain in the direction of the field, and change the basis with a unitary operator which eliminates the rotation of the field. IIRC we did this in 137A?
We're going to pick some unitary transformation so that we are in the rotating frame of reference. We can let $R(t) = e^{-\frac{i}{2}\Delta\omega t\sigma^z}$, so we get

$$\left|\tilde{\uparrow}\right\rangle = R(t)\,|\uparrow\rangle = e^{-\frac{i}{2}\Delta\omega t}\,|\uparrow\rangle \qquad \left|\tilde{\downarrow}\right\rangle = R(t)\,|\downarrow\rangle = e^{\frac{i}{2}\Delta\omega t}\,|\downarrow\rangle$$

which gives

$$\begin{aligned}|\psi(t)\rangle &= d_\uparrow(t)\,|\uparrow\rangle + d_\downarrow(t)\,|\downarrow\rangle\\ &= d_\uparrow(t)e^{\frac{i}{2}\Delta\omega t}\left|\tilde{\uparrow}\right\rangle + d_\downarrow(t)e^{-\frac{i}{2}\Delta\omega t}\left|\tilde{\downarrow}\right\rangle\end{aligned}$$

Our new schroedinger equation becomes

$$i\hbar\frac{\partial}{\partial t}d_\updownarrow(t) = i\hbar\frac{\partial}{\partial t}\left[e^{\mp\frac{i}{2}\Delta\omega t}\tilde{d}_\updownarrow(t)\right] = i\hbar\left[\mp\frac{i}{2}\Delta\omega e^{\mp\frac{i}{2}\Delta\omega t}\tilde{d}_\updownarrow(t) + e^{\mp\frac{i}{2}\Delta\omega t}\dot{\tilde{d}}_\updownarrow(t)\right]$$

This ends up coming out as

$$i\hbar\frac{\partial}{\partial t}d_{\uparrow,\downarrow}(t) = -\frac{B}{2}e^{\mp i\Delta\omega t}d_{\downarrow,\uparrow} = -\frac{B}{2}\tilde{d}_{\downarrow,\uparrow}(t)$$

more or less. We super ran out of time. Basically, we can get a time independent effective hamiltonian in our new basis, and rotate back to the old basis to get the result.'
Altman wrote this on the board at the beginning of lecture:

- Step 1: Rotating Wave Approximation,[23] we keep only slowly rotating terms. This will yield an effective spin-$\frac{1}{2}$ in a slowly rotating field.
- Step 2: Move to the rotating frame. $\left|\tilde{\uparrow}\right\rangle = R(t)\,|\uparrow\rangle = e^{-\frac{i}{2}\Delta\omega t}\,|\uparrow\rangle$, and similarly for ↓, but the conjugate. This yields the d coefficients $\tilde{d_\uparrow}(t) = d_\uparrow(t)e^{i\Delta\omega t/2}$ and likewise for ↓.

---

[23] Haeffner Covered in 137A.

This is going to give us a new schrodinger equation in $\tilde{d}_{\uparrow,\downarrow}$.

$$i\hbar e^{-\frac{i}{2}\Delta\omega t}\partial_t\tilde{d}_\uparrow = -\frac{\hbar\Delta\omega}{2}e^{-i\frac{\Delta\omega t}{2}}\tilde{d}_\uparrow\dots$$

which can be stacked as a matrix equation, after eliminating your time dependence

$$i\hbar\partial_t\begin{bmatrix}\tilde{d}_\uparrow\\ \tilde{d}_\downarrow\end{bmatrix} = \begin{bmatrix}-\frac{\hbar\Delta\omega}{2} & -\frac{1}{2}B\\ -\frac{1}{2}B & \frac{\hbar\Delta\omega}{2}\end{bmatrix}\begin{bmatrix}\tilde{d}_\uparrow\\ \tilde{d}_\downarrow\end{bmatrix} = -\frac{\hbar\Delta\omega}{2}\sigma^z - \frac{1}{2}B\sigma^x = -\vec{\Omega}\cdot\vec{S}$$

