

8.06 Spring 2016 Lecture Notes

1. Approximate methods for time-independent Hamiltonians

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Last updated: February 17, 2016

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Often we can't solve the Schrödinger equation exactly. This is in fact almost always the case. For example, consider the van der Waals force between two Hydrogen atoms. What happens then? Do we give up?

Of course not! We use *approximate methods*. The guiding philosophy is

- Reduce real system to toy model that can be exactly solved.
- “Solve” actual Schrödinger equation in some (hopefully controlled) approximation.

Our strategy will depend on how our real system is close to our toy system. If the difference is small (meaning not very much energy) we use perturbation theory. If we are dealing with a Hamiltonian changing slowly in time we use the adiabatic approximation and for a Hamiltonian varying slowly in space we use WKB. We can also consider perturbations that are localized in space, which leads to the framework of scattering.

1 Time-independent perturbation theory

1.1 Non-degenerate case

1.1.1 Setup

Suppose

$$H = H_0 + \delta H,$$

where H_0 has a known eigenspectrum

$$H_0|n^0\rangle = E_n^0|n^0\rangle \quad n = 0, 1, 2, \dots,$$

and δH is a “small” perturbation. We can make this precise by saying that $\|\delta H\| = O(\lambda)$, and λ is a small dimensionless number (say around 0.01). (Here the norm of a Hermitian matrix is defined to be the largest absolute value of its eigenvalues.) Some examples are:

- Relativistic effects: $\lambda \sim v/c$.
- spin-orbit coupling: $\lambda \sim \alpha \approx 1/137$.
- weak E or B field

We will solve for $|n\rangle$ and E_n order by order in λ ; i.e.

$$\begin{aligned} |n\rangle &= |n^0\rangle + |\delta n\rangle = \underbrace{|n^0\rangle}_{O(\lambda^0)} + \underbrace{|n^1\rangle}_{O(\lambda^1)} + \underbrace{|n^2\rangle}_{O(\lambda^2)} + \dots \\ E_n &= E_n^0 + \delta E_n = \underbrace{E_n^0}_{O(\lambda^0)} + \underbrace{E_n^1}_{O(\lambda^1)} + \underbrace{E_n^2}_{O(\lambda^2)} + \dots \end{aligned}$$

The definition of $|n^k\rangle$ is the $O(\lambda^k)$ piece of $|n\rangle$. Formally $|n^k\rangle = k! \frac{\partial^k}{\partial \lambda^k} |n\rangle|_{\lambda=0}$ and $E_n^k = k! \frac{\partial^k}{\partial \lambda^k} E_n|_{\lambda=0}$. While we know the energies and eigenstates of H_0 , we may not know so much about δH . However, we will need to assume that at least we know its matrix elements in the unperturbed eigenbasis. Denote these by

$$\delta H_{mn} \equiv \langle m^0 | \delta H | n^0 \rangle.$$

Today we will consider the non-degenerate case; i.e. when $E_m^0 \neq E_n^0$ for $m \neq n$. Next time we will consider the degenerate case. Your antennae should be going up at this: the difference between $E_m^0 \neq E_n^0$ and $E_m^0 = E_n^0$ can be arbitrarily small, so how can they really lead to different physical theories? In fact, we will see that for non-degenerate perturbation theory to make sense, the energy levels need to be not only different, but also far enough apart, in a sense that we will make precise later.

Difference from Griffiths We will work in a basis where $\langle n^0 | \delta n \rangle = 0$. Equivalently $\langle n^0 | n^k \rangle = 0$ for all $k > 0$. Since $|n^0\rangle$ is normalized, this means that

$$\langle n | n \rangle = \langle n^0 | n^0 \rangle + \langle \delta n | \delta n \rangle = 1 + \langle \delta n | \delta n \rangle \geq 1.$$

Of course $|n\rangle$ is still a valid eigenvector even it is not a unit vector. But if we want a unit vector, we will need to take

$$|n\rangle_{\text{norm}} = \frac{|n^0\rangle + |\delta n\rangle}{\sqrt{1 + \langle \delta n | \delta n \rangle}}.$$

This convention is used in Sakurai.

As a result of this convention

$$\langle n^0 | n \rangle = 1 \quad (1)$$

$$\langle m^0 | n \rangle = \langle m^0 | \delta n \rangle \quad \text{for } m \neq n \quad (2)$$

1.1.2 Perturbative solutions

We want to solve the eigenvalue equation

$$H|n\rangle = E_n|n\rangle. \quad (3)$$

Instead of expanding every term, we will make choices that will be justified in hindsight:

$$(H_0 + \delta H)|n\rangle = E_n(|n^0\rangle + |\delta n\rangle) \quad (4)$$

Thus we avoid for now expanding $|n\rangle$ on the LHS and E_n on the RHS. Now left-multiply (4) by $\langle n^0 |$ and use $\langle n^0 | H_0 = \langle n^0 | E_n^0$ and $\langle n^0 | n \rangle = 1$ to obtain

$$\langle n^0 | \delta H | n \rangle = E_n - E_n^0. \quad (5)$$

What if we instead left-multiply by $\langle m^0 |$ for some $m \neq n$? Then we obtain (using $\langle m^0 | n^0 \rangle = 0$)

$$\langle m^0 | \delta H | n \rangle = (E_n - E_m^0) \langle m^0 | \delta n \rangle. \quad (6)$$

So far everything is still exact, but further progress will require approximation. We now solve (5) and (6) order by order in λ .

Replacing the $|n\rangle$ in (5) with $|n^0\rangle + O(\lambda)$ we obtain

$$\boxed{E_n = E_n^0 + \langle n^0 | \delta H | n^0 \rangle + O(\lambda^2)}. \quad (7)$$

This is the *first-order energy shift*. It will soon become an old friend.

Performing the same substitution in a rearranged version of (6) yields

$$\langle m^0 | \delta n \rangle = \frac{\langle m^0 | \delta H | n \rangle}{E_n - E_m^0} = \frac{\langle m^0 | \delta H | n^0 \rangle + O(\lambda^2)}{E_n^0 - E_m^0 + O(\lambda)} \quad (8)$$

Repeating for all values of $m \neq n$ (recall that $\langle n^0 | \delta n \rangle = 0$ by fiat) we obtain

$$|\delta n\rangle = \sum_{m \neq n} |m^0\rangle \frac{\langle m^0 | \delta H | n^0 \rangle}{E_n^0 - E_m^0} + O(\lambda^2) \quad (9)$$

This yields the *first-order shift in the wavefunction*. We need to be a little careful here. Clearly we are using the non-degenerate condition here by assuming that $E_n^0 - E_m^0 \neq 0$ for $n \neq m$. But we have actually used a robust version of this assumption

On to second order!

$$E_n = E_n^0 + \langle n^0 | \delta H | n \rangle \quad \text{exact} \quad (10a)$$

$$= E_n^0 + \langle n^0 | \delta H | n^0 \rangle + \langle n^0 | \delta H | \delta n \rangle \quad \text{still exact} \quad (10b)$$

$$= E_n^0 + \delta H_{nn} + \langle n^0 | \delta H \sum_{m \neq n} |m^0\rangle \frac{\langle m^0 | \delta H | n \rangle + O(\lambda^2)}{E_n - E_m^0} \quad \text{using (9)} \quad (10c)$$

$$= E_n^0 + \delta H_{nn} + \sum_{m \neq n} \frac{|\delta H_{mn}|^2}{E_n^0 - E_m^0} + O(\lambda^3) \quad (10d)$$

We will generally not need the second-order shift in the wavefunction, but it can be computed to be

$$|n^2\rangle = \sum_{k \neq n} \sum_{l \neq n} \frac{|k^0\rangle \delta H_{k,l} \delta H_{l,n}}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} - \sum_{k \neq n} \frac{|k^0\rangle \delta H_{n,n} \delta H_{k,n}}{(E_n^0 - E_k^0)^2}. \quad (11)$$

For higher-order corrections, Sakurai is the best reference. For 8.06, we will never go beyond second order in energy or first order in wavefunction, although below we will see that (11) is relevant to degenerate perturbation theory.

To summarize, we have

$$\begin{aligned} E_n^0 &= E_n^0 \\ E_n^1 &= \delta H_{nn} \\ E_n^2 &= \sum_{m \neq n} \frac{|\delta H_{mn}|^2}{E_n^0 - E_m^0} \\ |n^0\rangle &= |n^0\rangle \\ |n^1\rangle &= \sum_{m \neq n} |m^0\rangle \frac{\langle m^0 | \delta H | n^0 \rangle}{E_n^0 - E_m^0} \end{aligned}$$

What about normalization? We should multiply by $(1 + \langle \delta n | \delta n \rangle)^{-1/2} = 1 - \frac{1}{2} \langle n^1 | n^1 \rangle + O(\lambda^4)$ so this affects only $|n^2\rangle$ and not $|n^1\rangle$.

1.1.3 Energy shifts of the ground state

The first-order energy shift can of course be either positive or negative; e.g. suppose $\delta H = \pm \lambda I$. But there is one thing we can always say about it: it always *overstates* the true ground-state energy of the perturbed system. Here is the proof. The first-order estimate of the ground-state energy is

$$E_0^0 + E_0^1 = \langle 0^0 | H_0 | 0^0 \rangle + \langle 0^0 | \delta H | 0^0 \rangle = \langle 0^0 | H | 0^0 \rangle \geq \langle 0 | H | 0 \rangle = E_0.$$

The second equality is from the identity $H = H_0 + \delta H$ and the inequality is the variational principle: $\langle \psi | H | \psi \rangle \geq \langle 0 | H | 0 \rangle$ for all unit vectors $|\psi\rangle$.

In this case, we would hope that the second-order term E_0^2 would improve things by being negative. And this is indeed the case.

$$E_0^2 = \sum_{m \neq 0} \frac{|\delta H_{m0}|^2}{E_0^0 - E_m^0}.$$

Every term in the sum is ≤ 0 so we always have $E_0^2 \leq 0$.

More generally at 2nd order we observe “level repulsion.” The n ’th energy level is pushed up by levels with $m < n$ and pushed down by levels with $m > n$ (assuming that $E_0 < E_1 < \dots$).

1.1.4 Range of validity and a two-state example

As we go to higher orders of perturbation theory, we multiply by entries of δH (e.g. δH_{mn}) and divide by *differences* of eigenvalues of H_0 , e.g. $E_n^0 - E_m^0$. So the perturbation has to be small w.r.t the level spacing. See diagram on blackboard plotting $E(\lambda)$ as a function of λ .

Here's probably the simplest possible example.

$$H = \begin{pmatrix} E_0^0 & \lambda \\ \lambda & E_1^0 \end{pmatrix} = \underbrace{\begin{pmatrix} E_0^0 & 0 \\ 0 & E_1^0 \end{pmatrix}}_{H_0} + \underbrace{\begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}}_{\delta H}.$$

Let's write $E_0^0, E_1^0 = \bar{E} \pm \Delta$ so that $H_0 = \bar{E} + \Delta \sigma_z$. The first-order shifts are $\delta H_{00} = \delta H_{11} = 0$. The second-order shifts are

$$E_0^2 = \frac{|\delta H_{01}|^2}{E_0^0 - E_1^0} = -\frac{\lambda^2}{2\Delta}$$

$$E_1^2 = \frac{|\delta H_{01}|^2}{E_1^0 - E_0^0} = \frac{\lambda^2}{2\Delta}$$

Of course this problem can be solved directly more easily, as you will explore on your pset. There you will find that the energy levels are (exactly)

$$E_0, E_1 = \bar{E} \pm \sqrt{\lambda^2 + \Delta^2}$$

In the $|\Delta| \gg |\lambda|$ limit this can be written as

$$\bar{E} \pm \Delta \sqrt{1 + \left(\frac{\lambda}{\Delta}\right)^2},$$

while in the $|\lambda| \gg |\Delta|$ limit we can write this as

$$\bar{E} \pm \lambda \sqrt{1 + \left(\frac{\Delta}{\lambda}\right)^2}.$$

The splitting in energy levels is 2Δ for $\lambda = 0$ and then has a $O(\lambda^2)$ term for small λ and finally becomes approximately linear in λ for large λ . This type of behavior is called an “avoided crossing” because of the fact that generically Hamiltonians tend to have non-degenerate eigenvalues. See figure drawn in lecture.

1.1.5 Anharmonic oscillator

$$H = \underbrace{\frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}}_{H_0} + \underbrace{\lambda x^4}_{\delta H}. \quad (12)$$

How does the ground-state energy change? The unperturbed ground-state energy is $E_0^0 = \frac{1}{2}\hbar\omega$.

Using $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ we can calculate

$$\begin{aligned} E_0^1 &= \lambda \langle 0 | \left(\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \right)^4 | 0 \rangle \\ &= \lambda \frac{\hbar^2}{4m^2\omega^2} \left| (a + a^\dagger)^2 | 0 \rangle \right|^2 \\ &= \lambda \frac{\hbar^2}{4m^2\omega^2} \left| (a + a^\dagger) | 1 \rangle \right|^2 \\ &= \lambda \frac{\hbar^2}{4m^2\omega^2} \left| | 0 \rangle + \sqrt{2} | 2 \rangle \right|^2 \\ &= \frac{3}{4} \lambda \frac{\hbar^2}{m^2\omega^2} \end{aligned}$$

Here is an alternate derivation using integrals. This one is hairier, so let's set $\hbar = m = \omega = 1$. We will use $\langle x|0\rangle = N e^{-x^2/2}$, for some normalization N . Then we can compute

$$E_0^1 = \lambda \langle 0|x^4|0\rangle = \lambda \frac{\int_{-\infty}^{\infty} dx e^{-x^2} x^4}{\int_{-\infty}^{\infty} dx e^{-x^2}}.$$

Here our job becomes easier if we introduce a parameter.

$$\begin{aligned} \int dx e^{-ax^2} &= \sqrt{\frac{\pi}{a}} \\ \frac{d}{da} \int dx e^{-ax^2} &= \int dx (-x^2) e^{-ax^2} = -\frac{1}{2} \frac{\sqrt{\pi}}{a^{3/2}} \\ \frac{d^2}{da^2} \int dx e^{-ax^2} &= \int dx x^4 e^{-ax^2} = \left(-\frac{1}{2}\right) \left(-\frac{3}{2}\right) \frac{\sqrt{\pi}}{a^{5/2}} \end{aligned}$$

Thus $\langle x^4\rangle = 3/4$.

Moral of the story: Gaussian integrals involve some beautiful tricks that you should learn. But raising and lowering operators are easier.

1.2 Degenerate perturbation theory

1.2.1 Overview

The first-order corrections to the wavefunction and the second-order corrections to the energy all have factors of $E_n^0 - E_m^0$ in the denominator. So when two energy levels become equal, these give nonsense answers. But in fact, even the first-order energy shift will be wrong in this case. Let us revisit the case of two-level systems. Suppose that $E_0^0 = E_1^1$. For simplicity, assume $E_0^0 = E_1^1 = 0$ so the overall Hamiltonian is

$$H = \delta H = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}.$$

The eigenvalues are $\pm\lambda$, which is first order in δH . But the diagonal elements of δH are zero, so (7) would say that the first-order energy shifts are zero. To summarize, the first-order energy shift is wrong, and the second-order energy shift and first-order wavefunction shift are infinite. The situation looks grim.

There is one point in the above paragraph where I pulled a fast one. The reference to “diagonal elements” refers to the eigenbasis of H_0 . In the above example, this is labeled $|0^0\rangle$ and $|1^0\rangle$, which we took to be $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. But since H_0 has degenerate eigenvalues, the corresponding eigenvectors are not unique. We can make a unitary change of basis within the degenerate eigenspace and obtain new eigenvectors. In that example, we could take

$$|0^0\rangle = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}} \quad \text{and} \quad |1^0\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$$

so that the matrix for δH would be diagonal in the $\{|0^0\rangle, |1^0\rangle\}$ basis. In this case the first-order energy shift is exactly correct and the second-order energy shift is zero.

General rule for degeneracy in H_0 . For a general Hamiltonian where H_0 has degenerate eigenvalues, the strategy is:

1. Choose an eigenbasis $\{|n^0\rangle\}$ for H_0 where $\delta H_{mn} = 0$ for each $m \neq n$ with $E_m^0 = E_n^0$. This is called a “good basis.”
2. Apply non-degenerate perturbation theory to handle the remaining off-diagonal terms in δH (which now will only be nonzero when $E_m^0 \neq E_n^0$).

Why is this possible? By the spectral theorem, we can write H_0 as

$$H_0 = \sum_i E_i^0 \Pi_i, \quad (13)$$

where Π_i is a projection operator supported on the space of E_i^0 -eigenvectors. Call this space V_i . We will think of H_0 as block diagonal with blocks corresponding to the subspaces V_1, V_2, \dots

We can write $\delta H = \sum_{i,j} \Pi_i \delta H \Pi_j$. The diagonal blocks are the components of the form $\Pi_i \delta H \Pi_i$. These are the blocks we would like to diagonalize. Since each $\Pi_i \delta H \Pi_i$ is a Hermitian matrix we can write

$$\Pi_i \delta H \Pi_i = \sum_{a=1}^{\dim V_i} \Delta_{i,a} |i, a\rangle \langle i, a| \quad (14)$$

where $\Delta_{i,a}$ are the eigenvalues of $\Pi_i \delta H \Pi_i$ (when considered an operator on V_i) and $\{|i, a\rangle\}_{a=1, \dots, \dim V_i}$ forms an orthonormal basis for V_i . Since each $|i, a\rangle \in V_i$, we also have $H_0 |i, a\rangle = E_i^0 |i, a\rangle$. Now the first-order energy shifts are given by the $\Delta_{i,a}$ and the second-order energy shifts and first-order wavefunction corrections involve off-diagonal elements of δH between eigenvectors of H_0 with different eigenvalues. *If* this fully breaks the degeneracy of H_0 , then we can follow the lines of the non-degenerate case. We first introduce a little more notation: let n stand for the pair (i, a) , denote $|n\rangle^{\text{rotated}} = |i, a\rangle$ and let $\delta H^{\text{rotated}}$ denote δH in the $\{|n\rangle^{\text{rotated}}\}$ basis.

$$E_n = E_n^0 + \delta H_{nn}^{\text{rotated}} + \sum_{m: E_m^0 \neq E_n^0} \frac{|\delta H_{mn}^{\text{rotated}}|^2}{E_n^0 - E_m^0} + O(\lambda^3) \quad (15)$$

The above equations work in many cases, including all the examples on problems sets or exams that you will encounter. However, it may be that the diagonal elements of δH do not fully break the degeneracy. In this case, higher-order corrections may encounter new degeneracies which may require new changes of basis¹. In the next section we will describe systematically what to do in this case.

¹Here is an example. Take $\lambda \ll \Delta$ and let

$$H = \begin{pmatrix} 0 & 0 & \lambda \\ 0 & 0 & \lambda \\ \lambda & \lambda & \Delta \end{pmatrix}.$$

Graphically, H_0 might look something like

$$H_0 = \left(\begin{array}{c|c|c} E_1^0 & & \\ \hline & E_1^0 & \\ \hline & & E_2^0 \\ & & E_2^0 \\ & & E_2^0 \\ \hline & & E_3^0 \end{array} \right) \quad (16)$$

We can write δH in this basis and generically it could have every matrix element nonzero, e.g.

$$\delta H = \left(\begin{array}{c|c|c} * & * & * & * & * & * \\ * & * & * & * & * & * \\ \hline * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ \hline * & * & * & * & * & * \end{array} \right) \quad (17)$$

By choosing a new basis for each block, H_0 stays the same and δH takes on the form

$$\delta H^{\text{rotated}} = \left(\begin{array}{c|c|c} * & 0 & * & * & * & * \\ 0 & * & * & * & * & * \\ \hline * & * & * & 0 & 0 & * \\ * & * & 0 & * & 0 & * \\ * & * & 0 & 0 & * & * \\ \hline * & * & * & * & * & * \end{array} \right) \quad (18)$$

There are still off-diagonal terms but only between different eigenvalues of H_0 .

Why is it reasonable to ask that we find a new basis in this way? After all, the whole point of perturbation theory was that it was too hard to diagonalize $H_0 + \delta H$. However, now we only need to diagonalize δH in each block of degenerate eigenvalues. Typically these will be much lower dimension than the overall space.

1.2.2 First-order wavefunction correction - degenerate case

Note: This section is included for completeness, but contains material that goes beyond lecture and will not appear on any problem sets or exams.

What about the perturbed wavefunction $|n\rangle$? The zeroth order wavefunction should be $|n^0\rangle^{\text{rotated}}$. It is tempting to state that the first-order correction to $|n\rangle = |i, a\rangle$ is

$$|n^1\rangle \stackrel{?}{=} \sum_{m: E_m^0 \neq E_n^0} |m^0\rangle^{\text{rotated}} \frac{\delta H_{mn}^{\text{rotated}}}{E_n^0 - E_m^0} = \sum_{j \neq i} \sum_{b=1}^{\dim V_j} |j, b\rangle^{\text{rotated}} \frac{\delta H_{jb,ia}^{\text{rotated}}}{E_i^0 - E_j^0} \quad (19)$$

but this is only part of the story (the $\stackrel{?}{=}$ is a warning that this equation is not quite correct). (19) does indeed describe the contribution to $|i, a\rangle$ from states $|j, a^0\rangle^{\text{rotated}}$ with $i \neq j$, but there are also contributions within the same block, i.e. from states with $j = i$. This can be thought of as representing the need to *further rotate* our rotated basis to account for degeneracies that arise at higher order in perturbation theory.

Another way to think about that is that if we go to second order in perturbation theory, we get the contribution (following (11)):

$$|n^2\rangle \stackrel{?}{=} |i, a^2\rangle \stackrel{?}{=} \sum_{(j,b) \neq (i,a)} \sum_{(k,c) \neq (i,a)} \frac{|j, b\rangle^{\text{rotated}} \delta H_{jb,kc}^{\text{rot}} \delta H_{kc,ia}^{\text{rot}}}{(E_{ia} - E_{jb})(E_{ia} - E_{kc})} - \sum_{(j,b) \neq (i,a)} \frac{|j, b\rangle^{\text{rotated}} \delta H_{ia,ia}^{\text{rot}} \delta H_{jb,ia}^{\text{rot}}}{(E_{ia} - E_{jb})^2} \quad (20)$$

Is this really a second-order (i.e. $O(\lambda^2)$) correction? First look at the second term. Because we have rotated into a block-diagonal basis $\delta H_{jb,ia}$ is zero unless $i \neq j$. Thus the denominator is $O(1)$ and the numerator is $O(\lambda^2)$, and the second term gives a $O(\lambda^2)$ correction. What about the first term? Now the block-diagonal constraint means that only the $i \neq k \neq j$ terms survive, and again the numerator is $O(\lambda^2)$. However, it is legal to have $i = j$ (as long as $a \neq b$. In this case, the energy splitting between i, a and i, b is $O(\lambda)$. Thus, this term contributes $O(\frac{\lambda^2}{\lambda}) = O(\lambda)$. In other words, it is a first-order contribution, despite appearing in the expansions of the second-order term. (For similar reasons, (20) gives only part of the true second-order contribution, for which we need to go to third order.) We conclude that the true first-order correction to the wavefunction is

$$|i, a^1\rangle = \sum_{j \neq i} \sum_{b=1}^{\dim V_j} |j, b\rangle^{\text{rotated}} \frac{\delta H_{jb,ia}^{\text{rotated}}}{E_i^0 - E_j^0} + \sum_{b \neq a} \sum_{j \neq i} \sum_{c=1}^{\dim V_j} \frac{|i, b\rangle^{\text{rotated}} \delta H_{ib,jc}^{\text{rot}} \delta H_{jc,ia}^{\text{rot}}}{(\delta H_{ia}^{\text{rot}} - \delta H_{ib}^0)(E_i^0 - E_j^0)} \quad (21)$$

1.2.3 Hydrogen preview

An important application of degenerate perturbation theory is to the spectrum of hydrogen. Here

$$H_0 = \frac{p^2}{2m_e} - \frac{e^2}{r}.$$

The eigenbasis can be taken to be $|n, l, m, m_s\rangle$ where n is the principle quantum number, l denote total orbital angular momentum, m its z -component and m_s the z -component of the electron spin. Another valid basis is $|n, l, j, m_j\rangle$ where j denotes the total overall angular momentum (i.e. corresponding to the operator \vec{J}^2 where $\vec{J} = \vec{L} + \vec{S}$) and m_j its z component.

In both cases, the eigenvalues of H_0 depend only on n and all the other degrees of freedom are degenerate. Indeed

$$E_{nlmm_s}^0 = -\frac{1}{n^2} \frac{m_e e^4}{2\hbar^2} \approx -\frac{13.6\text{eV}}{n^2}.$$

Next week we will discuss a number of corrections to this that are smaller by factors of either $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ (the fine structure constant) or $\frac{m_e}{m_p} \approx \frac{1}{1800}$. (Indeed even $\frac{m_e e^2}{\hbar^2}$ can be written as $m_e c^2 \alpha^2$, where $m_e c^2$ is the energy scale from the energy from the rest mass of the electron. And this of course is smaller by a factor of roughly $\frac{m_e}{m_p}$ than the mass of the entire atom. We ignore these larger energies in what follows because they are not relevant to experiments in which the electron or proton are not created or destroyed.) The contributions to the energy of hydrogen are summarized as follows.

We mention here also the “spectroscopic notation” convention, which is used for the coupled basis. The state $|n, l, j, m_j\rangle$ is written as nL_j where “L” is a letter that expresses the orbital angular momentum according to the rule:

what	where discussed	magnitude
0th order	8.04/8.05	$E_n^0 \sim \frac{m_e e^4}{\hbar^2} \sim m_e c^2 \alpha^2$
fine structure	8.05	$E_{\text{fs}} \sim m_e c^2 \alpha^4$
Lamb shift	QFT	$E_{\text{Lamb}} \sim m_e c^2 \alpha^5$
hyperfine structure	8.05	$E_{\text{hf}} \sim m_e c^2 \alpha^4 \frac{m_e}{m_p}$
proton radius	pset	$\sim m_e c^2 \alpha^3 \left(\frac{m_e}{m_p}\right)^2$
Zeeman effect	Griffiths	depends on \vec{B} field
Stark effect	pset	depends on \vec{E} field

Table 1: Contributions to the hydrogen energy levels.

$L =$	S	P	D	F	G	...
$l =$	0	1	2	3	4	...

Some examples are

nL_j	n	l	j
$1S_{1/2}$	1	0	1/2
$2S_{1/2}$	2	0	1/2
$2P_{1/2}$	2	1	1/2
$2P_{3/2}$	2	1	3/2

1.2.4 Two-spin example

Let's see how these ideas work with a simple example. Consider two spin-1/2 particles with Hamiltonian

$$H_0 = \frac{E_0}{\hbar^2} \vec{S}_1 \cdot \vec{S}_2 = \frac{E_0}{\hbar^2} (S_x \otimes S_x + S_y \otimes S_y + S_z \otimes S_z).$$

To diagonalize this, define $\vec{J} = \vec{S}_1 + \vec{S}_2$ and observe that $\vec{J}^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$. Thus

$$H_0 = \frac{E_0}{\hbar^2} \frac{\vec{J}^2 - \vec{S}_1^2 - \vec{S}_2^2}{2} = E_0 \left(\frac{\vec{J}^2}{2\hbar^2} - \frac{3}{4} \right).$$

The eigenvalues of \vec{J}^2 are 0 (degeneracy 1) and $2\hbar^2$ (degeneracy 3); these correspond to total spin 0 and 1 respectively. Thus spectrum of H_0 is $-\frac{3}{4}E_0$ (with degeneracy 1) and $\frac{1}{4}E_0$ (with degeneracy 3).

Case 1 Now suppose we add a perturbation

$$\delta H = \frac{\Delta}{\hbar}(S_{z,1} + S_{z,2}) = \frac{\Delta}{\hbar}J_z.$$

(This might arise from applying a magnetic field in the \hat{z} direction.) We need to choose a good basis. Fortunately, δH and H_0 commute and the coupled basis $|j, m\rangle$ (with $j = 0, 1$ and $-j \leq m \leq j$) works. In this basis we have

$$\begin{aligned} H_0|j, m\rangle &= E_0 \left(\frac{j(j+1)}{2} - \frac{3}{4} \right) |j, m\rangle \\ \delta H|j, m\rangle &= \Delta m |j, m\rangle \end{aligned}$$

[Draw energy level diagram of this.]

This was too easy! When everything commutes, this is what it looks like. Of course, we could have chosen a more foolish eigenbasis of H_0 . Any eigenbasis would include the singlet $|0, 0\rangle = \frac{|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle}{\sqrt{2}}$, but it could be completed with any additional three orthonormal states in the triple space. If we chose these to be anything other than $|1, 1\rangle, |1, 0\rangle, |1, -1\rangle$, then even first-order perturbation theory would give the wrong answer. (Working this out is an exercise left to the reader.)

Case 2 Let us try a slightly more interesting perturbation.

$$\delta H = \frac{\Delta}{\hbar}(S_{z,1} - S_{z,2}).$$

This could arise from applying a magnetic field to positronium. We calculate its matrix elements in the coupled basis as follows:

$$\begin{aligned} \delta H|1, 1\rangle &= \delta H|+\rangle \otimes |+\rangle = 0 \\ \delta H|1, -1\rangle &= \delta H|-\rangle \otimes |-\rangle = 0 \\ \delta H|1, 0\rangle &= \delta H \frac{|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle}{\sqrt{2}} = \Delta \frac{|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle}{\sqrt{2}} = \Delta|0, 0\rangle \end{aligned}$$

Since δH is Hermitian we know also that $\delta H|0, 0\rangle = \Delta|1, 0\rangle$.

Thus, in the coupled basis we have

$$H_0 = \begin{matrix} & \begin{matrix} 1, 1 & 1, 0 & 1, -1 & 0, 0 \end{matrix} \\ \begin{matrix} 1, 1 \\ 1, 0 \\ 1, -1 \\ 0, 0 \end{matrix} & \begin{pmatrix} \frac{E_0}{4} & 0 & 0 & 0 \\ 0 & \frac{E_0}{4} & 0 & 0 \\ 0 & 0 & \frac{E_0}{4} & 0 \\ 0 & 0 & 0 & -\frac{3}{4}E_0 \end{pmatrix} \end{matrix} \quad \text{and} \quad \delta H = \begin{matrix} & \begin{matrix} 1, 1 & 1, 0 & 1, -1 & 0, 0 \end{matrix} \\ \begin{matrix} 1, 1 \\ 1, 0 \\ 1, -1 \\ 0, 0 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Delta \\ 0 & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 \end{pmatrix} \end{matrix} \quad (22)$$

First-order perturbation theory (correctly) gives us zero energy shift to first order in Δ . The second-order shifts are

$$\begin{aligned} E_{(1,0)}^2 &= \frac{|\delta H_{(1,0),(0,0)}|^2}{E_{(1,0)}^0 - E_{(0,0)}^0} = \frac{\Delta^2}{E_0} \\ E_{(0,0)}^2 &= \frac{|\delta H_{(0,0),(1,0)}|^2}{E_{(0,0)}^0 - E_{(1,0)}^0} = \frac{\Delta^2}{-E_0}, \end{aligned}$$

where we have used the fact that $E_0 = E_{j=1}^0 - E_{j=0}^0$.

2 The Hydrogen spectrum

See Section 1.2.3 for an overview.

2.1 Fine structure

The term “fine structure” refers to three different contributions to the energy that are $O(m_e c^2 \alpha^4)$, compared with the $O(m_e c^2 \alpha^2)$ zeroth order contribution: relativistic corrections, spin-orbit coupling and the Darwin term. The contributions all arise from the Dirac equation for a particle with charge q and mass m :

$$H_{\text{Dirac}} = c \vec{\alpha} \cdot (\vec{p} - \frac{q}{c} \vec{A}) + \beta m c^2 + q \phi,$$

where \vec{A}, ϕ are the vector and scalar potentials of the EM field, and $\vec{\alpha}$ and β are given by

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} = \sigma_x \otimes \vec{\sigma} \quad \text{and} \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \sigma_z \otimes I.$$

The Hilbert space here is the space of well-behaved functions from $\mathbb{R}^3 \rightarrow \mathbb{C}$ as well as a four-dimensional discrete space. Why four dimensions? Two are to account for spin, and another two are to allow a particle to be either an electron or positron. While the Dirac equation was originally motivated by the need to properly account for the fine structure of hydrogen and to unify quantum mechanics with special relativity, it as a bonus generated the prediction of antimatter.

We will not further explore the Dirac equation in 8.06, but at this point we should observe its symmetry under *collective* rotation. That is, if R is a 3×3 rotation matrix and we replace $(\sigma_1, \sigma_2, \sigma_3)$ with $(\sum_i R_{i1} \sigma_i, \sum_i R_{i2} \sigma_i, \sum_i R_{i3} \sigma_i)$ and (p_1, p_2, p_3) with $(\sum_i R_{i1} p_i, \sum_i R_{i2} p_i, \sum_i R_{i3} p_i)$ (and similarly transform \vec{A}, ϕ), then H^{Dirac} is unchanged.

This means that H^{Dirac} commutes with the collective rotation operators $\vec{J} = \vec{L} + \vec{S}$, although not necessarily the individual rotations \vec{L} and \vec{S} . As a result, a good basis for the Dirac-equation version of hydrogen is likely to be $|n, l, j, m_j\rangle$ (since the Hamiltonian should be block-diagonal in n, j and independent of m_j) instead of the alternative $|n, l, m_l, m_s\rangle$. After much calculation we will see this fact confirmed.

2.1.1 Relativistic correction

Let's first do some back-of-the-envelope estimates of how important relativity is to the hydrogen atom. The unperturbed ground-state wavefunction is

$$\psi_{100}(\vec{r}) = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}}, \quad a_0 = \frac{\hbar^2}{m e^2} = \frac{1}{\alpha} \frac{\hbar}{m c}.$$

We can then estimate

$$p \approx \frac{\hbar}{a_0} = \alpha m c$$

$$v \approx \frac{p}{m} = \alpha c$$

Thus the electron velocity is $\approx 1/137$ the speed of light. This is non-relativistic, but still fast enough that relativistic corrections will be non-negligible. Let's compute them!

$$\begin{aligned}\text{KE} &= \sqrt{m^2 c^4 + \vec{p}^2 c^2} - mc^2 \\ &= \underbrace{\frac{\vec{p}^2}{2m}}_{\text{usual term}} - \underbrace{\frac{\vec{p}^4}{8m^3 c^2}}_{\delta H_{\text{rel}}}\end{aligned}$$

The first-order contribution to the energy is

$$\begin{aligned}E_{nlj}^1 &= \langle n, l, j | \delta H_{\text{rel}} | n, l, j \rangle && \text{independent of } m_j \\ &= \langle n, l, j | -\frac{\vec{p}^4}{8m^3 c^2} | n, l, j \rangle \\ &= \text{calculation omitted, see textbooks} \\ &= -\frac{\alpha^4 m c^2}{8n^4} \left(\frac{4n}{l + \frac{1}{2}} - 3 \right)\end{aligned}$$

One key feature of this calculation is that the answer indeed scales as $\alpha^4 m c^2$ (since $\frac{p^4}{m^3 c^2} \sim \frac{(\alpha m c)^4}{m^3 c^2} = \alpha^4 m c^2$) which is smaller than E_n^0 by a factor of α^2 . Also note that the answer depends on l but not j . This is not surprising since spin never appeared. But it is inconsistent with the prediction from the Dirac equation that the energy should depend instead on j . To get there we will need to consider additional terms.

2.1.2 Spin-orbit coupling

See Lecture 23 of the 2015 8.05 notes (or Griffiths) for more detail. The general formula for the energy of a dipole in a magnetic field is $\delta H = -\vec{\mu} \cdot \vec{B}$. For an electron, the dipole moment is

$$\vec{\mu}_e = -\underbrace{\mu_B}_{\frac{e\hbar}{2mc}} \underbrace{g_e}_{2} \frac{\vec{S}}{\hbar} = -\frac{e}{mc} \vec{S}.$$

Compute the \vec{B} field from the proton in the rest frame of the electron, which see the proton orbiting it. If \vec{r} is the vector pointing from the proton to the electron, then the magnetic field strength is

$$\vec{B} = -\frac{\vec{v}}{c} \times \frac{e\vec{r}}{r^3} = \frac{e}{c} \frac{\vec{v} \times \vec{r}}{r^3} = \frac{e}{mc} \frac{\vec{L}}{r^3}$$

(In both cases, the “mass” is technically the reduced mass $\frac{m_e m_p}{m_e + m_p}$ which we can approximate with $m \approx m_e$.) Putting this together we get a semi-classical estimate of δH :

$$\delta H^{\text{semi-classical}} = \frac{e^2}{m^2 c^2 r^3} \vec{S} \cdot \vec{L}.$$

This is close, but not quite, the true answer that can be obtained from the Dirac equation, which is exactly half the semi-classical estimate.

$$\delta H^{\text{Dirac}} = \frac{e^2}{2m^2 c^2 r^3} \vec{S} \cdot \vec{L}.$$

Now we compute the first-order correction to the energies. We will use the facts that

$$\langle nlj | \vec{S} \cdot \vec{L} | nlj \rangle = \frac{\hbar^2}{2} \left(j(j+1) - l(l+1) - \frac{3}{4} \right) \quad (23a)$$

$$\langle nlj | \frac{1}{r^3} | nlj \rangle = \frac{1}{n^3 l(l + \frac{1}{2})(l+1) a_0^3} \quad (\text{see Griffiths problem 6.35(c)}) \quad (23b)$$

Now we can calculate:

$$\begin{aligned} E_{nlj,\text{SO}}^1 &= \frac{e^2}{2m^2c^2} \langle nlj | \frac{\vec{S} \cdot \vec{L}}{r^3} | nlj \rangle \\ &= \frac{\alpha^4 mc^2}{4n^4} \left(\frac{n(j(j+1) - l(l+1) - \frac{3}{4})}{l(l + \frac{1}{2})(l+1)} \right) \end{aligned}$$

While the exact form of this equation is a bit hairy, we can see that its order of magnitude is $\sim \alpha^4 mc^2$, which is comparable to the relativistic correction. Also note that now there is a j and l dependence, because spin is part of the picture as well.

2.1.3 Fine structure

Combining the relativistic and spin-orbit coupling leads to a miraculous cancelation

$$E_{nlj,\text{FS}}^1 = E_{nlj,\text{rel}}^1 + E_{nlj,\text{SO}}^1 = \frac{\alpha^4 mc^2}{8n^4} \left(3 - \frac{4n}{j + \frac{1}{2}} \right). \quad (24)$$

This derivation used the fact that $j = l \pm 1/2$ and can be proved to hold separately for each case $j = l+1/2$ and $j = l-1/2$. An additional complication is that the above formulas for the relativistic and spin-orbit corrections were not quite right when $l = 0$ (e.g. the spin-orbit coupling should really be zero then, and p^4 is not a Hermitian operator for $l = 0$); additionally, there is a *third* correction of order $\alpha^4 mc^2$ called the *Darwin shift*, due to the fact that the electron is delocalized across a distance given by its Compton wavelength (which is $\sim \alpha a_0$). However, this term affects only the $l = 0$ term and, together with the correct $l = 0$ versions of the spin-orbit and relativistic couplings, ends up giving precisely the formula in (24).

To summarize, while the previous calculations had limited validity, (24) is exactly correct for all values of n and j . It can also be derived directly from the Dirac equation. We reassuringly find that it depends only on n and j and not on other quantum numbers.

Draw a diagram showing the $n = 2$ states of hydrogen. The zeroth order energy is $-\frac{\alpha^2 mc^2}{8}$. The fine structure then contributes energy $-5\frac{\alpha^4 mc^2}{8}$ to the $2S_{1/2}$ and $2P_{1/2}$ states and energy $-\frac{\alpha^4 mc^2}{8}$ to the $2P_{3/2}$ states. Are the $2S_{1/2}$ and $2P_{1/2}$ states degenerate? It turns out that the *Lamb shift* leads to a further splitting of these two levels, of order $\alpha^3 \ln(1/\alpha) 5mc^2$. The Lamb shift comes from the interaction of the electron with the electromagnetic field (since even a harmonic oscillator in the ground state has nonzero expectation value for observables like \hat{x}^2) and a precise derivation of the Lamb shift requires QED.

2.2 Hyperfine splitting

This was covered in 8.05, but I want to review the derivation and briefly justify one point that we previously did not have the tools for.

The electron and proton are both magnetic dipoles and thus contribute to the Hamiltonian a term

$$\delta H_{\text{HF}} = -\vec{\mu}_e \cdot \vec{B}_{\text{proton dipole}},$$

where the \vec{B} field coming from the dipole moment of the proton is

$$\vec{B}_{\text{proton dipole}} = \frac{1}{r^3} (3(\vec{\mu}_p \cdot \hat{r})\hat{r} - \vec{\mu}_p) + \frac{8\pi}{3} \vec{\mu}_p \delta^{(3)}(\vec{r}). \quad (25)$$

The first term has the property that $\langle \psi | \text{first term} | \psi \rangle = 0$ if $|\psi\rangle$ is an $l = 0$ state (because the rotational invariance of $|\psi\rangle$ means we can replace $\hat{r}_i \hat{r}_j$ with its average over rotations, which is $\frac{1}{3} \delta_{ij}$). This was discussed in 8.05, but now first-order perturbation theory lets us rigorously justify that this means that the first term contributes zero to the energy of $l = 0$ states at first order in perturbation theory.

The second term is called the “contact term” because of the presence of the delta function. Again we can use perturbation theory to obtain that the first-order correction to the wavefunction $|\psi_{\text{spatial}}\rangle \otimes |\psi_{\text{spin}}\rangle$ is

$$\begin{aligned} E_{\text{HF}}^1 &= -\langle \psi_{\text{spatial}} | \otimes \langle \psi_{\text{spin}} | \left(\frac{8\pi}{3} \vec{\mu}_e \cdot \vec{\mu}_p \delta^{(3)}(\vec{r}) \right) | \psi_{\text{spatial}} \rangle \otimes | \psi_{\text{spin}} \rangle \\ &= \frac{g_e g_p}{m_e m_p} \frac{2\pi e^2}{3c^2} \langle \psi_{\text{spin}} | \vec{S}_e \cdot \vec{S}_p | \psi_{\text{spin}} \rangle \langle \psi_{\text{spatial}} | \delta^{(3)}(\vec{r}) | \psi_{\text{spatial}} \rangle \end{aligned}$$

We now should pause to consider good bases. In fact, treating the spatial and spin wavefunctions as a tensor product was already an assumption that cannot always be justified, since the fine structure wants a basis where j (involving both spatial and electron-spin degrees of freedom) is well-defined. However for the $n = 1$ state of hydrogen, we always have $l = 0$ and $j = 1/2$. Thus $|\psi_{\text{spatial}}\rangle = |1, 0, 0\rangle$ and we obtain a factor of $\frac{1}{\pi a_0^3}$ from the $\langle \psi_{\text{spatial}} | \delta^{(3)}(\vec{r}) | \psi_{\text{spatial}} \rangle$ term.

For the electron and nuclear spins, we have so far a degenerate Hamiltonian. Thus we will choose a basis for the spin space that diagonalizes the hyperfine splitting. The eigenvalues of $\vec{S}_e \cdot \vec{S}_p$ are $\frac{\hbar^2}{4}$ with degeneracy 3 (the triplet states) and $-\frac{3}{4}\hbar^2$ (the singlet state). Thus we find that the hyperfine splitting is

$$\begin{aligned} \Delta E_{1,0,0}^{\text{HF}} &= E_{1,0,0,\text{triplet}}^1 - E_{1,0,0,\text{singlet}}^1 \\ &= \frac{2}{3} g_e g_p \frac{m_e}{m_p} \alpha^4 m_e c^2 = 5.9 \cdot 10^{-6} \text{eV} \end{aligned}$$

The wavelength $\lambda = \frac{hc}{\Delta E}$ is 21cm, and radiation at this wavelength plays a central role in radio astronomy.

2.3 Zeeman effect

We have so far considered internal magnetic fields, but what happens when we apply an *external* magnetic field? Then the contribution to energy from the interaction of this field with the electron orbital angular momentum and spin angular momentum is

$$\begin{aligned} \delta H_{\text{Zeeman}} &= -\left(\underbrace{\vec{\mu}_L}_{-\mu_B \frac{\vec{L}}{\hbar}} + \underbrace{\vec{\mu}_S}_{-2\mu_B \frac{\vec{S}}{\hbar}} \right) \cdot \underbrace{\vec{B}_{\text{ext}}}_{(0,0,B)} \\ &= \frac{\mu_B B}{\hbar} (L_z + 2S_z) \\ &= \frac{eB}{2mc} (L_z + 2S_z) \quad \text{using } \mu_B = \frac{\hbar e}{2mc} \end{aligned}$$

Because \vec{L} and \vec{S} are multiplied by different g-factors (1 and ≈ 2 respectively), we do *not* simply end up with something that depends on \vec{J} . As a result, the states $|n, l, j, m_j\rangle$ that were good for the fine structure do not diagonalize δH_{Zeeman} . One basis that would diagonalize the Zeeman Hamiltonian is $|n, l, m_l, m_s\rangle$. However, if we use this, then the fine structure is no longer diagonal! This is a fundamental problem: δH_{FS} and δH_{Zeeman} do not commute, and thus there is no basis that simultaneously diagonalizes them.

To solve this problem we will use perturbation theory. But which Hamiltonian is the base Hamiltonian and which is the perturbation will depend on how strong the magnetic field is.