This gives us a total larmor precession from $\hbar\Omega = \sqrt{B^2 + (\hbar\Delta\omega)^2}$.
So, we have at $t = 0$, $|\psi(0)\rangle = |\uparrow\rangle = \left|\tilde{\uparrow}(0)\right\rangle$.
We want to write this in terms of the eigenstates of our hamiltonian, which gives

$$|\psi(0)\rangle = \left|\tilde{\uparrow}\right\rangle = \cos\frac{\theta}{2}\left|\tilde{\uparrow}\right\rangle - \sin\frac{\theta}{2}\left|\tilde{\downarrow}\right\rangle$$

with

$$\tan\theta = \frac{B}{\hbar\Delta\Omega} \qquad\qquad \sin\theta = \frac{B}{\hbar\Omega}$$

which gives

$$|\psi(t)\rangle = \cos\frac{\theta}{2}e^{i\Omega t/2}\left(\cos\frac{\theta}{2}\left|\tilde{\uparrow}\right\rangle + \sin\frac{\theta}{2}\left|\tilde{\downarrow}\right\rangle\right) - \sin\frac{\theta}{2}e^{-i\Omega t/2}\left(\sin\frac{\theta}{2}\left|\tilde{\uparrow}\right\rangle + \cos\frac{\theta}{2}\left|\tilde{\downarrow}\right\rangle\right)$$

Now, we have to multiply through by $R^\dagger$ to get back to the lab frame, and collect terms

$$|\psi(t)\rangle = \left(\cos^2\left(\frac{\theta}{2}\right)e^{i\frac{\Omega}{2}t} + \sin^2\left(\frac{\theta}{2}\right)e^{-i\frac{\Omega}{2}t}\right)e^{-i\frac{\Delta\omega}{2}t}|\uparrow\rangle + \left(\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{i\frac{\Omega}{2}t} - \cos\frac{\theta}{2}\sin\frac{\theta}{2}\right)e^{-i\frac{\Delta\omega}{2}t}|\downarrow\rangle$$

where we can now compute the transition probability as

$$P_e(t) = |\langle\downarrow|\psi(t)\rangle|^2 = \sin^2(\theta)\sin^2\left(\frac{\Omega t}{2}\right) = \frac{B^2}{(\hbar\Delta\omega)^2 + B^2}\sin^2\left(\frac{\sqrt{\Delta\omega^2 + B^2/\hbar^2}}{2}t\right)$$

But, since B isn't an actual magnetic field, it's $B^2 = \frac{1}{4}|\langle e|\hat{V}|g\rangle|^2$. This itself is Rabi's Formula!
Comparing this to our first order perturbation theory, we haev

$$P_e^{(1)}(t) = \frac{B^2}{(\hbar\Delta\omega)^2}\sin\left(\frac{\Delta\omega}{2}\right)$$

which isn't terrible, but fails for small detuning.

7 Coupling to an Electric Field

7.1 Lagrangian Formalism for Electrodynamics

Magnetic fields are a little stranger than electric fields. Recall, we have some Lorentz force,

$$\vec{F} = q\vec{E} + \frac{q}{c}\vec{v}\times\vec{B}$$

which leads to the equation of motion

$$\ddot{\vec{x}} = \frac{q}{m}\left(\vec{E} + \frac{1}{c}\dot{\vec{x}}\times\vec{B}\right)$$

We are going to write this down in Lagrangian formalism, so that we can use the canonical commutation relations to quantize our field.
Recall the typical form of the lagrangian for a solely potential force.

$$\mathcal{L} = \frac{1}{2}m\dot{\vec{x}}^2 - q\phi(x)$$

But, the magnetic field is not a potential force (no monopoles), so we need to guess some correcting term

$$\mathcal{L} = \frac{1}{2}\dot{\vec{x}} - q\phi(x) + \frac{q}{c}\dot{\vec{x}} \cdot \vec{A}$$

where $\vec{A}$ is the vector potential such that $B = \vec{\nabla} \times \vec{A}$, and $\vec{E} = -\nabla\phi - \frac{1}{c}\dot{\vec{A}}$.
These fields though, aren't unique, they're just nice ways for us to define B, E. This redundancy is referred to as gauge invariance.