2.3.1 Strong-field Zeeman

If $E_{\text{Zeeman}} \gg E_{\text{FS}}$ then we treat $H_0 + \delta H_{\text{Zeeman}}$ as the base Hamiltonian, use the $|n, l, m_l, m_s\rangle$ basis and treat δH_{FS} as the perturbation. In this case the energy is

$$E_{n,l,m_l,m_s} = \underbrace{E_n^0}_{-\frac{\alpha^2 m_e c^2}{2n^2}} + \mu_B B(m_l + 2m_s) + E_{\text{FS}}^1 + \dots \quad (26)$$

To compute the fine-structure contribution we need to evaluate things like $\langle \vec{L} \cdot \vec{S} \rangle$ and $\langle p^4 \rangle$ with respect to the states $|n, l, m_l, m_s\rangle$. We will not fully carry out this calculation. One example is the spin-orbit coupling which is proportional to

$$\langle \vec{L} \cdot \vec{S} \rangle = \langle L_x \rangle \langle S_x \rangle + \langle L_y \rangle \langle S_y \rangle + \langle L_z \rangle \langle S_z \rangle = \langle L_z \rangle \langle S_z \rangle = \hbar^2 m_l m_s.$$

Here we have used the fact that if a state $|\psi\rangle$ satisfies $J_z|\psi\rangle = \lambda|\psi\rangle$ (for any operators J_x, J_y, J_z with the appropriate commutation relations for angular momentum) then

$$\langle \psi | J_x | \psi \rangle = \langle \psi | \frac{J_y J_z - J_z J_y}{i\hbar} | \psi \rangle = \langle \psi | \frac{J_y \lambda - \lambda J_y}{i\hbar} | \psi \rangle = 0$$

and similarly $\langle \psi | J_x | \psi \rangle = 0$.

After some (omitted) calculations we arrive at

$$E_{n,l,m_l,m_s}^{\text{FS}} = \begin{cases} \frac{\alpha^4 m_e c^2}{2n^3} \left(\frac{3}{4n} - 1 \right) & \text{if } l = 0 \\ \frac{\alpha^4 m_e c^2}{2n^3} \left(\frac{3}{4n} - \frac{l(l+1) - m_l m_s}{l(l+1/2)(l+1)} \right) & \text{otherwise} \end{cases} \quad (27)$$

The field strength needed for this is not unreasonable. Since the fine-structure splitting between $j = 1/2$ and $j = 3/2$ is $5.7 \cdot 10^{-5} \text{eV}$ and $\mu_B = 5.8 \cdot 10^{-5} \text{eV/T}$, we need a field of about one Tesla, which is large but achievable. This strong-field case is sometimes called the Paschen-Back effect.

2.3.2 Weak-field Zeeman effect

Now we write

$$H = \underbrace{H_0 + \delta H_{\text{FS}}}_{H_0^{\text{Zee}}} + \delta H_{\text{Zee}}. \quad (28)$$

As we've seen before, the eigenbasis of H_0^{Zee} is $|n, l, j, m_j\rangle$, so the first-order energy shift when we add a magnetic field is

$$\begin{aligned} E_{n,l,j,m_j}^{\text{Zee}} &= \frac{\mu_B B}{\hbar} \langle n, l, j, m_j | L_z + 2S_z | n, l, j, m_j \rangle \\ &= \frac{\mu_B B}{\hbar} \langle n, l, j, m_j | J_z + S_z | n, l, j, m_j \rangle \\ &= \mu_B B m_j + \frac{\mu_B B}{\hbar} \langle n, l, j, m_j | S_z | n, l, j, m_j \rangle \end{aligned}$$

How do we evaluate this \vec{S}_z term? One method is described in Griffiths, and involves an argument about the Heisenberg-picture time average of \vec{S} under the fine-structure Hamiltonian. A more direct method is to use Clebsch-Gordan coefficients. Indeed

$$|j = l \pm \frac{1}{2}, m_j\rangle = \pm \sqrt{\frac{l \pm m_j + \frac{1}{2}}{2l+1}} |m_l = m_j - \frac{1}{2}, m_s = \frac{1}{2}\rangle + \sqrt{\frac{l \mp m_j + \frac{1}{2}}{2l+1}} |m_l = m_j + \frac{1}{2}, m_s = -\frac{1}{2}\rangle \quad (29)$$

so if $\text{Pr}[\pm]$ denotes the probability of obtaining outcome $\pm\hbar/2$ when measuring the spin, then we have

$$\begin{aligned} \langle S_z \rangle &= \frac{\hbar}{2} (\text{Pr}[+] - \text{Pr}[-]) \\ &= \frac{\hbar}{2} \frac{1}{2l+1} \left(\left(l \pm m_j + \frac{1}{2} \right) - \left(l \mp m_j + \frac{1}{2} \right) \right) \\ &= \pm \frac{\hbar m_j}{2l+1} \end{aligned}$$

We conclude that

$$E_{n,l,j,m_j}^{\text{Zee}} = \frac{e\hbar B}{2m_e c} m_j \underbrace{\left(1 \pm \frac{1}{2l+1} \right)}_{g_J}.$$

The term in braces is called the Landé g -factor, after Alfred Landé, who discovered it in 1921. We see throughout the spectrum of the hydrogen atom many of the precursors of modern quantum theory.

3 WKB

3.1 Introduction to WKB

Perturbation theory covers the case when δH_{mn} is small relative to $|E_m^0 - E_n^0|$. The Wentzel-Kramers-Brillouin (WKB) approximation covers a different limit, when quantum systems are in some ways approximately classical. For this reason, it is an example of a *semi-classical* approximation. It will result in powers not of δH but of \hbar , and thus becomes exact in the “classical” limit $\hbar \rightarrow 0$.

We begin with some exact manipulations of the Schrödinger equation. For a spin-0 mass- m particle in 3-d, define

$$\begin{aligned} \rho(\vec{x}, t) &= |\psi(\vec{x}, t)|^2 && \text{probability density} \\ \vec{J}(\vec{x}, t) &= \frac{\hbar}{m} \text{Im}(\psi^* \vec{\nabla} \psi) && \text{probability flux} \end{aligned}$$

The flux \vec{J} has units of probability / area x time and can be seen to be related to momentum as follows:

$$\begin{aligned} \vec{J}(\vec{x}, t) &= \frac{\hbar}{m} \text{Im} \left(\psi^* \frac{i}{\hbar} \vec{p} \psi \right) \\ &= \frac{1}{m} \text{Re} (\psi^* \vec{p} \psi) \end{aligned}$$

Thus, if we integrate over all \vec{x} , we obtain

$$\int d^3x \vec{J} = \int d^3x \frac{1}{m} \text{Re} (\psi^* \vec{p} \psi) = \text{Re} \frac{\langle \vec{p} \rangle_t}{m} = \frac{\langle \vec{p} \rangle_t}{m}.$$

One can show (using the Schrödinger equation) the *conservation equation*

$$\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0}. \quad (30)$$

We can also re-express the wavefunction using ρ as

$$\boxed{\psi(\vec{x}, t) = \sqrt{\rho(\vec{x}, t)} e^{i \frac{S(\vec{x}, t)}{\hbar}} \quad (31)$$

with $S(\vec{x}, t)$ *real* so that the exponent contributes a pure phase. What does it mean physically? In terms of ρ, S we can compute

$$\begin{aligned} \vec{\nabla} \psi &= \frac{1}{2} \frac{\vec{\nabla} \rho}{\sqrt{\rho}} e^{iS/\hbar} + i \frac{\vec{\nabla} S}{\hbar} \psi \\ \psi^* \vec{\nabla} \psi &= \underbrace{\frac{1}{2} \vec{\nabla} \rho}_{\text{real}} + \underbrace{\frac{i}{\hbar} \rho \vec{\nabla} S}_{\text{imaginary}} \\ \vec{J}(\vec{x}, t) &= \frac{\hbar}{m} \text{Im}(\psi^* \vec{\nabla} \psi) = \frac{\hbar}{m} \frac{\rho}{\hbar} \vec{\nabla} S \end{aligned}$$

Thus we obtain a physical interpretation for the phase.

$$\vec{J}(\vec{x}, t) = \rho \frac{\vec{\nabla} S}{m}. \quad (32)$$

Namely its gradient relates to the probability flux. If $\vec{J} = \rho \vec{v}$ then $\vec{\nabla} S \approx \vec{p}$. These equivalences are pretty loose, but we will build on this intuition as we proceed. For now, observe that for a free particle, they indeed give the right idea:

$$\psi_{\text{free}}(\vec{x}, t) \sim e^{-\frac{i\vec{p} \cdot \vec{x}}{\hbar} - \frac{iEt}{\hbar}}.$$

So $S = \vec{p} \cdot \vec{x} - Et$ and we have $\vec{\nabla} S = \vec{p}$ exactly. We also have $\vec{\nabla}^2 S = 0$, and it will turn out later that this quantity will measure how “non-plane-wave-like” our wavefunction is.

Schrödinger equation for a general 1-D potential Consider a region where $V(x) \leq E$ (called “classically allowed”). Then

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} &= (E - V(x)) \psi(x) \\ -\hbar^2 \frac{d^2 \psi}{dx^2} &= \underbrace{2m(E - V(x))}_{p^2(x)} \psi(x) \end{aligned}$$

We can interpret $p(x)$ as a classical momentum. The solution of this corresponds (roughly) to oscillations with period $\lambda(x) \equiv \frac{2\pi\hbar}{p(x)}$, which is the De Broglie wavelength corresponding to momentum $p(x)$.

What if $V(x) > E$? These are called “classically forbidden.” Then we get

$$\hbar^2 \frac{d^2 \psi}{dx^2} = \underbrace{2m(V(x) - E)}_{\kappa^2(x)} \psi(x)$$

corresponding to solutions that exponentially decay at rate $\kappa(x)$.

The claims of “oscillating with period $\lambda(x)$ ” or “decaying at rate $\kappa(x)$ ” are only rigorous when $p(x)$ or $\kappa(x)$ are independent of x . But we will see how they can be good approximations even when $p(x)$ or $\kappa(x)$ are merely slowly varying with x .

Let’s write $\psi(x) = \exp(iS(x)/\hbar)$, for some S with units of angular momentum. Since S can be complex, this is without loss of generality.

Substituting (in the classically allowed region) we get

$$\begin{aligned} p^2(x)e^{\frac{iS(x)}{\hbar}} &= -\hbar^2 \frac{d^2}{dx^2} e^{\frac{iS(x)}{\hbar}} \\ &= -\hbar^2 \frac{d}{dx} \left(i \frac{S'(x)}{\hbar} e^{\frac{iS(x)}{\hbar}} \right) \\ &= -\hbar^2 \left(i \frac{S''(x)}{\hbar} - \frac{(S'(x))^2}{\hbar^2} \right) e^{\frac{iS(x)}{\hbar}} \end{aligned}$$

The $e^{\frac{iS(x)}{\hbar}}$ terms drop out and we obtain

$$\boxed{(S')^2 - i\hbar S'' = p^2(x)} \quad (33)$$

So far this is exact. But if the potential is slowly varying, then $p(x)$ is slowly varying, and the $-i\hbar S''$ term will be small. What does “slowly varying” mean? The wavelength $\lambda(x) = \frac{2\pi\hbar}{p(x)}$ should be small relative to the variation of $p(x)$. In the classical limit $\hbar \rightarrow 0$ we have $\lambda(x) \rightarrow 0$. Thus it makes sense to expand around this limit in powers of \hbar , in a way analogous to our perturbation-theory strategy of expanding in terms of the perturbation. Thus we write

$$S(x) = \underbrace{S_0(x) + \hbar S_1(x)}_{\text{WKB approximation}} + \hbar^2 S_2(x) + \dots$$

and will take only the first two terms to be the WKB approximation.

Let us now substitute $S(x) = S_0(x) + \hbar S_1(x)$ into (33). We obtain

$$\begin{aligned} (S'_0 + \hbar S'_1)^2 - i\hbar S''_0 - i\hbar^2 S''_1 &= p^2(x) \\ (S'_0)^2 + 2\hbar S'_0 S'_1 - i\hbar S''_0 + \hbar^2 ((S'_1)^2 - iS''_1) &= p^2(x) \end{aligned}$$

We want to equate powers of \hbar . Treat \hbar here as a former parameter, and we obtain

$$(S'_0)^2 = p^2(x) \quad \text{at } O(\hbar^0) \quad (34a)$$

$$2S'_0 S'_1 - iS''_0 = 0 \quad \text{at } O(\hbar^1) \quad (34b)$$

From (34a), we obtain $S'_0 = \pm p(x)$, which we can solve to obtain

$$S_0(x) = \pm \int_{x_0}^x p(x') dx',$$

where x_0 is arbitrary. Substituting $S'_0 = \pm p(x)$, $S''_0 = \pm p'(x)$ into (34b) we find

$$S'_1 = \frac{i}{2} \frac{p'(x)}{p(x)} = \frac{i}{2} \frac{d}{dx} \ln p(x).$$

This has solution

$$\boxed{S_1(x) = \frac{i}{2} \ln p(x) + C} \quad (35)$$

Substituting into our equation for $\psi(x)$ we get

$$\psi(x) = e^{iS(x)/\hbar} \approx e^{\frac{i}{\hbar}(S_0 + \hbar S_1)} = \exp\left(\pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right) \exp\left(-\frac{1}{2} \ln p(x) + C\right)$$

Thus in the classically allowed regions we have the solution

$$\boxed{\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right) + \frac{B}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right)} \quad (36)$$

with $p(x) = \sqrt{2m(V - E(x))}$. The solution in the classically forbidden regions is the same but with $p(x) = i\kappa(x)$. This corresponds to

$$\boxed{\psi(x) = \frac{C}{\sqrt{\kappa(x)}} \exp\left(\frac{1}{\hbar} \int_{x_0}^x \kappa(x') dx'\right) + \frac{D}{\sqrt{\kappa(x)}} \exp\left(-\frac{1}{\hbar} \int_{x_0}^x \kappa(x') dx'\right)} \quad (37)$$

3.2 Validity of WKB

Let's just look at the first part of the classically allowed solution: $\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right)$.

The probability density $\rho(x) = |\psi(x)|^2 = \frac{|A|^2}{p(x)} = \frac{|A|^2}{mv(x)}$, where $v(x)$ can be thought of as a classical velocity. This makes sense because it says that the particle spends less time in regions where it is moving faster.

Another check is to look at the probability current: $J = \frac{\hbar}{m} \text{Im}(\psi^* \frac{\partial}{\partial x} \psi)$. We calculate

$$\begin{aligned} \psi' &= -\frac{1}{2} \frac{p'(x)}{p(x)} \psi + \frac{i}{\hbar} p(x) \psi \\ \psi^* \psi' &= -\frac{1}{2} \frac{p'(x)}{p(x)} |\psi|^2 + i \frac{p(x)}{\hbar} |\psi|^2 \\ J &= \frac{\hbar}{m} \frac{p(x)}{\hbar} \rho = \rho \frac{p(x)}{m} = \rho v(x). \end{aligned}$$

Next, let's look at the first discarded term. Our approximation assumed that $|\hbar^2 (S'_1)^2| \ll |\hbar S'_0 S'_1|$, or equivalently, $|\hbar S'_1| \ll |S'_0|$. In terms of $p(x)$ this condition states that

$$\left| \hbar \frac{p'}{p} \right| \ll |p| \iff 1 \gg \left| \hbar \frac{p'}{p^2} \right| = \left| \partial_x \frac{\hbar}{p} \right| = |\partial_x \lambda(x)|. \quad (38)$$

In other words, the de Broglie wavelength should be slowly varying. How slowly? Return to $1 \gg \left| \hbar \frac{p'}{p^2} \right|$. Rearranging, we obtain

$$|p| \gg \frac{\hbar}{|p|} |p'| = \lambda(x) \left| \frac{dp}{dx} \right|.$$

In other words, the change of p over a de Broglie wavelength should be $\ll |p|$.

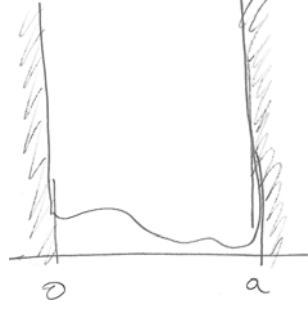


Figure 1: Example of a potential $V(x)$ that is finite only in the interval $0 < x < a$.

We can relate this back to the potential energy.

$$\begin{aligned}
 p^2 &= 2m(E - V) \\
 |2pp'| &= 2m|V'| \\
 \hbar|p'| &= m \frac{\hbar}{p} |V'| = m\lambda(x)|V'| \\
 \hbar|p'| &\ll |p|^2 && \text{from (38)} \\
 m\lambda(x)|V'| &\ll |p|^2 \\
 \lambda(x)|V'| &\ll \frac{|p|^2}{m}
 \end{aligned}$$

The change of potential energy over one wavelength should be \ll the kinetic energy.

3.3 Bohr-Sommerfeld quantization

The WKB approximation can be used to generalize the old idea that quantum “orbits” should have action (integral of $p dx$) that is an integer multiple of $h = 2\pi\hbar$. This idea is part of what is called “old quantum mechanics” because it predates the modern (ca. 1925) formulation in terms of the Schrödinger equation.

We illustrate this with an example. Consider a potential $V(x)$ such that $V(x) = \infty$ for $x \leq 0$ or $x \geq a$ and $V(x)$ is finite for $0 < x < a$. This is depicted in Fig. 1.

Assume that $E > V(x)$ for all $0 < x < a$. Then the solution has the form

$$\begin{aligned}
 \psi(x) &= \frac{1}{\sqrt{p(x)}} \left(A \exp \left(\frac{i}{\hbar} \int_0^x p(x') dx' \right) + B \exp \left(-\frac{i}{\hbar} \int_0^x p(x') dx' \right) \right) \\
 &= \frac{1}{\sqrt{p(x)}} \left(A e^{i\phi(x)} + B e^{-i\phi(x)} \right) && \phi(x) = \frac{1}{\hbar} \int_0^x p(x') dx' \\
 &= \frac{1}{\sqrt{p(x)}} (C \cos(\phi(x)) + D \sin(\phi(x)))
 \end{aligned}$$

From the boundary condition $\psi(0) = 0$ and the fact that $\phi(0) = 0$ we obtain $C = 0$. From the condition $\psi(a) = 0$ we find that $\phi(a) = n\pi$. Plugging in the definition of $\phi(x)$ we find the quantization condition:

$$\frac{1}{\hbar} \int_0^a dx \sqrt{2m(E_n - V(x))} = n\pi, \tag{39}$$

where we have defined E_n to be the n^{th} energy level.

As a sanity check, if $V(x) = 0$ then (39) yields

$$\frac{1}{\hbar} a \sqrt{2mE_n} = n\pi \quad \Rightarrow \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}. \quad (40)$$

What if we have “soft” walls? For this we need to connect the oscillating solutions in the allowed regions with the decaying solutions in the forbidden regions. This is achieved by the connection formulae.

To see the need for this, let’s examine the integral of $p(x)$ over the classically allowed region of a harmonic oscillator.

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2.$$

The energy levels are of course $E_n = \hbar \omega (n + 1/2)$. The turning points are given by solution to the equation $\frac{1}{2} m \omega^2 x^2 = \hbar \omega (n + 1/2)$. These are

$$x = \pm l \sqrt{2n+1} \quad l \equiv \sqrt{\frac{\hbar}{m\omega}}. \quad (41)$$

Let’s see what happens when we integrate $p(x)/\hbar$ between these turning points. We obtain

$$\begin{aligned} \frac{1}{\hbar} \int_{-l\sqrt{2n+1}}^{l\sqrt{2n+1}} p(x) dx &= \frac{1}{\hbar} \int_{-l\sqrt{2n+1}}^{l\sqrt{2n+1}} \sqrt{2m(\hbar\omega(n+1/2) - \frac{1}{2} m \omega^2 x^2)} dx \\ &= \int_{-l\sqrt{2n+1}}^{l\sqrt{2n+1}} \frac{1}{l} \sqrt{2n+1 - \frac{x^2}{l^2}} dx \\ &= (2n+1) \int_{-1}^1 \sqrt{1-u^2} du \quad \text{defining } u \equiv l\sqrt{2n+1} \\ &= \pi(n+1/2). \end{aligned}$$

There is an extra factor of $\pi/2$ relative to what happens with hard walls. We will see below why this is.

Before continuing, we can see that the WKB approximation does give a pretty accurate picture of the harmonic oscillator. In the forbidden region ($|x| > l$) they describe the wavefunction as exponentially decaying. Specifically suppose that $|x| \gg l$ so that $\kappa(x) = \sqrt{2m(V(x) - E_n)} \approx \sqrt{2mV(x)} = m\omega|x|$. Integrating this we get

$$\psi(x) \propto \exp\left(-\frac{m\omega}{\hbar} \frac{x^2}{2}\right) = e^{-\frac{x^2}{2l^2}}, \quad (42)$$

which gives the correct rate of exponential decay.

In the classically allowed region WKB also correctly predicts the number of oscillations of the wavefunction. But how can WKB predict the $\pi(n+1/2)$ result we found above?

3.4 Connection formulae

When $E = V(a)$ then we say that a is a “turning point”. Turning points separate allowed from forbidden regions, and therefore oscillating from decaying solutions. However, near a turning point, the WKB approximation breaks down. So if we want to glue together oscillating and decaying solutions, we cannot just match boundary conditions at the border. Something nontrivial will happen at the turning point, which could involve reflection/transmission as well as phase shifts.

There are two approaches to this, both difficult. One that we will not explore is to use complex analysis and analytically continue the wavefunction to complex-valued x . In this way we can avoid going near a : x goes up to $a - \epsilon$ along the real line, then follows a half-circle in the complex plane to $a + \epsilon$ and then continues along the real line.

Instead we will follow Griffiths and use Airy functions. Near a turning point, we can approximate $V(x) = V(a) + (a - x)V'(a) + \dots$. To simplify notation shift the origin and the overall energy level so that $a = 0$ and $E = V(0) = 0$. In the vicinity of the turning point, the Schrödinger equation looks like

$$-\frac{\hbar^2}{2m}\psi''(x) + xV'(0)\psi(x) = 0 \quad (43)$$

$$\psi''(x) = \underbrace{\frac{2mV'(0)}{\hbar^2}}_{\alpha^3} x\psi(x). \quad (44)$$

We define α in this way so that when we change coordinates to $z = \alpha x$ then z is dimensionless and we obtain the dimensionless equation

$$\psi''(z) = z\psi(z). \quad (45)$$

This is a second-order differential equation and thus has a two-dimensional space of solutions. These are called the Airy function $Ai(z)$ and the Airy function of the second kind $Bi(z)$. There are exact expressions for these that are somewhat unilluminating (see Griffiths or wikipedia for details), but what will be more useful are the asymptotic formulas. These are oscillatory for $z < 0$ and exponentially decaying or growing for $z > 0$. Specifically:

	$Ai(z)$	$Bi(z)$
$z \ll 0$	$\frac{1}{\sqrt{\pi(-z)^{1/4}}} \sin\left(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right)$	$\frac{1}{\sqrt{\pi(-z)^{1/4}}} \cos\left(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right)$
$z \gg 0$	$\frac{e^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi z^{1/4}}}$	$\frac{e^{\frac{2}{3}z^{3/2}}}{\sqrt{\pi z^{1/4}}}$

We can then match up the Airy function near the turning point with the decaying and oscillating solutions that are valid far from the turning point. This yield connection formulas. The high-level picture is that in the classically allowed region we have two oscillating solutions, near the turning point we have two Airy functions as solutions and in the forbidden region we have two exponentially decaying/growing solutions. At each boundary we have two constraints given by continuity of $\psi(x)$ and $\psi'(x)$. These give the following connection formulae:

Allowed on the left, forbidden on the right Consider the turning point depicted in Fig. 2(a).

Then we find

$$\frac{2A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_x^a p(x') dx' + \frac{\pi}{4}\right) + \frac{B}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_x^a p(x') dx' + \frac{\pi}{4}\right) \quad x \ll a \quad (46a)$$

$$\iff \frac{A}{\sqrt{\kappa(x)}} \exp\left(-\frac{1}{\hbar} \int_a^x \kappa(x') dx'\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\frac{1}{\hbar} \int_a^x \kappa(x') dx'\right) \quad x \gg a \quad (46b)$$

A few words of caution. If $B \neq 0$ then in the $x \gg a$ we might be tempted to neglect the A term. But this will give a bad error in the $x \ll a$ region.

Conversely if $|B| \ll |A|$, then we have to be careful about neglecting it in the $x \gg a$ region because it can become dominant for large x .

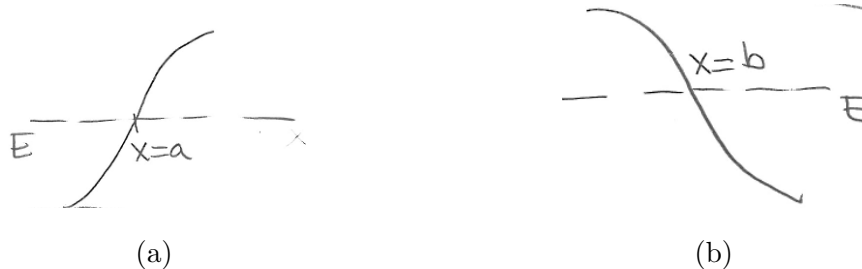


Figure 2: Turning points. In (a) the classically allowed region is on the left and the classically forbidden region is on the right. In (b) the classically allowed region is on the right and the classically forbidden region is on the left.

Allowed on the right, forbidden on the left Suppose the turning point is at $x = b$, as depicted in Fig. 2(b). Now the connection formula is

$$\frac{A}{\sqrt{\kappa(x)}} \exp\left(-\frac{1}{\hbar} \int_x^b \kappa(x') dx'\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\frac{1}{\hbar} \int_x^b \kappa(x') dx'\right) \quad x \ll b \quad (47a)$$

$$\Longleftrightarrow \frac{2A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_b^x p(x') dx' + \frac{\pi}{4}\right) + \frac{B}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar} \int_b^x p(x') dx' + \frac{\pi}{4}\right) \quad x \gg b \quad (47b)$$

Application to harmonic oscillator Applying these to the harmonic oscillator predicts that (calculation omitted - see Griffiths)

$$\int_{-x_0}^{x_0} p(x) dx = (n - 1/2)\pi,$$

where $\pm x_0$ are the turning points. Here we take $n = 1, 2, 3, \dots$, which is why it matches what we observed above (where $n = 0, 1, 2, \dots$ is from the conventional way to label the harmonic oscillator energy levels). To summarize, the Bohr-Sommerfeld quantization condition for $\frac{1}{\hbar} \int_a^b p(x) dx$ (where

	two hard walls	$n\pi$
$[a, b]$ is the classically allowed region)	one hard wall, one soft wall	$(n - 1/4)\pi$
	two soft walls	$(n - 1/2)\pi$

3.5 Tunneling

We can also use WKB to estimate the rate at which a particle will “tunnel” through a classically forbidden region, as depicted in Fig. 3(a). This is useful for modeling phenomena such as radioactive decay.

The transmission probability is

$$T = \frac{|F|^2}{|A|^2} \approx \exp\left[-\frac{2}{\hbar} \int_b^c \kappa(x) dx\right].$$

This approximation is valid if the barrier is broad and high.

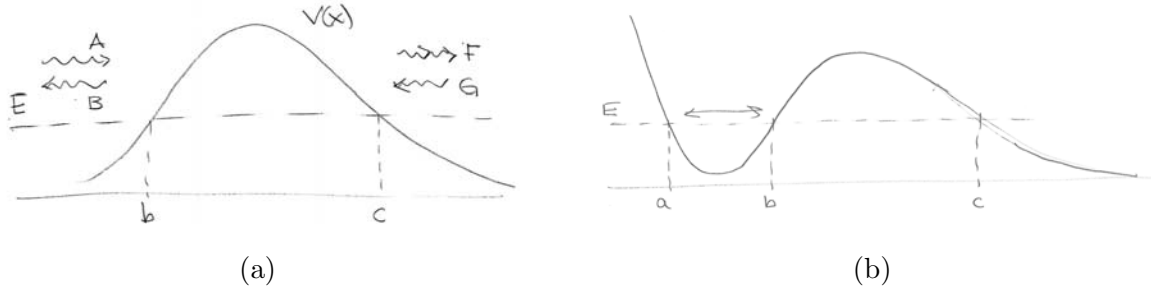


Figure 3: (a) Tunneling through a classically forbidden region. (b) A particle localized in the region $a < x < b$ will eventually tunnel into the region $x > c$.

How do we get a lifetime from this? Suppose that the particle is localized in the region $a < x < b$ in Fig. 3(b). Then we can approximate

$$\text{lifetime} = \frac{1}{\text{tunnel prob per unit time}} \simeq \frac{1}{T \cdot \# \text{ hits per unit time}} = \frac{1}{T \frac{1}{\tau}} = \frac{\tau}{T}$$

where τ is the period of oscillation within the region $a < x < b$. This can be approximated by

$$\tau = 2 \int_a^b \frac{dx}{v(x)} = 2 \int_a^b m \frac{dx}{p(x)}.$$

Putting this together we can approximate the lifetime as

$$\text{lifetime} \approx 2 \int_a^b m \frac{dx}{p(x)} \cdot \exp \left[\frac{2}{\hbar} \int_b^c \kappa(x) dx \right].$$

The fact that lifetime scales exponentially with barrier height explains the vast differences we see in alpha decay. The halflife at which ^{238}U decays to ^{234}Th is 4.5 billion years while the halflife for the decay of ^{214}Po to ^{210}Pb is 0.164ms; see Fig. 4 for the full decay chain. This difference is due to the difference in barrier height relative to the energy of the ejected alpha particle.

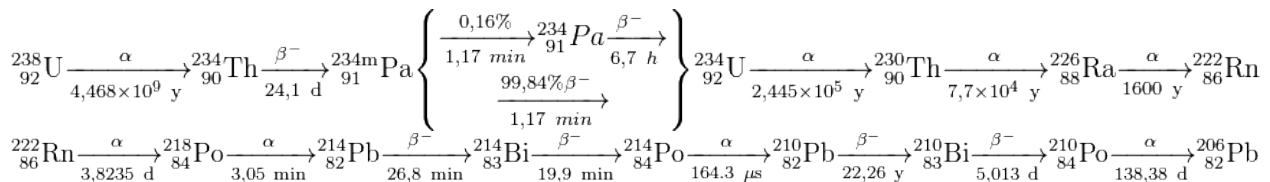


Figure 4: Decay chain of ^{238}U . From wikipedia article on Uranium-238.

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8.06 Quantum Physics III
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8.06 Spring 2016 Lecture Notes

2. Time-dependent approximation methods

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Last updated: March 12, 2016

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1 Time-dependent perturbation theory

Perturbation theory can also be used to analyze the case when we have a large static Hamiltonian H_0 and a small, possibly time-dependent, perturbation $\delta H(t)$. In other words

$$H(t) = H_0 + \delta H(t). \quad (1)$$

However, the more important difference from time-independent perturbation theory is in our *goals*: we will seek to analyze the dynamics of the wavefunction (i.e. find $|\psi(t)\rangle$ as a function of t) rather than computing the spectrum of H . In fact, when we use a basis, we will work in the eigenbasis of H_0 . For example, one common situation that we will analyze is that we start in an eigenstate of H_0 , temporarily turn on a perturbation $\delta H(t)$ and then measure in the eigenbasis of H_0 . This is a bit abstract, so here is a more concrete version of the example. H_0 is the natural Hamiltonian of

the hydrogen atom and $\delta H(t)$ comes from electric and/or magnetic fields that we temporarily turn on. If we start in the $1s$ state, then what is the probability that after some time we will be in the $2p$ state? (Note that the very definition of the states depends on H_0 and not the perturbation.) Time-dependent perturbation theory will equip us to answer these questions.

1.1 Rotating frame

We want to solve the time-dependent Schrödinger equation $i\hbar\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle$. We will assume that the dynamics of H_0 are simple to compute and that the computational difficulty comes from $\delta H(t)$. At the same time, if H_0 is much larger than $\delta H(t)$ then most of the change in the state will come from H_0 . In classical dynamics when an object is undergoing two different types of motion, it is often useful to perform a change of coordinates to eliminate one of them. We will do the same thing here. Define the state

$$|\tilde{\psi}(t)\rangle = e^{\frac{iH_0 t}{\hbar}}|\psi(t)\rangle. \quad (2)$$

We say that $|\tilde{\psi}(t)\rangle$ is in the *rotating frame* or alternatively the *interaction picture*. Multiplying by $e^{\frac{iH_0 t}{\hbar}}$ cancels out the natural time evolution of H_0 . In particular, if $\delta H(t) = 0$ then we would have $|\tilde{\psi}(t)\rangle = |\tilde{\psi}(0)\rangle = |\psi(0)\rangle$. Thus, any change in $|\tilde{\psi}(t)\rangle$ must come from $\delta H(t)$.

Aside: comparison to Schrödinger and Heisenberg pictures. In 8.05 we saw the Schrödinger picture and the Heisenberg picture. In the former, states evolve according to H and operators remain the same; in the latter, states stay the same and operators evolve according to H . The interaction picture can be thought of as intermediate between these two. We pick a frame rotating with H_0 , which means that the operators evolve according to H_0 and the states evolve with the remaining piece of the Hamiltonian, namely δH . As we will see below, to calculate this evolution correctly we need δH to rotate with H_0 , just like all other operators. This is a little vague but below we will perform an exact calculation to demonstrate what happens.

Now let's compute the time evolution of $|\tilde{\psi}(t)\rangle$.

$$\begin{aligned} i\hbar \frac{d}{dt}|\tilde{\psi}(t)\rangle &= i\hbar \frac{d}{dt} \left(e^{\frac{iH_0 t}{\hbar}} |\psi(t)\rangle \right) \\ &= -H_0 e^{\frac{iH_0 t}{\hbar}} |\psi(t)\rangle + e^{\frac{iH_0 t}{\hbar}} (H_0 + \delta H(t)) |\psi(t)\rangle \\ &= e^{\frac{iH_0 t}{\hbar}} \delta H(t) |\psi(t)\rangle && \text{since } H_0 \text{ and } e^{\frac{iH_0 t}{\hbar}} \text{ commute} \\ &= \underbrace{e^{\frac{iH_0 t}{\hbar}} \delta H(t) e^{-\frac{iH_0 t}{\hbar}}}_{\widetilde{\delta H}(t)} |\tilde{\psi}(t)\rangle \end{aligned}$$

Thus we obtain an effective Schrödinger equation in the rotating frame

$$\boxed{i\hbar \frac{d}{dt}|\tilde{\psi}(t)\rangle = \widetilde{\delta H}(t)|\tilde{\psi}(t)\rangle} \quad (3)$$

where we have defined

$$\widetilde{\delta H}(t) = e^{\frac{iH_0 t}{\hbar}} \delta H(t) e^{-\frac{iH_0 t}{\hbar}}.$$

This has a simple interpretation as a matrix. Suppose that the eigenvalues and eigenvectors of H_0 (reminder: we work with the eigenbasis of H_0 and *not* $H(t)$) are given by

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

Define $\delta H_{mn}(t) = \langle m | \delta H(t) | n \rangle$. Then

$$\widetilde{\delta H}_{mn}(t) = \langle m | e^{\frac{iH_0 t}{\hbar}} \delta H(t) e^{-\frac{iH_0 t}{\hbar}} | n \rangle = e^{\frac{i(E_m - E_n)t}{\hbar}} \delta H_{mn}(t) \equiv e^{i\omega_{mn}t} \delta H_{mn},$$

where we have defined $\omega_{mn} = \frac{E_m - E_n}{\hbar}$. If we define $c_n(t)$ according to

$$|\tilde{\psi}(t)\rangle = \sum_n c_n(t) |n\rangle \quad \implies \quad |\psi(t)\rangle = \sum_n e^{-\frac{iE_n t}{\hbar}} c_n(t) |n\rangle$$

then we obtain the following coupled differential equations for the $\{c_n\}$.

$$i\hbar \dot{c}_m(t) = \sum_n \widetilde{\delta H}_{mn}(t) c_n(t) = \sum_n e^{i\omega_{mn}t} \delta H_{mn} c_n(t).$$

1.2 Perturbation expansion

So far everything has been exact, although sometimes this is already enough to solve interesting problems. But often we will need approximate solutions. So assume that $\delta H(t) = O(\lambda)$ and expand the wavefunction in powers of λ , i.e.

$$\begin{aligned} c_m(t) &= c_m^{(0)}(t) + c_m^{(1)}(t) + c_m^{(2)}(t) + \dots \\ &\quad O(1) \quad O(\lambda) \quad O(\lambda^2) \\ |\tilde{\psi}(t)\rangle &= |\tilde{\psi}^{(0)}(t)\rangle + |\tilde{\psi}^{(1)}(t)\rangle + |\tilde{\psi}^{(2)}(t)\rangle + \dots \end{aligned}$$

We can solve these order by order. Applying (3) we obtain

$$\underbrace{i\hbar \partial_t |\tilde{\psi}^{(0)}(t)\rangle}_{O(1)} + \underbrace{i\hbar \partial_t |\tilde{\psi}^{(1)}(t)\rangle}_{O(\lambda)} + \underbrace{i\hbar \partial_t |\tilde{\psi}^{(2)}(t)\rangle}_{O(\lambda^2)} + \dots = \underbrace{\widetilde{\delta H}(t) |\tilde{\psi}^{(0)}(t)\rangle}_{O(\lambda)} + \underbrace{\widetilde{\delta H}(t) |\tilde{\psi}^{(1)}(t)\rangle}_{O(\lambda^2)} + \dots \quad (4)$$

The solution is much simpler than in the time-dependent case. There is no zeroth order term on the RHS, so the zeroth order approximation is simply that nothing happens:

$$\boxed{|\tilde{\psi}^{(0)}(t)\rangle = |\tilde{\psi}^{(0)}(0)\rangle = |\psi(0)\rangle} \quad (5)$$

The first-order terms yield

$$i\hbar \partial_t |\tilde{\psi}^{(1)}(t)\rangle = \widetilde{\delta H}(t) |\tilde{\psi}^{(0)}(t)\rangle = \widetilde{\delta H}(t) |\psi(0)\rangle. \quad (6)$$

Integrating, we find

$$\boxed{|\tilde{\psi}^{(1)}(t)\rangle = \int_0^t dt' \frac{\widetilde{\delta H}(t')}{i\hbar} |\psi(0)\rangle.} \quad (7)$$

This leads to one very useful formula. If we start in state $|n\rangle$, turn on $H(t)$ for times $0 \leq t \leq T$ and then measure in the energy eigenbasis of H_0 , then we find that the probability of ending in state $|m\rangle$ is

$$P_{n \rightarrow m} = \left| \int_0^t dt' \frac{\delta H_{mn}(t') e^{i\omega_{mn}t'}}{i\hbar} \right|^2$$

We can also continue to higher orders. The second-order solution is

$$\boxed{|\tilde{\psi}^{(2)}(t)\rangle = \int_0^t dt' \int_0^{t'} dt'' \frac{\widetilde{\delta H}(t')}{i\hbar} \frac{\widetilde{\delta H}(t'')}{i\hbar} |\psi(0)\rangle.} \quad (8)$$

1.3 NMR

In some cases the rotating frame already helps us solve nontrivial problems *exactly* without going to perturbation theory. Suppose we have a single spin-1/2 particle in a magnetic field pointing in the \hat{z} direction. This field corresponds to a Hamiltonian

$$H_0 = \omega_0 S_z = \frac{\hbar}{2} \omega_0 \sigma_z.$$

If the particle is a proton (i.e. hydrogen nucleus) and the field is typical for NMR, then ω_0 might be around 500 MHz.

Static magnetic field Now let's add a perturbation consisting of a magnetic field in the \hat{x} direction. First we will consider the *static* perturbation

$$\delta H(t) = \Omega S_x,$$

where we will assume $\Omega \ll \omega_0$, e.g. Ω might be on the order of 20 KHz. (Why are we considering a time-independent Hamiltonian with time-dependent perturbation theory? Because really it is the time-dependence of the *state* and not the Hamiltonian that we are after.)

We can solve this problem exactly without using any tools of perturbation theory, but it will be instructive to compare the exact answer with the approximate one. The exact evolution is given by precession about the

$$\frac{\omega_0 \hat{z} + \Omega \hat{x}}{\sqrt{\omega_0^2 + \Omega^2}}$$

axis at an angular frequency of $\sqrt{\omega_0^2 + \Omega^2}$. If $\Omega \ll \omega_0$ then this is very close to precession around the \hat{z} axis.

Now let's look at this problem using first-order perturbation theory.

$$\begin{aligned} \widetilde{\delta H}(t) &= e^{i\frac{\omega_0 t}{2}\sigma_z} \Omega S_x e^{-i\frac{\omega_0 t}{2}\sigma_z} = \Omega (\cos(\omega_0 t) S_x - \sin(\omega_0 t) S_y) \\ |\tilde{\psi}^{(1)}(t)\rangle &= \int_0^t dt' \frac{\widetilde{\delta H}(t')}{i\hbar} |\psi(0)\rangle \\ &= \int_0^t dt' \frac{\Omega}{i\hbar} (\cos(\omega_0 t') S_x - \sin(\omega_0 t') S_y) |\psi(0)\rangle \\ &= \frac{1}{i\hbar} \frac{\Omega}{\omega_0} (\sin(\omega_0 t) S_x + (\cos(\omega_0 t) - 1) S_y) |\psi(0)\rangle \end{aligned}$$

We see that the total change is proportional to Ω/ω_0 , which is $\ll 1$. Since this is the difference between pure rotating around the \hat{z} axis, this is consistent with the exact answer we obtained.

The result of this calculation is that if we have a strong \hat{z} field, then adding a weak static \hat{x} field doesn't do very much. If we want to have a significant effect on the state, we will need to do something else. The rotating-frame picture suggests the answer: the perturbation should rotate along with the frame, so that in the rotating frame it appears to be static.

Rotating magnetic field Now suppose we apply the perturbation

$$\delta H(t) = \Omega (\cos(\omega_0 t) S_x + \sin(\omega_0 t) S_y).$$

We have already computed \tilde{S}_x above. In the rotating frame we have

$$\begin{aligned}\tilde{S}_x &= (\cos(\omega_0 t) S_x - \sin(\omega_0 t) S_y) \\ \tilde{S}_y &= (\cos(\omega_0 t) S_y + \sin(\omega_0 t) S_x)\end{aligned}$$

Thus

$$\widetilde{\delta H}(t) = \Omega S_x.$$

The rotating-frame solution is now very simple:

$$|\tilde{\psi}(t)\rangle = e^{-\frac{i\Omega t}{2}\sigma_x} |\psi(0)\rangle.$$

This can be easily translated back into the stationary frame to obtain

$$|\psi(t)\rangle = e^{-\frac{i\omega_0 t}{2}\sigma_z} e^{-\frac{i\Omega t}{2}\sigma_x} |\psi(0)\rangle.$$

1.4 Periodic perturbations

The NMR example suggests that transitions between eigenstates of H_0 happens most effectively when the perturbation rotates at the frequency ω_{mn} . We will show that this holds more generally in first-order perturbation theory. Suppose that

$$\delta H(t) = V \cos(\omega t),$$

for some time-independent operator V . If our system starts in state $|n\rangle$ then at time t we can calculate

$$\begin{aligned}c_m^{(1)}(t) &= \langle m | \tilde{\psi}^{(1)}(t) \rangle = \int_0^t dt' \frac{\widetilde{\delta H}_{mn}(t')}{i\hbar} \\ &= \int_0^t dt' \frac{\delta H_{mn}(t')}{i\hbar} e^{i\omega_{mn}t'} \\ &= \int_0^t dt' \frac{V_{mn}}{i\hbar} \cos(\omega t') e^{i\omega_{mn}t'} \\ &= \frac{V_{mn}}{2i\hbar} \int_0^t dt' \left(e^{i(\omega_{mn}+\omega)t'} + e^{i(\omega_{mn}-\omega)t'} \right) \\ &= \frac{V_{mn}}{2i\hbar} \left[\frac{e^{i(\omega_{mn}+\omega)t} - 1}{\omega_{mn} + \omega} + \frac{e^{i(\omega_{mn}-\omega)t} - 1}{\omega_{mn} - \omega} \right]\end{aligned}$$

The $\omega_{mn} \pm \omega$ terms in the denominator mean that we will get the largest contribution when $\omega \approx |\omega_{mn}|$. (A word about signs. By convention we have $\omega > 0$, but ω_{mn} is a difference of energies and so can have either sign.) For concreteness, let's suppose that $\omega \approx \omega_{mn}$; the $\omega \approx -\omega_{mn}$ case is similar. Then we have

$$c_m^{(1)}(t) \approx \frac{V_{mn}}{2i\hbar} \frac{e^{i(\omega_{mn}-\omega)t} - 1}{\omega_{mn} - \omega}.$$

If we now measure, then the probability of obtaining outcome m is

$$P_{n \rightarrow m}(t) \approx |c_m^{(1)}(t)|^2 = \frac{|V_{mn}|^2}{\hbar^2} \frac{\sin^2\left(\frac{(\omega_{mn}-\omega)t}{2}\right)}{(\omega_{mn} - \omega)^2} = \frac{|V_{mn}|^2}{\hbar^2} \frac{\sin^2\left(\frac{\alpha t}{2}\right)}{\alpha^2},$$

where we have defined the *detuning* $\alpha \equiv \omega_{mn} - \omega$. The t, α dependence is rather subtle, so we examine it separately. Define

$$f(t, \alpha) = \frac{\sin^2\left(\frac{\alpha t}{2}\right)}{\alpha^2} \quad (9)$$

For fixed α , $f(t, \alpha)$ is periodic in t .

It is more interesting to consider the case of fixed t , for which f has a sinc-like appearance (see Fig. 1).