$$\vec{A} \to \vec{A} + \nabla\chi = \vec{A}$$

$$\phi \to \phi - \frac{1}{c}\partial_t\chi + c = \phi$$

As an excercise, derive the equation of motion from this lagrangian.
I'm going to start treating vectors and constants the same. It'll be up to you to determine which is which from context, future connor.
We have the lagrangian

$$\mathcal{L} = \frac{1}{2}m\dot{x} - q\phi(x) + \frac{q}{c}\dot{x} \cdot A(x)$$

where A is the vector potential. Recall, these ϕ, A are not unique only up to a gauge transformation.
We can stick this into the Euler-Lagrange equations to get the Lorentz force back out. Recall, the ELE are given as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}$$

where we go component-by-component in $x, \dot{x}$. If we wanted the associated conjugate momentum, we'd have $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$. This is going to be important for our formulation of hamiltonian mechanics. We can take the legendre transform

$$H(x, p) = p\dot{x} - \mathcal{L}$$

For now, we resort to showing that our notion of electrodynamics falls out of the lagrangian postulated by Altman.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(m\dot{x} + \frac{q}{c}A(x)\right) = m\ddot{x} + \frac{q}{c}\left(\dot{A}(x) + \dot{x} \cdot \nabla A\right)$$

We also have

$$\frac{\partial}{\partial x}\mathcal{L} = -q\nabla\phi + \frac{q}{c}\nabla\dot{x} \cdot A$$

We can just collect terms, and equate the two sides of the Euler-Lagrange equation to get

$$m\ddot{x} = q\left(-\nabla\phi - \frac{\partial A}{\partial t}\right) + \frac{q}{c}\left(\nabla(\dot{x} \cdot A) - (\dot{x} \cdot \nabla)A\right) = -qE + \frac{q}{c}\dot{x} \times (\nabla \times A) = -qE + \frac{q}{c}\dot{x} \times B$$

Using the vector identity

$$b(a \cdot c) + c(a \cdot b) = a \times b \times c$$

We want the canonical momentum p of our lagrangian,

$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}} = m\dot{x} + \frac{q}{c}A(x)$$

Note that this canonical momentum is **not** gauge invariant.
You might see $\vec{\pi} = m\dot{x} = p - \frac{q}{c}A(x)$ as the mechanical momentum.

7.2 Quantizing our Hamiltonian

Now, we Legendre Transform the Lagrangian to get

$$H(x, p) = p\dot{x} - \mathcal{L} = \left(m\dot{x} + \frac{q}{c}A(x)\right)\dot{x} - \frac{1}{2}m\dot{x} + q\phi(x) - \frac{q}{c}\dot{x}A(x) = \frac{1}{2}m\dot{x}^2 + q\phi(x)$$

We need to write this in terms of the canonical momentum, p, so

$$H(x, p) = \frac{1}{2m}\left(p - \frac{q}{c}A(x)\right) + \frac{q}{c}\dot{x}\phi(x)$$

We promote x, p to observables, so now $[x_k, p_j] = i\hbar\delta_{kj}$. We should also include the contribution of our particle to the electric field in principle. Then, we'd have to quantize the field and the particle. Here, we're treating them as static fields, which are set externally. We will quantize them later though!!

7.2.1 Velocities don't Commute

Here's a weird result.

$$[v_j, v_k] = \frac{1}{m^2}\left[p_j - \frac{q}{c}A_j(x), p_k - \frac{q}{c}A_k(x)\right] = \frac{q}{m^2c}\left([p_j, A_k(x)] + [A_j(x), p_k]\right) = \frac{i\hbar q}{m^2c}\left(\partial_j A_k - \partial_k A_j\right) = \frac{i\hbar q}{m^2c}\left(\nabla \times A\right)_i = \frac{i\hbar q}{m^2c}B_i$$

So, in 3-d coordinates,

$$[v_x, v_y] = \frac{i\hbar q}{m^2c}B_z$$

7.3 The Schrödinger Equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}A\right)^2\psi + q\phi\psi$$

7.3.1 It's Not Gauge Invariant

This is not gauge invariant. This is something we should prove to ourselves, but we can make a quantum correction to our gauge transformation. This is going to make our new gauge transformation (Altman Claims)

$$\begin{aligned} A \to A' &= A + \nabla\Lambda \\ \phi \to \phi' &= \frac{1}{c}\partial_t\Lambda \\ \psi \to \psi' &= e^{i\frac{q}{\hbar c}\Lambda(x,t)}\psi(x,t) \end{aligned}$$

This is very spicy, because our phase is **not global**, which means we can't just yeet it. In fact, it very much changes the physics since for two different x,

$$e^{i\lambda(x)}e^{-i\lambda(x')} = e^{i(\lambda(x)-\lambda(x'))} \neq 1$$