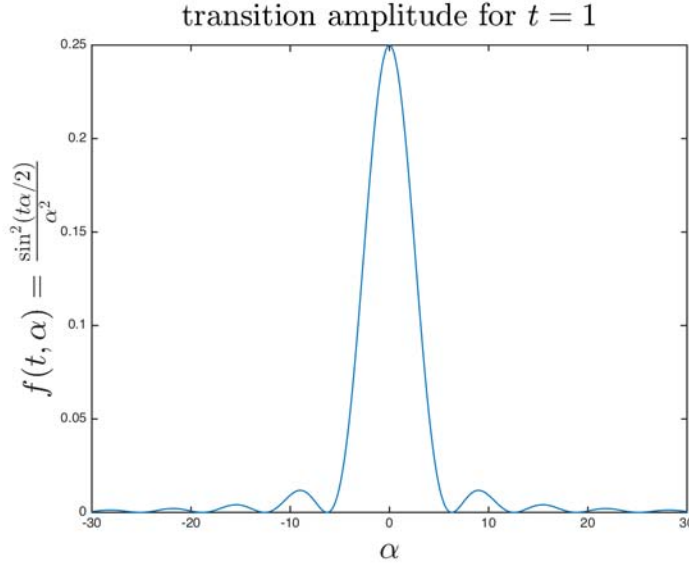


Figure 1: The function $f(\alpha, t)$ from (9), representing the amount of amplitude transferred at a fixed time t as we vary the detuning $\alpha \equiv \omega_{mn} - \omega$.

It has zeroes as $\alpha = \frac{2\pi}{t}n$ for integers $n \neq 0$. Since the closest zeros to the origin are at $\pm 2\pi/t$, we call the region $\alpha \in [-2\pi/t, 2\pi/t]$ the “peak” and the rest of the real line (i.e. $|\alpha| \geq \frac{2\pi}{t}$) the “tails.” For $\alpha \rightarrow \infty$, $f(t, \alpha) \leq 1/\alpha^2$. Thus, the tail has total area bounded by $2 \int_{2\pi/t}^{\infty} 1/\alpha^2 = O(t)$.

For the peak, as $\alpha \rightarrow 0$, $f(t, \alpha) \rightarrow t^2/4$. On the other hand, \sin is concave, so for $0 \leq \theta \leq \pi/2$ we have $\sin(\theta) \geq \frac{\sin(\pi/2)}{\pi/2}\theta = \frac{2}{\pi}\theta$. Thus for $|\alpha| \leq \frac{\pi}{t}$ we have $f(\alpha, t) \geq \frac{t^2}{\pi}$. While these crude bounds do not determine the precise multiplicative constants, this does show that there is a region of width $\sim 1/t$ and height $\sim t^2$, and so the peak also has area $O(t)$.

We conclude that $\int_{-\infty}^{\infty} d\alpha f(t, \alpha) \sim t$. Dividing by t , we obtain

$$\int_{-\infty}^{\infty} d\alpha \frac{f(t, \alpha)}{t} \sim 1.$$

On the other hand, $\frac{f(t, \alpha)}{t} \rightarrow 0$ as $t \rightarrow \infty$ for all $\alpha \neq 0$. So as $t \rightarrow \infty$ we see that $\frac{f(t, \alpha)}{t}$ is always nonnegative, always has total mass roughly independent of t , but approaches zero for all nonzero α . This means that it approaches a delta function. A more detailed calculation (omitted, but it uses complex analysis) shows that

$$\lim_{t \rightarrow \infty} \frac{f(t, \alpha)}{t} = \frac{\pi}{2} \delta(\alpha).$$

The reason to divide by t is that this identifies the rate of transitions per unit time. Define $R_{n \rightarrow m} = \frac{P_{n \rightarrow m}}{t}$. Then the above arguments imply that

$$R_{n \rightarrow m} \approx \frac{\pi}{2} \frac{|V_{mn}|^2}{\hbar^2} \delta(|\omega_{mn}| - \omega) \quad \text{for large } t. \quad (10)$$

Linewidth In practice the frequency dependence is not a delta function. The term “linewidth” refers to the width of the region of ω that drives a transition; more concretely, FWHM stands for “full-width half-maximum” and denotes the width of the region that achieves $\geq 1/2$ the peak transition rate. The above derivation already suggests some reasons for nonzero linewidth.

1. *Finite lifetime.* If we apply the perturbation for a limited amount of time, or if the state we are driving to/from has finite lifetime, then this will contribute linewidth on the order of $1/t$.
2. *Power broadening.* If $|V_{mn}|$ is large, then we will still see transitions for larger values of $|\alpha|$. For this to prevent us from seeing the precise location of a peak, we need also the phenomenon of *saturation* in which transition rates all look the same above some threshold. (For example, we might observe the fraction of a beam that is absorbed by some sample, and by definition this cannot go above 1.)

There are many other sources of linewidth. In general we can think of both the driving frequency ω and the gap frequency ω_{mn} as being distributions rather than δ functions. The driving frequency might come from a thermal distribution or a laser, both of which output a distribution of frequencies. The linewidth of a laser is much lower but still nonzero. The energy difference $\hbar\omega_{mn}$ seems like a universal constant, can also be replaced by a distribution by phenomena such as Doppler broadening, in which the thermal motion of an atom will redshift or blueshift the incident light. This is just one example of a more general phenomenon in which interactions with other degrees of freedom can add to the linewidth; e.g. consider the hyperfine splitting, which measures the small shifts in an electron’s energy from its interaction with the nuclear spin. This can be thought of as adding to linewidth in two different, roughly equivalent, ways. We might think of the nuclear spins as random and thus the interaction adds a random term to the electron’s Hamiltonian. Alternatively, we might view the interaction with the nuclear spin as a source of decoherence and thus as contributing to the finite lifetime of the electron’s excited state. We will not explore those issues further here.

The other contribution to the rate is the matrix element $|V_{mn}|$. This depends not only on the strength of the perturbation, but also expresses the important point that we only see transitions from $n \rightarrow m$ if $V_{mn} \neq 0$. This is called a *selection rule*. In Griffiths it is proved that transitions from electric fields (see the next section) from Hydrogen state $|n, l, m\rangle$ to $|n', l', m'\rangle$ are only possible when $|l - l'| = 1$ and $|m - m'| \leq 1$ (among other restrictions). Technically these constraints hold only for first-order perturbation theory, but still selection rules are important, since they tell us when we need to go to higher-order perturbation theory to see transitions (known as “forbidden transitions”). In those cases transition rates are much lower. One dramatic example is that $2p \rightarrow 1s$ transition in hydrogen takes 1.6ns because it occurs at first order while the $2s \rightarrow 1s$ transition takes 0.12 seconds. For this reason states such as the 2s states are called “metastable.”

We now consider the most important special case, which gets its own top-level section, despite being an example of a periodic perturbation, which itself is an example of first-order perturbation theory.

2 Light and atoms

Light consists of oscillating \vec{E} and \vec{B} fields. The effects of the \vec{B} fields are weaker by a factor $O(v/c) \sim \alpha$, so we will focus on the \vec{E} fields. Let

$$\vec{E}(\vec{r}) = E_0 \hat{z} \cos(\omega t - kx).$$

However, optical wavelengths are 4000-8000Å, while the Bohr radius is $\approx 0.5\text{Å}$, so to leading order we can neglect the x dependence. Thus we approximate

$$\delta H(t) = eE_0 z \cos(\omega t). \quad (11)$$

We now can apply the results on transition rates from the last section with $V_{mn} = eE_0 \langle m|z|n \rangle$. (This term is responsible for selection rules and for the role of polarization.) Thus the rate of transitions is

$$R_{n \rightarrow m} = \frac{\pi}{2} \frac{e^2 E_0^2}{\hbar^2} |\langle m|z|n \rangle|^2 \delta(|\omega_{mn}| - \omega). \quad (12)$$

We get contributions at $\omega_{mn} = \pm\omega$ corresponding to both absorption and stimulated emission.

Aside: quantizing light What about spontaneous emission? This does not appear in the semiclassical treatment we've described here. Nor do the photons. "Absorption" means jumping from a low-energy state to a higher-energy state, and "stimulated emission" means jumping from high energy to low energy. In the former case, we reason from energy conservation that a photon must have been absorbed, and in the latter, a photon must have been emitted. However, these arguments are rather indirect. A much more direct explanation of what happens to the photon comes from a more fully quantum treatment. This also yields the phenomenon of spontaneous emission. Recall from 8.05 that oscillating electromagnetic fields can be quantized as follows:

$$E_0 = \mathcal{E}_0(\hat{a} + \hat{a}^\dagger) \quad \mathcal{E}_0 = \sqrt{\frac{2\pi\hbar\omega}{V}} \text{ (Gaussian units)} \quad = \sqrt{\frac{\hbar\omega}{\epsilon_0 V}} \text{ (SI units)}$$

Using $\delta H = eE_0 z$, we obtain

$$\delta H = eE_0 z \otimes (\hat{a} + \hat{a}^\dagger).$$

If we look at the action of z in the $\{1s, 2p_z\}$ basis, then it has the form $\begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix}$ with $\alpha = \langle 1s|z|2p_z \rangle$.

We then obtain the form of the Hamiltonian examined on pset 3.

This perspective also can be used to give a partial derivation of the Lamb shift, which can be thought of as the interaction of the electron with fluctuations in the electric field of the vacuum. In the vacuum (i.e. ground state of the photon field) we have $\langle E_0 \rangle \sim \langle \hat{a} + \hat{a}^\dagger \rangle = 0$ but $\langle E_0^2 \rangle \sim \langle (\hat{a} + \hat{a}^\dagger)^2 \rangle > 0$. These vacuum fluctuations lead to a small separation in energy between the 2s and 2p levels of hydrogen.

Dipole moment In the Stark effect we looked at the interaction of the hydrogen atom with an electric field. This was a special case of the interaction between a \vec{E} field and the dipole moment of a collection of particles. Here we discuss the more general case.

Suppose that we have charges q_1, \dots, q_N at positions $\vec{x}^{(1)}, \dots, \vec{x}^{(N)}$, and we apply an electric field $\vec{E}(\vec{x})$. The energy is determined by the scalar potential $\phi(\vec{x})$ which is related to the electric

field by $\vec{E} = -\vec{\nabla}\phi$. If $\vec{E}(\vec{x}) = \vec{E}$ (i.e. independent of position \vec{x}) then one possible solution is $\phi(\vec{x}) = -\vec{x} \cdot \vec{E}$. In this case the Hamiltonian will be

$$H = \sum_{i=1}^N q_i \phi(\vec{x}^{(i)}) = - \sum_{i=1}^N q_i \vec{x}^{(i)} \cdot \vec{E} = -\vec{d} \cdot \vec{E}$$

where we have defined the dipole moment $\vec{d} = \sum_{i=1}^N q_i \vec{x}^{(i)}$. Our choice of ϕ was not unique, and we could have chosen $\phi(\vec{x}) = C - \vec{x} \cdot \vec{E}$ for any constant C . However, this would only have added an overall constant to the Hamiltonian, which would have no physical effect.

What if the electric field is spatially varying? If this spatial variation is small and we are near the origin, we use the first few terms of the Taylor expansion to approximate the field:

$$\vec{E}(\vec{x}) = \vec{E}(0) + \sum_{i,j=1}^3 \frac{\partial E_i}{\partial x_j} \hat{e}_i x_j + \dots$$

This corresponds to a scalar potential of the form

$$\phi = \sum_{i=1}^3 x_i E_i(0) + \frac{1}{2} \sum_{i,j=1}^3 x_i x_j \frac{\partial E_i}{\partial x_j} + \dots$$

For the quadratic terms we see that the field couples not to the dipole moment, but to the *quadrupole moment*, defined to be $\sum_{i=1}^N q_i \vec{x}^{(i)} \otimes \vec{x}^{(i)}$. This is related to emission lines such as $1s \rightarrow 3d$ in which ℓ may change by up to ± 2 . Of course higher moments such as octupole moments can be also be considered. We will not explore these topics further in 8.06.

2.1 Incoherent light

While we have so far discussed monochromatic light with a definite polarization, it is easier to produce light with a wide range of frequencies and with random polarization. To analyze the rate of transitions this causes we will average (12) over frequencies and polarizations.

Begin with polarizations. Instead of the field being $E_0 \hat{z}$, let the electric field be $E_0 \hat{P}$ for some random unit vector \hat{P} . We then replace V with $-E_0 \hat{P} \cdot \vec{d}$. The only operator here is the dipole moment $\vec{d} = (d_1, d_2, d_3)$, so the matrix elements of V are given by

$$V_{mn} = -E_0 \hat{P} \cdot \vec{d}_{mn} = -E_0 \sum_{i=1}^3 P_i \langle m | d_i | n \rangle.$$

Since the transition rate depends on $|V_{mn}|^2$, we will average this quantity over the choice of polar-

ization. Denote the average over all unit vectors \hat{P} by $\langle \cdot \rangle_{\hat{P}}$.

$$\begin{aligned}
\langle |V_{mn}|^2 \rangle_{\hat{P}} &= E_0^2 \left\langle |\hat{P} \cdot \vec{d}_{mn}|^2 \right\rangle_{\hat{P}} \\
&= E_0^2 \sum_{i,j=1}^3 \langle \langle m|P_i d_i|n \rangle \langle n|P_j d_j|m \rangle \rangle_{\hat{P}} \\
&= E_0^2 \sum_{i,j=1}^3 \langle P_i P_j \rangle_{\hat{P}} \langle m|d_i|n \rangle \langle n|d_j|m \rangle \\
&= E_0^2 \sum_{i,j=1}^3 \frac{\delta_{ij}}{3} \langle m|d_i|n \rangle \langle n|d_j|m \rangle \quad \text{explained below} \\
&= \frac{E_0^2}{3} \sum_i |\langle m|d_i|n \rangle|^2 \\
&\equiv \frac{E_0^2}{3} |\vec{d}_{mn}|^2
\end{aligned}$$

How did we calculate $\langle P_i P_j \rangle_{\hat{P}}$? This can be done by explicit calculation, but it is easier to use symmetry. First, observe that the uniform distribution over unit vectors is invariant under reflection. Thus, if $i \neq j$, then $\langle P_i P_j \rangle = \langle (-P_i) P_j \rangle = 0$. On the other hand rotation symmetry means that $\langle P_i^2 \rangle$ should be independent of i . Since $P_1^2 + P_2^2 + P_3^2 = 1$, we also have $\langle P_1^2 + P_2^2 + P_3^2 \rangle = 1$ and thus $\langle P_i^2 \rangle = 1/3$. Putting this together we obtain

$$\langle P_i P_j \rangle_{\hat{P}} = \frac{\delta_{ij}}{3}. \quad (13)$$

Next, we would like to average over different frequencies. The energy density of an electric field is $U = \frac{E_0^2}{8\pi}$ (using Gaussian units). Define $U(\omega)$ to be the energy density at frequency ω , so that $U = \int U(\omega) d\omega$. If we consider light with this power spectrum, then we should integrate the rate times this distribution over $U(\omega)$ to obtain

$$\begin{aligned}
R_{n \rightarrow m} &= \int d\omega U(\omega) \frac{4\pi^2}{3\hbar^2} |\vec{d}_{mn}|^2 \delta(\omega - |\omega_{mn}|) \\
&= \boxed{\frac{4\pi^2}{3\hbar^2} |\vec{d}_{mn}|^2 U(|\omega_{mn}|)}
\end{aligned}$$

This last expression is known as *Fermi's Golden Rule*. (It was discovered by Dirac, but Fermi called it “Goldren Rule #2”.)

2.2 Spontaneous emission

The modern description of spontaneous emission requires QED, but the first derivation of it predates even modern quantum mechanics! In a simple and elegant argument, Einstein:

- (a) derived an exact relation between rates of spontaneous emission, stimulated emission and absorption; and
- (b) proposed the phenomenon of stimulated emission, which was not observed until 1960.

He did this in 1917, more than a decade before even the Schrödinger equation!

Here we will reproduce that argument. It assumes a collection of atoms that can be in either state a or state b . Suppose that there are N_a atoms in state a and N_b atoms in state b , and that the states have energies E_a, E_b with $E_b > E_a$. Define $\omega_{ba} = \frac{E_b - E_a}{\hbar}$ and $\beta = 1/k_B T$. Assume further that the atoms are in contact with a bath of photons and that the entire system is in thermal equilibrium with temperature T . From this we can deduce three facts:

Fact 1. Equilibrium means no change: $\dot{N}_a = \dot{N}_b = 0$.

Fact 2. At thermal equilibrium we have $\frac{N_b}{N_a} = \frac{e^{-\beta E_b}}{e^{-\beta E_a}} = e^{-\beta \hbar \omega_{ba}}$.

Fact 3. At thermal equilibrium the black-body radiation spectrum is

$$U(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\beta \hbar \omega} - 1}. \quad (14)$$

We would like to understand the following processes:

Process	Explanation	Rate
<i>Absorption</i>	A photon of frequency ω_{ba} is absorbed and an atom changes from state a to state b .	$B_{ab} N_a U(\omega_{ba})$
<i>Spontaneous emission</i>	A photon of frequency ω_{ba} is emitted and an atom changes from state b to state a .	$A N_b$
<i>Stimulated emission</i>	A photon of frequency ω_{ba} is emitted and an atom changes from state b to state a .	$B_{ba} N_b U(\omega_{ba})$

These processes depend on the *Einstein coefficients* A , B_{ab} and B_{ba} for spontaneous emission, absorption and stimulated emission respectively. They also depend on the populations of atoms and/or photons that they involve; e.g. absorption requires an atom in state a and a photon of frequency ω_{ba} , so its rate is proportional to $N_a U(\omega_{ba})$. Here it is safe to posit the existence of stimulated emission because we have not assumed that B_{ba} is nonzero.

Having set up the problem, we are now almost done! Adding these processes up, we get

$$\dot{N}_b = -N_b A - N_b B_{ba} U(\omega_{ba}) + N_a B_{ab} U(\omega_{ba}). \quad (15)$$

From Fact 1, $\dot{N}_b = 0$ and so we can rearrange (15) to obtain

$$U(\omega_{ba}) = \frac{A}{\frac{N_a}{N_b} B_{ab} - B_{ba}} \stackrel{\text{Fact 2}}{=} \frac{A}{e^{\beta \hbar \omega_{ba}} B_{ab} - B_{ba}} \stackrel{\text{Fact 3}}{=} \frac{\hbar \omega^3}{\pi^2 c^3} \frac{1}{e^{\beta \hbar \omega_{ba}} - 1}$$

Since this relation should hold for all values of β , we can equate coefficients and find

$$B_{ab} = B_{ba} \quad (16a)$$

$$A = \frac{\hbar \omega_{ba}^3}{\pi^2 c^3} B_{ab} \quad (16b)$$

We see that these three processes are tightly related! All from a simple thought experiment, and not even the one that Einstein is most famous for.

Today we can understand this as the fact that the electric field enters into the Hamiltonian as a Hermitian operator proportional to $\hat{a} + \hat{a}^\dagger$, and so the photon-destroying processes containing \hat{a}

are inevitably accompanied by photon-creating processes containing \hat{a}^\dagger . Additionally the relation between spontaneous and stimulated emission can be seen in the fact that both involve an a^\dagger operator acting on the photon field. If there are no photons, then the field is in state $|0\rangle$ and we get the term $a^\dagger|0\rangle = |1\rangle$, corresponding to spontaneous emission. If there are already n photon in the mode, then we get the term $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. Since the probabilities are the square of the amplitudes, this means that we see photons emitted at $n+1$ times the spontaneous emission rate. In Einstein's terminology, the n here is from stimulated emission and the $+1$ is from the spontaneous emission which always occurs independent of the number of photons present.

Returning to (16), we plug in Fermi's Golden Rule and obtain the rates

$$B_{ab} = B_{ba} = \frac{4\pi^2}{3\hbar^2} |\vec{d}_{ab}|^2 \quad \text{and} \\ A = \frac{4\omega_{ba}^3}{3\hbar c^3} |\vec{d}_{ab}|^2.$$

2.3 The photoelectric effect

So far we have considered transitions between individual pairs of states. Ionization (aka the photoelectric effect) involves a transition from a bound state of some atom to one in which the electron is in a free state. This presents a few new challenges. First, we are used to treating unbound states as unnormalized, e.g. $\psi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}$. Second, to calculate the ionization rate, we need to sum over final states, since the quantity of physical interest is the total rate of electrons being dislodged from an atom, and not the rate at which they transition to any specific final state. (A more refined analysis might look at the angular distribution of the final state.)

Suppose our initial state is our old friend, the ground state of the hydrogen atom, and the final state is a plane wave. If the final state is unnormalized, then matrix elements such as $\langle\psi_{\text{final}}|V|\psi_{\text{initial}}\rangle$ become less meaningful. One way to fix this is to put the system in a box of size $L \times L \times L$ with $L \gg a_0 \equiv \frac{\hbar^2}{me^2}$ and to impose periodic boundary conditions. The resulting plane-wave states are now

$$\psi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k} \cdot \vec{x})}{L^{3/2}},$$

where $|\vec{k}\rangle = \frac{2\pi}{L}\vec{n}$ and $\vec{n} = (n_1, n_2, n_3)$ is a vector of integers. (We use \vec{k} instead of $\vec{p} = \hbar\vec{k}$ to keep the notation more compact.) We will assume that $L \gg a_0$ and also that the final energy of the electron is $\gg 13.6$ eV. This means that we can approximate the final state as a free electron and can ignore the interaction with the proton.

Apply an oscillating electric field to obtain the time-dependent potential

$$\delta H = eE_0 x_3 \cos(\omega t) \equiv V \cos(\omega t).$$

The rate of the transitions will be governed by the matrix element

$$\langle\vec{k}|V|1,0,0\rangle = \frac{eE_0}{\sqrt{\pi a_0^3 L^3}} \underbrace{\int d^3x \, x_3 \exp\left(-\frac{r}{a_0} - i\vec{k} \cdot \vec{x}\right)}_A \equiv \frac{eE_0}{\sqrt{\pi a_0^3 L^3}} A.$$

We have defined A to equal the difficult-to-evaluate integral. The factor of x_3 can be removed by

writing $A = i \frac{\partial}{\partial k_3} B$, where

$$\begin{aligned}
B &= \int d^3x \exp\left(-\frac{r}{a_0} - i\vec{k} \cdot \vec{x}\right) \\
&= 2\pi \int_0^\infty r^2 \int_{-1}^1 d\mu \exp\left(-\frac{r}{a_0} - ikr\mu\right) && \text{defining } \mu = \frac{\vec{k} \cdot \vec{x}}{kr}, k = |\vec{k}|, r = |\vec{x}| \\
&= 4\pi \int_{-1}^1 d\mu \frac{1}{\left(\frac{1}{a_0} + ik\mu\right)^3} && \text{using } \int_0^\infty r^n e^{-\alpha r} = \frac{n!}{\alpha^{n+1}} \\
&= \frac{4\pi i}{k^3} \int_{-1}^1 d\mu \frac{1}{\left(\mu + \frac{i}{ka_0}\right)^3} \\
&= -\frac{2\pi i}{k^3} \left[\frac{1}{\left(1 + \frac{i}{ka_0}\right)^2} - \frac{1}{\left(1 - \frac{i}{ka_0}\right)^2} \right] = \frac{2\pi i}{k^3} \left[\frac{\left(1 + \frac{1}{ika_0}\right)^2 - \left(1 - \frac{1}{ika_0}\right)^2}{\left(1 + \frac{1}{k^2 a_0^2}\right)^2} \right] \\
&= \frac{8\pi i}{k^3} \frac{\frac{1}{ika_0}}{\left(1 + \frac{1}{k^2 a_0^2}\right)^2} = \frac{8\pi}{k^4 a_0 \left(1 + \frac{1}{k^2 a_0^2}\right)^2} = \boxed{\frac{8\pi}{a_0 (k^2 + a_0^{-2})^2}}
\end{aligned}$$

To compute A , we use the fact that $\frac{\partial}{\partial k_3} k^2 = 2k_3$. Thus

$$A = i \frac{\partial}{\partial k_3} B = \frac{-32\pi i k_3}{a_0 (k^2 + a_0^{-2})^3}.$$

We can simplify this expression using our assumption that the photon energy (and therefore also the final state energy) is much larger than the binding energy. The final energy is $\frac{\hbar^2 k^2}{2m}$ and the binding energy is $\frac{\hbar^2}{2ma_0^2}$. Thus

$$\frac{\hbar^2 k^2}{2m} \gg \frac{\hbar^2}{2ma_0^2} \implies ka_0 \gg 1.$$

We can use this to simplify A by dropping the a_0^{-2} term in the dominator:

$$A \approx \frac{-32\pi i k_3}{a_0 k^6} = \frac{-32\pi i \cos(\theta)}{a_0 k^5},$$

where θ is the angle between \vec{k} and the z -axis.

We can now compute the squared matrix element to be (canceling a factor of π from numerator and denominator)

$$|\langle \vec{k} | V | 1, 0, 0 \rangle|^2 = \frac{e^2 E_0^2}{a_0^3 L^3} \frac{1024\pi \cos^2(\theta)}{a_0^2 k^{10}}.$$

To compute the average rate over some time t , we will multiply this by $\frac{1}{\hbar^2} \frac{f(t, \alpha)}{t}$, where $f(t, \alpha) \equiv \frac{\sin^2(\alpha t/2)}{\alpha^2}$ and $\hbar\alpha$ is the difference in energy between the initial and final states. If we neglect the energy of the initial state, we obtain

$$R_{1,0,0 \rightarrow \vec{k}} = \frac{1024\pi e^2 E_0^2 \cos^2(\theta)}{\hbar^2 a_0^5 k^{10} L^3} \frac{f\left(t, \frac{\hbar k^2}{2m} - \omega\right)}{t}.$$

We can simplify this a bit by averaging over all the polarizations of the light. (In fact, the angular dependence of the free electron can often carry useful information, but here it will help simplify some calculations.) The average of $\cos^2(\theta)$ over the sphere is $1/3$ (by the same arguments we used in the derivation of Fermi's golden rule), so we obtain

$$\langle R_{1,0,0 \rightarrow \vec{k}} \rangle = \frac{1024\pi e^2 E_0^2}{3\hbar^2 a_0^5 k^{10} L^3} \frac{f\left(t, \frac{\hbar k^2}{2m} - \omega\right)}{t}.$$

Let's pause for a minute to look at what we've derived. One strange feature is the $1/L^3$ term, because the rate of ionization should not depend on how much empty space surrounds the atom. Another strange thing appears to happen when we take t large, so that $f(t, \alpha)/t$ will approach $\frac{\pi}{2}\delta(\alpha)$. This would cause the transition rates to be nonzero only when $2m\omega/\hbar$ exactly equals k^2 for some valid vector \vec{k} (i.e. of the form $\frac{2\pi}{L}\vec{n}$). We do not generally expect physical systems to have such sensitive dependence on their parameters.

As often happens when two things look wrong, these difficulties can be made to “cancel each other out.” Let us take t to be large but finite. It will turn out that t needs to be large only relative to $\frac{\hbar^2}{L^2 m}$, which is not very demanding when L is large. In this case, we can approximate $f(t, \alpha)$ with a step function:

$$f(t, \alpha) \approx \tilde{f}(t, \alpha) \equiv \begin{cases} \frac{\pi}{2}t^2 & \text{if } 0 \leq \alpha \leq \frac{1}{t} \\ 0 & \text{otherwise} \end{cases}$$

In what sense is this a good approximation? We argue that for large t , $\tilde{f}(t, \alpha)/t \approx \frac{\pi}{2}\delta(\alpha)$, just like $f(t, \alpha)/t$. Suppose that $g(\alpha)$ is a function satisfying $|g'(\alpha)| \leq C$ for all α . Then

$$\begin{aligned} \left| \int_{-\infty}^{\infty} d\alpha \left(\frac{\tilde{f}(t, \alpha)}{\frac{\pi}{2}t} - \delta(\alpha) \right) g(\alpha) \right| &= \left| \left(t \int_0^{1/t} d\alpha g(\alpha) \right) - g(0) \right| \\ &= \left| t \int_0^{1/t} d\alpha (g(\alpha) - g(0)) \right| \\ &= \left| t \int_0^{1/t} d\alpha \int_0^\alpha d\beta g'(\beta) \right| \\ &\leq t \int_0^{1/t} d\alpha \int_0^\alpha d\beta |g'(\beta)| \quad \text{triangle inequality} \\ &\leq t \frac{1}{2t^2} C = \frac{C}{2t} \end{aligned}$$

This tends to 0 as $t \rightarrow \infty$. (This is an example of a more general principle that the “shape” of a δ function doesn't matter. For example, the limit of a Gaussian distribution with $\sigma^2 \rightarrow 0$ would also work.)

Now using $\tilde{f}(t, \alpha)$, we get a nonzero contribution for \vec{k} satisfying

$$\begin{aligned} 0 &\leq \frac{\hbar}{k^2} 2m - \omega \leq \frac{1}{t} \\ \Leftrightarrow \quad \frac{2m\omega}{\hbar} &\leq k^2 \leq \frac{2m\omega}{\hbar} \left(1 + \frac{1}{t\omega} \right) \\ \Leftrightarrow \quad \sqrt{\frac{2m\omega}{\hbar}} &\leq k \leq \sqrt{\frac{2m\omega}{\hbar} \left(1 + \frac{1}{t\omega} \right)} \approx \sqrt{\frac{2m\omega}{\hbar}} \left(1 + \frac{1}{2t\omega} \right) \end{aligned} \tag{17}$$

How many \vec{k} satisfy (17)? Valid \vec{k} live on a cubic lattice with spacing $2\pi/L$, and thus have density $(L/2\pi)^3$. Thus we can estimate the number of \vec{k} satisfying (17) by $(L/2\pi)^3$ times the volume of k -space satisfying (17). This in turn corresponds to a spherical shell of inner radius $\sqrt{\frac{2m\omega}{\hbar}}$ and thickness $\sqrt{\frac{2m\omega}{\hbar}} \frac{1}{2t\omega}$. Thus we have

$$\# \text{ valid } \vec{k} = \left(\frac{L}{2\pi}\right)^3 4\pi \left(\frac{2m\omega}{\hbar}\right)^{3/2} \frac{1}{2t\omega} = \frac{L^3 m}{2\pi^2 \hbar t} \sqrt{\frac{2m\omega}{\hbar}} = \frac{L^3 m k}{2\pi^2 \hbar t}.$$

In the last step we use the fact that spherical shell is thin to approximate $k \approx \sqrt{\frac{2m\omega}{\hbar}}$. Thus, when we sum $\tilde{f}(t, \alpha)/t$ over \vec{k} we obtain

$$\sum_{\vec{k}} \frac{\tilde{f}(t, \alpha)}{t} = \frac{\pi}{2} t \cdot \# \text{ valid } \vec{k} = \frac{L^3 m k}{4\pi \hbar}.$$

We have obtained our factor of L^3 that removes the unphysical dependence on the boundary conditions. Putting everything together we get

$$R_{1,0,0 \rightarrow \text{all } \vec{k}} = \frac{256 m e^2 E_0^2}{3 \hbar^3 a_0^5 k^9}.$$

3 Adiabatic evolution

3.1 The adiabatic approximation

We now turn to a different kind of approximation, in which we consider slowly varying Hamiltonians. We will consider a time-dependent Hamiltonian $H(t)$. Let $|\psi_n(t)\rangle$ and $E_n(t)$ be the “instantaneous” eigenbases and eigenenergies, defined by

$$H(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle \quad E_1(t) \leq E_2(t) \leq \dots \quad (18)$$

We also define $|\Psi(t)\rangle$ to be the solution of Schrödinger’s equation: i.e.

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \quad (19)$$

Beware that (18) and (19) are *not* the same. You might think of (18) as a naive attempt to solve (19). If the system starts in $|\psi_n(0)\rangle$ at time 0, there is of course no reason in general to expect that $|\psi_n(t)\rangle$ will be the correct solution for later t . And yet, the adiabatic theorem states that in some cases this is exactly what happens.

Theorem 1 (Adiabatic theorem). *Suppose at $t = 0$, $|\Psi(0)\rangle = |\psi_n(0)\rangle$ for some n . Then if H is changed slowly for $0 \leq t \leq T$, then at time T we will have $|\Psi(T)\rangle \approx |\psi_n(T)\rangle$.*

This theorem is stated in somewhat vague terms, e.g. what does “changed slowly” mean? \dot{H} should be small, but relative to what? One clue is the reference to the n^{th} eigenstate $|\psi_n(t)\rangle$. This is only well defined if $E_n(t)$ is unique, so clearly the theorem fails in the case of degenerate eigenvalues. And since the theorem should not behave discontinuously with respect to $H(t)$, it should also fail for “nearly” degenerate eigenvalues. This gives us another energy scale to compare with \dot{H} (which has units of energy/time, or energy squared once we multiply by \hbar). We will see later the sense in which this can be shown to be the right comparison.

Example. Suppose we have a spin-1/2 particle in a magnetic field $\vec{B}(t)$. Then the Hamiltonian is $H(t) = g_e \mu_B \frac{\vec{S}}{\hbar} \cdot \vec{B}(t)$. The adiabatic theorem says that if we start with the spin and \vec{B} both pointing in the $+\hat{z}$ direction and gradually rotate \vec{B} to point in the \hat{x} direction, then the spin will follow the magnetic field and also point in the \hat{x} direction. Given that the Schrödinger equation prescribes instead that the spin precess around the magnetic field, this behavior appears at first somewhat strange.

Derivation We will not rigorously prove the adiabatic theorem, but will describe most of the derivation. Begin by writing

$$|\Psi(t)\rangle = \sum_n c_n(t) |\psi_n(t)\rangle.$$

Taking derivatives of both sides we obtain

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = i\hbar \sum_n \dot{c}_n(t) |\psi_n(t)\rangle + c_n(t) |\dot{\psi}_n(t)\rangle = \sum_n c_n(t) E_n(t) |\psi_n(t)\rangle.$$

Multiply both sides by $\langle \psi_k(t) |$ and we obtain

$$i\hbar \dot{c}_k = E_k c_k - i\hbar \sum_n \langle \psi_k | \dot{\psi}_n \rangle c_n. \quad (20)$$

Now we need a way to evaluate $\langle \psi_k | \dot{\psi}_n \rangle$ in terms of more familiar quantities.

$$\begin{aligned} \text{Start with} & \quad H |\psi_n\rangle = E_n |\psi_n\rangle \\ \text{Apply } \frac{d}{dt} & \quad \dot{H} |\psi_n\rangle + H |\dot{\psi}_n\rangle = \dot{E}_n |\psi_n\rangle + E_n |\dot{\psi}_n\rangle \\ \text{Apply } \langle \psi_k | & \quad \langle \psi_k | \dot{H} |\psi_n\rangle + E_k \langle \psi_k | \dot{\psi}_n\rangle = \dot{E}_n \delta_{kn} + E_n \langle \psi_k | \dot{\psi}_n\rangle \end{aligned}$$

This equation has two interesting cases: $k = n$ and $k \neq n$. The former will not be helpful in estimating $\langle \psi_k | \dot{\psi}_n \rangle$, but does give us a useful result, called the Hellmann-Feynman theorem.

$$\begin{aligned} k = n & \quad \dot{E}_n = \langle \psi_n | \dot{H} | \psi_n \rangle \\ k \neq n & \quad \langle \psi_k | \dot{\psi}_n \rangle = \frac{\langle \psi_k | \dot{H} | \psi_n \rangle}{E_n - E_k} \equiv \frac{\dot{H}_{kn}}{E_n - E_k} \end{aligned}$$

In the last step, we used \dot{H}_{kn} to refer to the matrix elements of \dot{H} in the $\{|\psi_n\rangle\}$ basis.

Plugging this into (20) we find

$$i\hbar \dot{c}_k = \underbrace{(E_k - i\hbar \langle \psi_k | \dot{\psi}_k \rangle) c_k}_{\text{adiabatic approximation}} - \underbrace{i\hbar \sum_{n \neq k} \frac{\dot{H}_{kn}}{E_n - E_k} c_n}_{\text{error term}}. \quad (21)$$

If the part of the equation denoted “error term” did not exist, then $|c_k|$ would be independent of time, which would confirm the adiabatic theorem. Furthermore, the error term is suppressed by a factor of $1/\Delta_{nk}$, where $\Delta_{nk} \equiv E_n - E_k$ is the energy gap. So naively it seems that if \dot{H} is small relative to Δ_{nk} then the error term should be small. On the other hand, these two quantities do not even have the same units, so we will have to be careful.

Phases Before we analyze the error term, let's look at the phases we get if the error term were not there. i.e. suppose that $i\hbar\dot{c}_k = (E_k - i\hbar\langle\psi_k|\dot{\psi}_k\rangle)c_k$. The solution of this differential equation is

$$c_k(t) = c_k(0)e^{i\theta_k(t)}e^{i\gamma_k(t)} \quad (22a)$$

$$\theta_k(t) \equiv -\frac{1}{\hbar} \int_0^t E_k(t') dt' \quad \gamma_k(t) \equiv \int_0^t \nu_k(t') dt' \quad \nu_k(t) \equiv i\langle\psi_k|\dot{\psi}_k\rangle \quad (22b)$$

The $\theta_k(t)$ term is called the “dynamical” phase and corresponds to exactly what you'd expect from a Hamiltonian that's always on; namely the phase of state k rotates at rate $-E_k/\hbar$. The $\gamma_k(t)$ is called the “geometric phase” or “Berry phase” and will be discussed further in the next lecture. At this point, observe only that it is independent of \hbar and that $\nu_k(t)$ can be seen to be real by applying d/dt to the equation $\langle\psi_k|\psi_k\rangle = 1$.

Validity of the adiabatic approximation Let's estimate the magnitude of the error term in a toy model. Suppose that $H(t) = H_0 + \frac{t}{T}V$, where H_0, V are time-independent and T is a constant that sets the timescale on which V is turned on. Then $\dot{H} = V/T$. An important prediction about the adiabatic theorem is that if the more slowly H changes from H_0 to $H_0 + V$, the lower the probability of transition should be; i.e. increasing T should reduce the error term, even if we integrate over time from 0 to T .

Let's see how this works. If the gap is always $\gtrsim \Delta$, then we can upper-bound the transition rate by some matrix element of $\frac{V}{T\Delta}$. This decreases as T and Δ increase, which is good. But if we add up this rate of transitions over time T , then the total transition amplitude can be as large as $\sim V/\Delta$. Thus, going more slowly appears *not* to reduce the total probability of transition!

What went wrong? Well, we assumed that amplitude from state n simply added up in state k . But if the states have different energies, then over time the terms we add will have different phases, and may cancel out. This can be understood in terms of time-dependent perturbation theory. Define $\tilde{c}_k(t) = e^{-i\theta_k(t)}c_k(t)$. Observe that

$$\begin{aligned} i\hbar \frac{d}{dt} \tilde{c}_k(t) &= \hbar \dot{\theta}_k(t) e^{-i\theta_k(t)} c_k(t) + i\hbar e^{-i\theta_k(t)} \dot{c}_k(t) \\ &= -E_k(t) e^{-i\theta_k(t)} c_k(t) + e^{-i\theta_k(t)} (E_k(t) - \hbar \nu_k(t)) c_k(t) - i\hbar \sum_{n \neq k} \frac{\dot{H}_{kn}}{E_n - E_k} e^{-i\theta_k(t)} c_n(t) \\ &= -\hbar \nu_k(t) \tilde{c}_k(t) - i\hbar \sum_{n \neq k} \frac{\dot{H}_{kn}}{E_n - E_k} e^{i(\theta_n(t) - \theta_k(t))} \tilde{c}_n(t) \end{aligned}$$

In the last step we have used $c_n(t) = e^{i\theta_n(t)} \tilde{c}_n(t)$. Let's ignore the $\nu_k(t)$ geometric phase term (since our analysis here is somewhat heuristic). We see that the error term is the same as in (21) but with an extra phase of $e^{i(\theta_n(t) - \theta_k(t))}$. Analyzing this in general is tricky, but let's suppose that the energy levels are roughly constant, so we can replace it with $e^{-i\omega_{nk}t}$, where $\omega_{nk} = (E_n - E_k)/\hbar$. Now when we integrate the contribution of this term from $t = 0$ to $t = T$ we get

$$\int_0^T \frac{\dot{H}_{kn} e^{-i\omega_{nk}t}}{E_n - E_k} dt \sim \frac{V}{T} \frac{e^{-i\omega_{nk}T} - 1}{\hbar \omega_{nk}^2} \sim \frac{V}{T \hbar \omega_{nk}^2} \sim \frac{\hbar V}{\Delta^2 T}$$

Finally we obtain that the probability of transition decreases with T . This can be thought of as a rough justification of the adiabatic theorem, but it of course made many simplifying assumptions and in general it will be only qualitatively correct.

This was focused on a specific transition. In general adiabatic transitions between levels m and n are suppressed if

$$\boxed{\hbar|\dot{H}_{mn}| \ll \Delta^2 = \min_t (E_m(t) - E_n(t))^2}. \quad (23)$$

Landau-Zener transitions One example that can be solved exactly is a two-level system with a linearly changing Hamiltonian. Suppose a spin-1/2 particle experiences a magnetic field resulting in the Hamiltonian

$$H(t) = \Delta\sigma_x + \frac{vt}{T}\sigma_z,$$

for some constants Δ, v, T . The eigenvalues are $\pm\sqrt{\Delta^2 + (vt/T)^2}$. Assuming $v > 0$, then when $t = -\infty$ the top eigenstate is $|-\rangle$ and the bottom eigenstate is $|+\rangle$. When $t = \infty$ these are reversed; $|+\rangle$ is the top eigenstate and $|-\rangle$ is the bottom eigenstate. When $t = 0$, the eigenstates are $\frac{|+\rangle \pm |-\rangle}{\sqrt{2}}$. See diagram on black-board for energy levels.

Suppose that $\Delta = 0$ and we start in the $|-\rangle$ at $t = -\infty$. Then at $t = \infty$ we will still be in the $|-\rangle$ state, with only the phase having changed. But if $\Delta > 0$ and we move slowly enough then the adiabatic approximation says we will remain in the top eigenstate, which for $t = \infty$ will be $|+\rangle$. Thus, the presence of a very small transverse field can completely change the state if we move slowly enough through it.

In this case, the error term in the adiabatic approximation can be calculated rather precisely and is given by the Landau-Zener formula (proof omitted):

$$\text{Pr}[\text{transition}] \approx \exp\left(-\frac{2\pi^2\Delta^2T}{\hbar v}\right).$$

Observe that it has all the qualitative features that we expect in terms of dependence on Δ, v, T , but that it corresponds to a rate of transitions exponentially smaller than our above estimate from first-order perturbation theory. Note that here “transition” refers to transitions between energy level. Thus starting in $|-\rangle$ and ending in $|+\rangle$ corresponds to “no transition” while ending in $|-\rangle$ would correspond to “transition,” since it means starting in the higher energy level and ending in the lower energy level.

3.2 Berry phase

Recall that the adiabatic theorem states that if we start in state $|\psi_n(0)\rangle$ and change the Hamiltonian slowly, then we will end in approximately the state

$$e^{i\theta_n(t)}e^{i\gamma_n(t)}|\psi_n(t)\rangle \quad (24a)$$

$$\theta_n(t) \equiv -\frac{1}{\hbar} \int_0^t E_n(t')dt' \quad \gamma_n(t) \equiv \int_0^t \nu_n(t')dt' \quad \nu_n(t) \equiv i\langle\psi_n|\dot{\psi}_n\rangle \quad (24b)$$

The phase $\gamma_n(t)$ is called the geometric phase, or the Berry phase, after Michael Berry’s 1984 explanation of it.

Do the phases in the adiabatic approximation matter? This is a somewhat subtle question. Of course an overall phase cannot be observed, but a relative phase can lead to observable interference effects. The phases in (22) depend on the eigenstate label n , and so in principle interference is possible. But solutions to the equation $H(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle$ are not uniquely defined, and we can in general redefine $|\psi_n(t)\rangle$ by multiplying by a phase that can depend on both n and t .

To see how this works, let us consider the example of a spin-1/2 particle in a spatially varying magnetic field. If the particle moves slowly, we can think of the position $\vec{r}(t)$ as a classical variable causing the spin to experience the Hamiltonian $H(\vec{r}(t))$. This suggests that we might write the state as a function of $\vec{r}(t)$, as $|\psi_n(\vec{r}(t))\rangle$ or even $|\psi_n(\vec{r})\rangle$. If the particle's position is a classical function of time, then we need only consider interference between states with the same value of \vec{r} , and so we can safely change $|\psi_n(\vec{r})\rangle$ by any phase that is a function of n and \vec{r} .

In fact, even if the particle were in a superposition of positions as in the two-slit experiment, then we could still only see interference effects between branches of the wavefunction with the same value of \vec{r} . Thus, again we can define an arbitrary (n, \vec{r}) -dependent phase.

More generally, suppose that H depends on some set of coordinates $\vec{R}(t) = (R_1(t), \dots, R_N(t))$. The eigenvalue equation (18) becomes $H(\vec{R})|\psi_n(\vec{R})\rangle = E_n(\vec{R})|\psi_n(\vec{R})\rangle$ where we leave the time-dependence of \vec{R} implicit. This allows us to compute even in situations where \vec{R} is in a superposition of coordinates at a given time t .

To express $\gamma_n(t)$ in terms of $|\psi_n(\vec{R})\rangle$, we compute

$$\begin{aligned} \frac{d}{dt}|\psi_n(\vec{R})\rangle &= \sum_{i=1}^N \frac{d|\psi_n(\vec{R})\rangle}{dR_i} \frac{dR_i}{dt} = \vec{\nabla}_{\vec{R}}|\psi_n(\vec{R})\rangle \cdot \frac{d\vec{R}}{dt} \\ \gamma_n(t) &= i \int_0^t \langle \psi_n | \vec{\nabla}_{\vec{R}} | \psi_n \rangle \cdot \frac{d\vec{R}}{dt} dt = \int_{\vec{R}(0)}^{\vec{R}(t)} i \langle \psi_n | \vec{\nabla}_{\vec{R}} | \psi_n \rangle \cdot d\vec{R} \end{aligned}$$

The answer is in terms of a line integral, which depends only on the path and *not* on time (unlike the dynamical phase).

How does this change if we reparameterize $|\psi_n(\vec{R})\rangle$? Suppose we replace $|\psi_n(\vec{R})\rangle$ with $|\tilde{\psi}_n(\vec{R})\rangle = e^{-i\beta(\vec{R})}|\psi_n(\vec{R})\rangle$. Then the Berry phase becomes

$$\begin{aligned} \tilde{\gamma}_n(t) &= i \int_{\vec{R}(0)}^{\vec{R}(t)} \langle \tilde{\psi}_n(\vec{R}) | \vec{\nabla}_{\vec{R}} | \tilde{\psi}_n(\vec{R}) \rangle \cdot d\vec{R} = i \int_{\vec{R}(0)}^{\vec{R}(t)} \langle \psi_n(\vec{R}) | e^{i\beta(\vec{R})} \vec{\nabla}_{\vec{R}} e^{-i\beta(\vec{R})} | \psi_n(\vec{R}) \rangle \cdot d\vec{R} \\ &= \gamma_n(t) + \beta(\vec{R}(t)) - \beta(\vec{R}(0)) \end{aligned}$$

Changing β only changes phases as a function of the endpoints of the path. Thus, we can eliminate the phase for any fixed path with $\vec{R}(t) \neq \vec{R}(0)$, but not simultaneously for all paths. In particular, if a particle takes two different paths to the same point, the difference in their phases cannot be redefined away. More simply, suppose the path is a loop, so that $\vec{R}(0) = \vec{R}(t)$. Then regardless of β we will have $\gamma_n = \tilde{\gamma}_n$. This suggests an important point about the Berry phase, which is that it is uniquely defined on closed paths, but not necessarily open ones.

Suppose that $\vec{R}(t)$ follows a closed curve C . Then we can write

$$\gamma_n[C] = \oint \underbrace{i \langle \psi_n | \vec{\nabla}_{\vec{R}} | \psi_n \rangle}_{\vec{\mathcal{A}}_n(\vec{R})} \cdot d\vec{R} = \oint \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R},$$

where we have defined the *Berry connection* $\vec{\mathcal{A}}_n(\vec{R}) = i \langle \psi_n | \vec{\nabla}_{\vec{R}} | \psi_n \rangle$. Note that it is real for the same reason that $\nu_n(t)$ is real.

In some cases, we can simplify $\gamma_n[C]$. If $N = 1$ then the integral is always zero, since the line integral of a closed curve in 1-d is always zero. In 2-d or 3-d we can use Green's theorem or Stokes's theorem respectively to simplify the computation of $\gamma_n[C]$. Let's focus on 3-d, because it contains 2-d as a special case. Then if S denotes the surface enclosed by curve C , we have

$$\oint_C \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R} = \iint_S (\vec{\nabla}_{\vec{R}} \times \vec{\mathcal{A}}_n) \cdot d\vec{a} \equiv \iint_S \vec{D}_n \cdot d\vec{a}.$$

Here we define the *Berry curvature* $\vec{D}_n = \vec{\nabla}_{\vec{R}} \times \vec{\mathcal{A}}_n$ and the infinitesimal unit of area $d\vec{a}$. We can write \vec{D}_n in a more symmetric way as follows:

$$(D_n)_i = i \sum_{j,k} \epsilon_{ijk} \frac{d}{dR_j} \langle \psi_n | \frac{d}{dR_k} | \psi_n \rangle = i \sum_{j,k} \epsilon_{ijk} \left(\frac{d \langle \psi_n |}{dR_j} \frac{d | \psi_n \rangle}{dR_k} + \langle \psi_n | \frac{d}{dR_j} \frac{d}{dR_k} | \psi_n \rangle \right).$$

Because ϵ_{ijk} is antisymmetric in j, k and $\frac{d}{dR_j} \frac{d}{dR_k}$ is symmetric, the second term vanishes and we are left with

$$\vec{D}_n = i(\vec{\nabla}_r \langle \psi_n |) \times (\vec{\nabla}_r | \psi_n \rangle). \quad (25)$$

Example: electron spin in a magnetic field. The Hamiltonian is

$$H = \mu \vec{\sigma} \cdot \vec{B} \quad \mu = \frac{e\hbar}{mc}.$$

Suppose that $\vec{B} = B\vec{r}$ where B is fixed and we slowly trace out a closed path in the unit sphere with \vec{r} . Suppose that we start in the state

$$|\vec{r}; +\rangle = |\vec{r}\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix} \quad \text{with} \quad \vec{r} = \begin{pmatrix} \sin(\theta) \cos(\phi) \\ \sin(\theta) \sin(\phi) \\ \cos(\theta) \end{pmatrix}$$

Then the adiabatic theorem states that we will remain in the state $|\vec{r}\rangle$ at later points, up to an overall phase. To compute the geometric phase observe that

$$\vec{\nabla} = \frac{d}{dr} \hat{r} + \frac{1}{r} \frac{d}{d\theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{d}{d\phi} \hat{\phi}.$$

Since $\frac{d}{dr} |\vec{r}\rangle = 0$ we have

$$\vec{\nabla} |\vec{r}\rangle = \frac{1}{2r} \underbrace{\begin{pmatrix} -\sin(\theta/2) \\ e^{i\phi} \cos(\theta/2) \end{pmatrix}}_{|\vec{-r}\rangle} \hat{\theta} + \frac{1}{r \sin \theta} \begin{pmatrix} 0 \\ ie^{i\phi} \sin(\theta/2) \end{pmatrix} \hat{\phi}.$$

This first term will not contribute to the Berry connection, and so we obtain

$$\vec{\mathcal{A}}_+(\vec{r}) = i \langle \vec{r} | \vec{\nabla} | \vec{r} \rangle = -\frac{1}{r} \frac{\sin^2(\theta/2)}{\sin(\theta)} \hat{\phi}.$$

Finally the Berry curvature is

$$\vec{D}_+ = \vec{\nabla} \times \vec{\mathcal{A}}_+ = \frac{1}{r \sin \theta} \frac{d}{d\theta} (\sin \theta \mathcal{A}_{+, \phi}) \hat{r} = -\frac{\hat{r}}{r^2 \sin \theta} \frac{d}{d\theta} \sin^2(\theta/2) = -\frac{1}{2r^2} \hat{r}.$$

For this last computation, observe that $\frac{d}{d\theta} \sin^2(\theta/2) = \frac{d}{d\theta} \frac{1-\cos \theta}{2} = \sin \theta$. We can now compute the Berry phase as

$$\gamma_+[C] = \iint_S \vec{D}_+ \cdot \underbrace{d\vec{a}}_{r^2 d\Omega \hat{r}} = -\frac{1}{2} \Omega.$$

Here $d\Omega$ is a unit of solid angle, and Ω is the solid angle contained by C .

What if we used a different parameterization for $|\vec{r}\rangle$? An equally valid choice is

$$|\vec{r}\rangle = \begin{pmatrix} e^{-i\phi} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}. \quad (26)$$

If we carry through the same computation we find that now

$$\vec{\mathcal{A}}_+ = \frac{1}{r} \frac{\cos^2(\theta/2)}{\sin(\theta)} \hat{\phi} \quad \text{and} \quad \vec{\mathcal{D}}_+ = -\frac{1}{2r^2} \hat{r}.$$

We see that the $\frac{d}{d\theta} \sin^2(\theta/2)$ was replaced by a $\frac{d}{d\theta} (-\cos^2(\theta/2))$ which gives the same answer. This is an example of the general principle that the Berry connection is sensitive to our choice of phase convention but the Berry curvature is not. Accordingly the Berry curvature can be observed in experiments.

What if we started instead with the state $|\vec{r}; -\rangle = |-\vec{r}\rangle$? Then a similar calculation would find that

$$\gamma_-[C] = \frac{1}{2}\Omega.$$

Since the two states pick up different phases, this can be seen experimentally if we start in a superposition of $|\vec{r}; +\rangle$ and $|\vec{r}; -\rangle$.

More generally, if we have a spin- s particle, then its z component of angular momentum can be anything in the range $-s \leq m \leq s$ and one can show that

$$\gamma_m[C] = -m\Omega.$$

There is much more that can be said about Berry's phase. An excellent treatment is found in the 1989 book *Geometric phases in physics* by Wilczek and Shapere. There is a classical analogue called Hannay's phase. Berry's phase also has applications to molecular dynamics and to understanding electrical and magnetic properties of Bloch states. We will see Berry's phase again when we discuss the Aharonov-Bohm effect in a few weeks.

3.3 Neutrino oscillations and the MSW effect

In this section we will discuss the application of the adiabatic theorem to a phenomenon involving solar neutrinos. The name *neutrino* means "little neutral one" and neutrinos are spin-1/2, electrically neutral, almost massless and very weakly interacting particles. Neutrinos were first proposed by Pauli in 1930 to explain the apparent violation of energy, momentum and angular momentum conservation in beta decay. (Since beta decay involves the decay of a neutron into a proton, an electron and an electron antineutrino, but only the proton and electron could be readily detected, there was an apparent anomaly.)

Their almost complete lack of interaction with matter (it takes 100 lightyears of lead to absorb 50% of a beam of neutrinos) has made many properties of neutrinos remain mysterious. Corresponding to the charged leptons e^-, e^+ (electron/positron), μ^-, μ^+ (muon/antimuon) and τ^-, τ^+ (tau/antitau), neutrinos (aka neutral leptons) also exist in three flavors: ν_e, ν_μ, ν_τ , with antineutrinos denoted $\bar{\nu}_e, \bar{\nu}_\mu, \bar{\nu}_\tau$. Most, but not all, interactions preserve lepton number, defined to be the number of leptons minus the number of antileptons. Indeed, most interactions preserve $\#e^- + \#\nu_e - \#e^+ - \#\bar{\nu}_e$ (electronic number) and similarly for muons and taus. However, these quantities are not conserved by neutrino oscillations. Even the total lepton number is violated by a phenomenon known as the chiral anomaly.

Solar neutrinos Solar neutrinos are produced via the p - p chain reaction, which converts (via a series of reactions)

$$4\,^1H = 4p^+ + 4e^- \mapsto \underbrace{2p^+ + 2n + 2e^-}_{\,^4He} + 2\nu_e.$$

The resulting neutrinos are produced with energies in the range 0.5-20MeV. Almost all of neutrinos produced in the sun are electron neutrinos.

Detection Neutrinos can be detected via inverse beta decay, corresponding to the reaction

$$A + \nu_e \mapsto A' + e^-,$$

where A, A' are different atomic nuclei. For solar neutrinos this will only happen for electron neutrinos because the reaction $A + \nu_\mu \mapsto A' + \mu^-$ will only happen for mu neutrinos carrying at least 108 MeV of kinetic energy. So it is easiest to observe electron neutrinos. However other flavors of neutrinos can also be detected via more complicated processes, such as neutrino-mediated disassociation of deuterium.

Observations of solar neutrinos The first experiment to detect cosmic neutrinos was the 1968 Homestake experiment, led by Ray Davis, which used 100,000 gallons of dry-cleaning fluid (C_2Cl_4) to detect neutrinos via the process $^{37}Cl + \nu_e \mapsto ^{37}Ar + e^-$. However, this only found about 1/3 as many neutrinos as standard solar models predicted.

In 2002, the Sudbury Neutrino Observatory (SNO) measured the total neutrino flux and found that once mu- and tau-neutrinos were accounted for, the total number of neutrinos was correct. Thus, somehow electron neutrinos in the sun had become mu and tau neutrinos by the time they reached the Earth.

Neutrino oscillations The first high-confidence observations of neutrino oscillations were by the Super Kamiokande experiment in 1998, which could distinguish electron neutrinos from muon neutrinos. Since neutrinos oscillate, they must have energy, which means they must have mass (if we wish to exclude more speculative theories, such as violations of the principle of relativity). This means that a neutrino, in its rest frame, has a Hamiltonian with eigenstates $|\nu_1\rangle, |\nu_2\rangle, |\nu_3\rangle$ that in general will be different from the flavor eigenstates $|\nu_e\rangle, |\nu_\mu\rangle, |\nu_\tau\rangle$ that participate in weak-interaction processes such as beta decay.

We will treat this in a simplified way by neglecting $|\nu_3\rangle$ and $|\nu_\tau\rangle$. So the Hamiltonian can be modeled as (in the $|\nu_e\rangle, |\nu_\mu\rangle$ basis)

$$H = \begin{pmatrix} E_e & \Delta \\ \Delta & E_\mu \end{pmatrix}, \quad (27)$$

where E_e, E_μ are the energies (possibly equal) of the electron and muon neutrinos and Δ represents a mixing term. Unfortunately, plugging in known parameter estimates for the terms in (27) would predict that roughly a 0.57 fraction of solar neutrinos would end up in the $|\nu_e\rangle$ state, so this still cannot fully explain our observations.

The MSW effect It turns out that this puzzle can be resolved by a clever use of the adiabatic theorem. Electron neutrinos scatter off of electrons and thus the Hamiltonian in (27) should be

modified to add a term proportional to the local density of electrons. Thus after some additional rearranging, we obtain

$$H = E_0 + \begin{pmatrix} -\Delta_0 \cos(2\theta) & \Delta_0 \sin(2\theta) \\ \Delta_0 \sin(2\theta) & \Delta_0 \cos(2\theta) \end{pmatrix} + \begin{pmatrix} CN_e & 0 \\ 0 & 0 \end{pmatrix}, \quad (28)$$

where Δ_0, θ come from (27) ($\theta \approx \pi/6$ is the “mixing angle” that measures how far the flavor states are from being eigenstates), C is a constant and $N_e = N_e(\vec{r})$ is the local electron density. If the neutrino is traveling at speed $\approx c$ in direction \hat{x} , then $\vec{r} \approx ct\hat{x}$. Thus we can think of N_e as time-dependent. We then can rewrite H as

$$\text{const} \cdot I + \left(\frac{CN_e(t)}{2} - \Delta_0 \cos(2\theta) \right) \sigma_z + \Delta_0 \sin(2\theta) \sigma_x. \quad (29)$$

This looks like the adiabatic Landau-Zener transition we studied in the last lecture, although here the σ_z term is no longer being swept from $-\infty$ to $+\infty$. Instead, near the center of the sun, $N_e(0)$ is large and the eigenstates are roughly $|\nu_e\rangle, |\nu_\mu\rangle$. For large t , the neutrinos are in vacuum, where their eigenstates are $|\nu_1\rangle, |\nu_2\rangle$.

If the conditions of the adiabatic theorem are met, then neutrinos that start in state $|\nu_e\rangle$ (in the center of the sun) will emerge in state $|\nu_2\rangle$ (at the surface of the sun). They will then remain in this state as they propagate to the Earth. It turns out that this holds for neutrinos of energies $\gtrsim 2\text{MeV}$. In this case, the probability of observing the neutrino on Earth in the $|\nu_e\rangle$ state (thinking of neutrino detectors as making measurements in the flavor basis) is $\sin^2(\theta)$, which gives more or less the observed value of 0.31.

3.4 Born-Oppenheimer approximation

Consider a system with N nuclei and n electrons. Write the Hamiltonian as

$$H = - \sum_{j=1}^N \frac{\hbar^2}{2M_j} \vec{\nabla}_{\vec{R}_j}^2 + H_{\text{el}}(\mathbf{R}). \quad (30)$$

Here $\mathbf{R} = (\vec{R}_1, \dots, \vec{R}_N)$ denotes the positions of the N nuclei and $H_{\text{el}}(\mathbf{R})$ includes all the other terms, i.e. kinetic energy of the electrons as well as the potential energy terms which include electron-electron, nuclei-nuclei and electron-nuclei interactions. Let \mathbf{r} denote all of the coordinates of the electrons. While (30) may be too hard to solve exactly, we can use a version of the adiabatic theorem to derive an approximate solution.

We will consider a product ansatz:

$$\Psi(\mathbf{R}, \mathbf{r}) = \gamma(\mathbf{R}) \Phi_{\mathbf{R}}(\mathbf{r}), \quad (31)$$

where the many-electron wavefunction is an eigenstate of the reduced Hamiltonian:

$$H_{\text{el}}(\mathbf{R}) \Phi_{\mathbf{R}}(\mathbf{r}) = E_{\text{el}}(\mathbf{R}) \Phi_{\mathbf{R}}(\mathbf{r}). \quad (32)$$

(Typically this eigenstate will be simply the ground state.) This is plausible because of the adiabatic theorem. If the nuclei move slowly then as this happens the electrons can rapidly adjust to remain in their ground states. Then once we have solved (32) we might imagine that we can substitute

back to solve for the nuclear eigenstates. We might guess that they are solutions to the following eigenvalue equation

$$\left(-\sum_{j=1}^N \frac{\hbar^2}{2M_j} \vec{\nabla}_{\vec{R}_j}^2 + E_{\text{el}}(\mathbf{R}) \right) \gamma(\mathbf{R}) = E \gamma(\mathbf{R}). \quad (33)$$

However, this is not quite right. If we apply $\vec{\nabla}_{\vec{R}_j}$ to (31) we obtain

$$\vec{\nabla}_{\vec{R}_j} \Psi(\mathbf{R}, \mathbf{r}) = (\vec{\nabla}_{\vec{R}_j} \gamma(\mathbf{R})) \Phi_{\mathbf{R}}(\mathbf{r}) + \gamma(\mathbf{R}) \vec{\nabla}_{\vec{R}_j} \Phi_{\mathbf{R}}(\mathbf{r}). \quad (34)$$

Using the adiabatic approximation we neglect the overlap of $\vec{\nabla}_{\vec{R}_j} \Psi(\mathbf{R}, \mathbf{r})$ with all states to $|\Phi_{\mathbf{R}}\rangle$. Equivalently we can multiply on the left by $\langle \Phi_{\mathbf{R}} |$. This results in

$$\begin{aligned} \int d^3\mathbf{r} \Phi_{\mathbf{R}}(\mathbf{r})^* \vec{\nabla}_{\vec{R}_j} \Psi(\mathbf{R}, \mathbf{r}) &= \vec{\nabla}_{\vec{R}_j} \gamma(\mathbf{R}) + \gamma(\mathbf{R}) \int d^3\mathbf{r} \Phi_{\mathbf{R}}(\mathbf{r})^* \vec{\nabla}_{\vec{R}_j} \Phi_{\mathbf{R}}(\mathbf{r}) \\ &= (\vec{\nabla}_{\vec{R}_j} - i\vec{\mathcal{A}}_j) \gamma(\mathbf{R}), \end{aligned}$$

where $\vec{\mathcal{A}}_j$ is the familiar Berry connection

$$\vec{\mathcal{A}}_j = i \langle \Phi_{\mathbf{R}} | \vec{\nabla}_{\vec{R}_j} | \Phi_{\mathbf{R}} \rangle. \quad (35)$$

We conclude that the effective Hamiltonian actually experienced by the nuclei should be

$$H_{\text{eff}} = \sum_{j=1}^N \frac{\hbar^2}{2M_j} (\vec{\nabla}_{\vec{R}_j} - i\vec{\mathcal{A}}_j)^2 + E_{\text{el}}(\mathbf{R}). \quad (36)$$

We will see these $\vec{\mathcal{A}}_j$ terms again when we discuss electromagnetism later in the semester. In systems of nuclei and atoms we need at least three nuclei before the $\vec{\mathcal{A}}_j$ terms can have an effect, for the same reason that we do not see a Berry phase unless we trace out a loop in a parameter space of dimension ≥ 2 .

The Born-Oppenheimer applies not just to nuclei and electrons but whenever we can divide a system into fast and slow-moving degrees of freedom; e.g. we can treat a proton as a single particle and ignore (or “integrate out”) the motion of the quarks within the proton. This is an important principle that we often take for granted. Some more general versions of Born-Oppenheimer are called “effective field theory” or the renormalization group.

4 Scattering

4.1 Preliminaries

One of the most important types of experiments in quantum mechanics is *scattering*. A beam of particles is sent into a potential and scatters off it in various directions. The angular distribution of scattered particles is then measured. In 8.04 we studied scattering in 1-d, and here we will study scattering in 3-d. This is an enormous field, and we will barely scratch the surface of it. In particular, we will focus on the following special case:

- *Elastic scattering*. The outgoing particle has the same energy as the incoming particle. This means we can model the particles being scattered off semi-classically, as a static potential $V(\vec{r})$. The other types of scattering are inelastic scattering, which can involve transformation of the particles involved or creation of new particles, and absorption, in which there is no outgoing particle.

- *Non-relativistic scattering.* This is by contrast with modern accelerators such as the LHC. However, non-relativistic scattering is still relevant to many cutting-edge experiments, such as modern search for cosmic dark matter (which is believed to be traveling at non-relativistic speeds).

Even this special case can teach us a lot of interesting physics. For example, Rutherford scattering¹ showed that atoms have nuclei, thereby refuting the earlier “plum pudding” model of atoms. This led to a model of atoms in which electrons orbit nuclei like planets, and resolving the problems of this model in turn was one of the early successes of quantum mechanics.

Scattering cross section: In scattering problems it is important to think about which physical quantities can be observed. The incoming particles have a flux that is measured in terms of number of particles per unit area per unit time, i.e. $\frac{d^2 N_{\text{in}}}{dA dt}$. If we just count the total number of scattered particles, then this is measured in terms of particles per time: $\frac{dN_{\text{scat}}}{dt}$. The ratio of these quantities has units of area and is called the *scattering cross section*:

$$\frac{\frac{dN_{\text{scat}}}{dt}}{\frac{d^2 N_{\text{in}}}{dA dt}} = \sigma. \quad (37)$$

To get a sense of why these are the right units, consider scattering of classical particles off of a classical hard sphere of radius a . If a particle hits the sphere it will scatter, and if it does not hit the sphere it will not scatter. Assume that the beam of particles is much wider than the target, i.e. each particle has trajectory $\vec{r} = (x_0, y_0, z_0 + vt)$ with $\sqrt{x_0^2 + y_0^2}$ given by a distribution with standard deviation that is $\gg a$. The particles that scatter will be the ones with $\sqrt{x_0^2 + y_0^2} \leq a$ which corresponds to a region with area πa^2 , which is precisely the cross-sectional area of the sphere. Since we have $\frac{dN_{\text{scat}}}{dt} = \frac{d^2 N_{\text{in}}}{dA dt} \pi a^2$, it follows that $\sigma = \pi a^2$. This simple example is good to keep in mind to have intuition about the meaning of scattering cross sections.

Differential cross-section: We can get more information out of an experiment by measuring the angular dependence of the scattered particles. The number of scattered particles can then be measured in terms of a rate *per solid angle*, i.e. $\frac{d^2 N_{\text{scat}}}{d\Omega dt}$. The resulting *differential cross-section* $\frac{d\sigma}{d\Omega}$ is defined to be

$$\frac{d\sigma}{d\Omega}(\theta, \phi) \equiv \frac{\frac{d^2 N_{\text{scat}}}{d\Omega dt}}{\frac{d^2 N_{\text{in}}}{dA dt}} \quad (38)$$

Here the spherical coordinates (θ, ϕ) denote the direction of the outgoing particles. It is conventional to define the axes so that the incoming particles have momentum in the \hat{z} direction, so θ is the angle between the scattered particle and the incoming beam (i.e. $\theta = 0$ means no change in direction and $\theta = \pi$ means backwards scattering) while ϕ is the azimuthal angle. Integrating over all angles gives us the full cross-section, i.e.

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}. \quad (39)$$

Quantum mechanical scattering: Assume that the incoming particle states are wavepackets that are large relative to the target. This allows us to approximate the incoming particles as plane wave, i.e.

$$\psi_{\text{in}} \propto e^{ikz - \frac{iEt}{\hbar}}, \quad (40)$$

¹Rutherford scattering is named after Ernest Rutherford for his 1911 explanation of the 1909 experiment which was carried out by Geiger and Marsden.

where $E = \frac{\hbar^2 k^2}{2m}$. Here we need to assume that the potential $V(\vec{r}) \rightarrow 0$ as $r \rightarrow \infty$ so that plane waves are solutions to the Schrödinger equation for large r . For the scattered wave, we should seek solutions satisfying

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi_{\text{scat}} = E \psi_{\text{scat}} \quad \text{as } r \rightarrow \infty \quad (41)$$

$$-\left(\frac{1}{r} \frac{d^2}{dr^2} r + \frac{1}{r^2} \hat{L}^2\right) \psi_{\text{scat}} = k^2 \psi_{\text{scat}} \quad \text{in spherical coordinates} \quad (42)$$

A general solution can be written as a superposition of separable solutions. Separable solutions to (42) can in turn be written as

$$r\psi(r, \theta, \phi) = u(r)f(\theta, \phi), \quad (43)$$

in terms of some functions $u(r), f(\theta, \phi)$. In terms of these (42) becomes

$$u''f + \underbrace{\frac{1}{r^2} u \hat{L}^2 f}_{\rightarrow 0 \text{ as } r \rightarrow \infty} + k^2 u f = 0. \quad (44)$$

Thus, for large r , we can cancel the f from each side and simply have $u'' = -k^2 u$, which has solutions $e^{\pm ikr}$. The e^{ikr} solution corresponds to outgoing waves and the e^{-ikr} solution to incoming waves. A scattered wave should be entirely outgoing, and so we obtain

$$\psi_{\text{scat}} \stackrel{r \rightarrow \infty}{=} \frac{f(\theta, \phi)}{r} e^{ikr - \frac{iEt}{\hbar}} \quad (45)$$

or more precisely

$$\psi_{\text{scat}} = \frac{f(\theta, \phi)}{r} e^{ikr - \frac{iEt}{\hbar}} + O\left(\frac{1}{r^2}\right). \quad (46)$$

Because the scattering is elastic, the k and E here are the same as for the incoming wave.

Time-independent formulation: As with 1-d scattering problems, the true scattering process is of course time-dependent, but the quantities of interest (transmission/reflection in 1-d, differential cross section in 3-d) can be extracted by solving the time-independent Schrödinger equation with suitable boundary conditions. In the true process, the incoming wave should really be a wavepacket with well-defined momentum $\approx (0, 0, k)$ and therefore delocalized position. The outgoing wave will be a combination of an un-scattered part, which looks like the original wave packet continuing forward in the \hat{z} direction, and a scattered part, which is a spherical outgoing wavepacket with a $f(\theta, \phi)$ angular dependence. However, we can treat the incoming wave instead as the static plane wave e^{ikz} and the scattered wave instead as the static outgoing wave $\frac{f(\theta, \phi)}{r} e^{ikr}$. (Both of these are when $r \rightarrow \infty$.) Thus we can formulate the entire scattering problem as a time-independent boundary-value problem. The high-level strategy is then to solve the Schrödinger equation subject to the boundary conditions

$$\psi(\vec{r}) \stackrel{r \rightarrow \infty}{=} e^{ikz} + \frac{f(\theta, \phi)}{r} e^{ikr}. \quad (47)$$

This is analogous to what we did in 1-D scattering, where the boundary conditions were that $\psi(x)$ should approach $e^{ikx} + Re^{-ikx}$ for $x \rightarrow -\infty$ and should approach Te^{ikx} for $x \rightarrow \infty$. As in the 1-D case, we have to remember that this equation is an approximation for a time-dependent problem. As a result when calculating observable quantities we have to remember not to include interference terms between the incoming and reflected waves, since these never both exist at the same point in time.

Relation to observables. In the 1-D case, the probabilities of transmission and reflection are $|T|^2$ and $|R|^2$ respectively. In the 3-d case, the observable quantities are the differential cross sections $\frac{d\sigma}{d\Omega}$. To compute these, first evaluate the incoming flux

$$\vec{S}_{\text{in}} = \frac{\hbar}{m} \text{Im} \psi_{\text{in}}^* \vec{\nabla} \psi_{\text{in}} = \frac{\hbar}{m} \text{Im} \left(e^{-ikz} \vec{\nabla} e^{ikz} \right) = \frac{\hbar k}{m} \hat{z} = v \hat{z} \quad (48)$$

In the last step we have used $v = \hbar k/m$. The units here are off because technically the wavefunction should be not e^{ikz} but something more like e^{ikz}/\sqrt{V} , where V has units of volume. But neglecting this factor in both the numerator and denominator of (38) will cause this to cancel out. Keeping that in mind, we calculate the denominator to be

$$\frac{d^2 N_{\text{in}}}{dA dt} = |\vec{S}_{\text{in}}| = v. \quad (49)$$

Similarly the outgoing flux is (using $\vec{\nabla} = \frac{\partial}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\phi}$)

$$\vec{S}_{\text{scat}} = \frac{\hbar}{m} \text{Im} \left(\frac{e^{-ikr}}{r} f^* i k \hat{r} \frac{e^{ikr}}{r} f + O\left(\frac{1}{r^3}\right) \right) = v \frac{\hat{r}}{r^2} |f|^2 + O(1/r^3). \quad (50)$$

To relate this to the flux per solid angle we use $d\vec{a} = r^2 d\Omega \hat{r}$ to obtain

$$\frac{d^2 N_{\text{scat}}}{d\Omega dt} = \vec{S}_{\text{scat}} \cdot d\vec{a} = (v \frac{\hat{r}}{r^2} |f|^2 + O(r^{-3})) \cdot r^2 d\Omega \hat{r} = |f|^2 v d\Omega + O(1/r). \quad (51)$$

We can neglect the $O(1/r)$ term as $r \rightarrow \infty$ (and on a side note, we see now why the leading-order term in \vec{S}_{scat} was $O(1/r^2)$) and obtain the simple formula

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2}. \quad (52)$$

The Optical Theorem. (52) is valid everywhere except at $\theta = 0$. There we have to also consider interference between the scattered and the unscattered wave. (Unlike the incoming wave, the outgoing unscattered does coexist with the scattered wave.) The resulting flux is

$$\vec{S}_{\text{out}} = \frac{\hbar}{m} \text{Im} \left(e^{-ikz} + \frac{f^*}{r} e^{-ikr} \right) \left(i k \hat{z} e^{ikz} + \frac{i k \hat{r}}{r} f e^{ikr} + O(1/r^2) \right) \quad (53a)$$

$$= \underbrace{v \hat{z}}_{\vec{S}_{\text{unscat}}} + \underbrace{v \frac{\hat{r}}{r^2} |f|^2}_{\vec{S}_{\text{scat}}} + \underbrace{v \text{Re} \left(\frac{\hat{z} f^*}{r} e^{ik(z-r)} + \frac{\hat{r} f}{r} e^{ik(r-z)} \right)}_{\vec{S}_{\text{interference}}} \quad (53b)$$

This last term can be thought of as the effects of interference. We will evaluate it for large r and for $\theta \approx 0$. Here $\hat{r} \approx \hat{z}$ and we define $\rho = \sqrt{x^2 + y^2}$ so that (to leading order) $r = z + \frac{\rho^2}{2z}$. Then

$$\int \vec{S}_{\text{inter}} \cdot d\vec{a} = v \int_0^{2\pi} d\phi \int_0^\infty \rho d\rho \frac{\hat{z}}{z} \left(f^* e^{-ik \frac{\rho^2}{2z}} + f e^{ik \frac{\rho^2}{2z}} \right) \quad (54a)$$

$$= 4\pi \frac{v}{z} \text{Re} \int_0^\infty \frac{d\rho^2}{2} f e^{\frac{ik\rho^2}{2z}} \quad (54b)$$

$$= \frac{2\pi v}{z} \text{Re} \int_0^\infty dy e^{\frac{iky}{2z}} f(0) = -\frac{4\pi v}{k} \text{Im} f(0) \quad (54c)$$

Since the outgoing flux should equal the incoming flux, we can define A to be the beam area and find

$$Av = Av + v \int d\Omega |f(\theta, \phi)|^2 - \frac{4\pi v}{k} \text{Im } f(0). \quad (55)$$

Thus we obtain the following identity, known as the *optical theorem*:

$$\int d\Omega |f(\theta, \phi)|^2 = \frac{4\pi}{k} \text{Im } f(0) \quad (56)$$

All this is well and good, but we have made no progress at all in computing $f(\theta, \phi)$. We will discuss two approximation methods: the partial wave method (which is exact, but yields nice approximations when k is very small) and the Born approximation, which is a good approximation when we are scattering off a weak potential. This is analogous to approximations we have seen before (see Table 1). We will discuss the Born approximation in Section 4.2 and the partial-wave

perturbation type	time-independent	time-dependent	scattering
small	TIPT	TDPT	Born
slow	WKB	adiabatic	partial wave

Table 1: Summary of approximation techniques for scattering problems.

technique in Section 4.3.

4.2 Born Approximation

Zooming out, we want to solve the following eigenvalue equation:

$$(\vec{\nabla}^2 + k^2)|\psi\rangle = U|\psi\rangle \quad \text{where} \quad U \equiv \frac{2m}{\hbar^2} V. \quad (57)$$

This looks like a basic linear algebra question. Can we solve it by inverting $(\vec{\nabla}^2 + k^2)$ to obtain

$$\psi \stackrel{?}{=} (\vec{\nabla}^2 + k^2)^{-1} U|\psi\rangle? \quad (58)$$

To answer this, we first review some basic linear algebra. Suppose we want to solve the equation

$$A\vec{x} = \vec{b} \quad (59)$$

for some normal matrix A . We can write $\vec{b} = A^{-1}\vec{x}$ only if A is invertible. Otherwise the solution will not be uniquely defined. More generally, suppose that our vectors live on a space V . Then we can divide up V as

$$V = \text{Im } A \oplus \ker A \quad \text{where} \quad \ker A = \{\vec{x}_0 : A\vec{x}_0 = 0\}. \quad (60)$$

If we restrict A to the subspace $\text{Im } A$ then it is indeed invertible. The solutions to (59) are then given by

$$\vec{x} = (A|_{\text{Im } A})^{-1}\vec{b} + \vec{x}_0 \quad \text{where} \quad \vec{x}_0 \in \ker A. \quad (61)$$

Returning now to the quantum case, the operator $(\vec{\nabla}^2 + k^2)$ is certainly not invertible. States satisfying $(\vec{\nabla}^2 + k^2)|\psi_0\rangle = 0$ exist, and are plane waves with momentum $\hbar k$. But if we restrict

$(\vec{\nabla}^2 + k^2)$ to the subspace of states with momentum $\neq \hbar k$ then it is invertible. Define the Green's operator G to be $(\vec{\nabla}^2 + k^2)|_{p \neq \hbar k}^{-1}$. The calculation of G is rather subtle and the details can be found in Griffiths. However, on general principles we can make a fair amount of progress. Since $(\vec{\nabla}^2 + k^2)$ is diagonal in the momentum basis, then G should be as well. Thus G should be written as an integral over $|\vec{p}\rangle\langle\vec{p}|$ times some function of \vec{p} . By Fourier transforming this function we can equivalently write G in terms of translation operators as

$$G = \int d^3\vec{r} G(\vec{r}) T_{\vec{r}} \quad \text{where} \quad T_{\vec{r}} \equiv e^{-i\frac{\vec{r}\cdot\vec{p}}{\hbar}}. \quad (62)$$

Let's go through this more concretely. In the momentum basis we have the completeness relation $\int d^3\vec{p} |\vec{p}\rangle\langle\vec{p}| = I$ which implies

$$\vec{\nabla}^2 + k^2 = \int d^3\vec{p} (-\hbar^2 p^2 + k^2) |\vec{p}\rangle\langle\vec{p}|. \quad (63)$$

To invert this we might naively write $G = \int' d^3\vec{p} (-\hbar^2 p^2 + k^2)^{-1} |\vec{p}\rangle\langle\vec{p}|$ where \int' denotes the integral over all \vec{p} with $p \neq \hbar k$. To handle the diverging denominator, one method is to write

$$G = \lim_{\epsilon \rightarrow 0} \int d^3\vec{p} (-\hbar^2 p^2 + k^2 + i\epsilon)^{-1} |\vec{p}\rangle\langle\vec{p}|. \quad (64)$$

Finally we can write this in the position basis according to (62) and obtain the position-space Green's function $G(\vec{r})$ by Fourier-transforming $(-\hbar^2 p^2 + k^2 + i\epsilon)^{-1}$. In Griffiths this integral is carried out obtaining the answer:

$$G(\vec{r}) = -\frac{e^{ikr}}{4\pi r}. \quad (65)$$

This function $G(\vec{r})$ is called a Green's function. We can thus write

$$G = \int d^3\vec{r} \frac{-e^{ikr}}{4\pi r} T_{\vec{r}}. \quad (66)$$

Having computed G , we can now solve (57) and obtain

$$|\psi\rangle = |\psi_0\rangle + GU|\psi\rangle \quad (67)$$

for some free-particle solution $|\psi_0\rangle$. Indeed for a scattering problem, we should have $\psi_0(\vec{r}) = e^{ikz}$. (67) is exact, but not very useful because $|\psi\rangle$ appears on both the LHS and RHS. However, it will let us expand $|\psi\rangle$ in powers of U .

The *first Born approximation* consists of replacing the $|\psi\rangle$ on the RHS of (67) by $|\psi_0\rangle$, thus yielding

$$|\psi\rangle = |\psi_0\rangle + GU|\psi_0\rangle. \quad (68)$$

The second Born approximation consists of using (68) to approximate $|\psi\rangle$ in the RHS of (67), which yields

$$|\psi\rangle = |\psi_0\rangle + GU(|\psi_0\rangle + GU|\psi_0\rangle) = |\psi_0\rangle + GU|\psi_0\rangle + GUGU|\psi_0\rangle. \quad (69)$$

Of course we could also rewrite (67) as $|\psi\rangle = (I - GU)^{-1}|\psi_0\rangle = \sum_{n \geq 0} (GU)^n |\psi_0\rangle$ (since $(I - GU)$ is formally invertible) and truncate this sum at some finite value of n .

These results so far have been rather abstract. Plugging in (65) and $\psi_0(\vec{r}) = e^{ikz}$ we find that the first Born approximation is

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3\vec{r}' \psi_0(\vec{r}') G(\vec{r} - \vec{r}') U(\vec{r}') \quad (70a)$$

$$= e^{ikz} - \int d^3\vec{r}' e^{ikz'} \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} U(\vec{r}') \quad (70b)$$

If we assume that the potential is short range and we evaluate this quantity for r far outside the range of U , then we will have $r \gg r'$ for all the points where the integral has a nonzero contribution. In this case $|\vec{r} - \vec{r}'| \approx r - \hat{r} \cdot \vec{r}'$. Let us further define

$$\vec{k} = k\hat{r} \quad \text{and} \quad \vec{k}' = k\hat{z}, \quad (71)$$

corresponding to the outgoing and incoming wavevectors respectively. Then we have (still in the first Born approximation)

$$\psi_{\text{scat}}(\vec{r}) = - \int d^3\vec{r}' e^{ikz'} \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} U(\vec{r}') \quad (72a)$$

$$\approx - \int d^3\vec{r}' e^{ikz'} \frac{e^{ikr - ik\hat{r} \cdot \vec{r}'}}{4\pi r} U(\vec{r}') \quad (72b)$$

$$= \left(- \int d^3\vec{r}' e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}'} \frac{U(\vec{r}')}{4\pi} \right) \frac{e^{ikr}}{r} \quad (72c)$$

The quantity in parentheses is then $f(\theta, \phi)$. If we define $\tilde{V}(\vec{q})$ to be the Fourier transform of $V(\vec{r})$ then we obtain

$$f_1(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \tilde{V}(\vec{k}' - \vec{k}), \quad (73)$$

where f_1 refers to the first Born approximation. One very simple example is when $V(\vec{r}) = V_0\delta(\vec{r})$. Then we simply have $f_1 = -\frac{mV_0}{2\pi\hbar^2}$.

A further simplification occurs in the case when $V(\vec{r})$ is centrally symmetric. Then

$$\tilde{V}(\vec{q}) \equiv \int d^3\vec{r} V(r) e^{i\vec{q} \cdot \vec{r}} = 2\pi \int_0^\infty dr \int_{-1}^1 d\mu r^2 V(r) e^{iqr\mu} = \frac{4\pi}{q} \int_0^\infty dr r V(r) \sin(qr). \quad (74)$$

Finally the momentum transfer $\vec{q} = \vec{k}' - \vec{k}$ satisfies $q = 2k \sin(\theta/2)$.

One application of this (see Griffiths for details) is the Yukawa potential: $V(r) = -\beta e^{-\mu r}/r$. The first Born approximation yields

$$f_1^{\text{Yukawa}}(\theta) = -\frac{2m\beta^2}{\hbar^2(\mu^2 + q^2)}.$$

Taking $\beta = -eQ$ and $\mu = 0$ recovers Rutherford scattering, with

$$f_1^{\text{Rutherford}}(\theta) = \frac{2meQ}{\hbar^2 q^2} = \frac{meQ}{2\hbar^2 k^2 \sin^2(\theta/2)}.$$

A good exercise is to rederive the Born approximation by using Fermi's Golden Rule and counting the number of outgoing states in the vicinity of a given \vec{k} . See section 7.11 of Sakurai for details. Another version is in Merzbacher, section 20.1.

Rigorous derivation of Green's functions. The above derivation of G was somewhat informal. However, once the form of $G(\vec{r})$ is derived informally or even guessed, it can be verified that $(\vec{\nabla}^2 + k^2)G$ acts as the identity on all states with no component in the null space of $(\vec{\nabla}^2 + k^2)$. This is the content of Griffiths problem 11.8. Implicit is that we are working in a Schwartz space which rules out exponentially growing wavefunctions, and in turn implies that $\vec{\nabla}^2$ has only real eigenvalues and is in fact Hermitian. A more rigorous derivation of the Born approximation can also be obtained by using time-dependent perturbation theory as described by Sakurai section 7.11 and Merzbacher section 20.1. I particularly recommend the discussion in Merzbacher.

4.3 Partial Waves

In this section assume we have a central potential, i.e. $V(\vec{r}) = V(r)$. Since our initial conditions are invariant under rotation about the \hat{z} axis, our scattering solutions will also be independent of ϕ (but not θ).

Assume further that

$$\lim_{r \rightarrow \infty} r^2 V(r) = 0. \quad (75)$$

We will see the relevance of this condition shortly.

A wavefunction with no ϕ dependence can be written in terms of Legendre polynomials² (corresponding to the $m = 0$ spherical harmonics) as

$$\psi(r, \theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos \theta). \quad (76)$$

If we define $u_l(r) = r R_l(r)$, then the eigenvalue equation becomes (for each l)

$$-u_l'' + V_{\text{eff}} u_l = k^2 u_l \quad \text{where} \quad V_{\text{eff}} \equiv \frac{2mV}{\hbar^2} + \frac{l(l+1)}{r^2}. \quad (77)$$

If (75) holds, then for sufficiently large r , we can approximate $V_{\text{eff}} \approx l(l+1)/r^2$. In this region the solutions to (77) are given by the *spherical Bessel functions*. Redefining $x \equiv kr$ and using the assumption $V_{\text{eff}} \approx l(l+1)/r^2$, (77) becomes

$$u_l'' - \frac{l(l+1)}{x^2} u_l = -u_l. \quad (78)$$

This has two linearly independent solutions: $x j_l(x)$ and $x n_l(x)$ where $j_l(x), n_l(x)$ are the spherical Bessel functions of the first and second kind respectively, and are defined as

$$j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin(x)}{x} \quad \text{and} \quad n_l(x) = -(-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\cos(x)}{x} \quad (79)$$

These can be thought of as “sin-like” and “cos-like” respectively. For $l = 0, 1$, (79) becomes

$$j_0(x) = \frac{\sin(x)}{x} \quad j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \quad (80a)$$

$$n_0(x) = -\frac{\cos(x)}{x} \quad n_1(x) = -\frac{\cos(x)}{x^2} - \frac{\sin(x)}{x} \quad (80b)$$

²What are Legendre polynomials? One definition starts with the orthogonality condition $\int_{-1}^1 P_m(x) P_n(x) dx = \frac{2}{2n+1} \delta_{mn}$. (The δ_{mn} is the important term here; $\frac{2}{2n+1}$ is a somewhat arbitrary convention.) Then if we apply the Gram-Schmidt procedure to $1, x, x^2, \dots$, we obtain the Legendre polynomials $P_0 = 1, P_1 = x, P_2 = \frac{1}{2}(3x^2 - 1), \dots$. Thus any degree- n polynomial can be written as a linear combination of P_0, \dots, P_n and vice-versa.

The reason for (76) is that if $\psi(r, \theta)$ is independent of ϕ then we can write it as a power series in r and z , or equivalently r and $\frac{z}{r} = \cos(\theta)$. These power series can always be written in the form of (76).

One can check (by evaluating the derivatives in (79) repeatedly and keeping only the lowest power of $1/x$) that as $x \rightarrow \infty$ we have the asymptotic behavior

$$j_l(x) \rightarrow \frac{1}{x} \sin(x - l\pi/2) \quad \text{and} \quad n_l(x) \rightarrow -\frac{1}{x} \cos(x - l\pi/2). \quad (81)$$

On the other hand, in the $x \rightarrow 0$ limit we can keep track of only the lowest power of x to find that as $x \rightarrow 0$ we have

$$j_l(x) \rightarrow \frac{x^l}{(2l+1)!!} \quad \text{and} \quad n_l(x) \rightarrow -\frac{(2l-1)!!}{x^{l+1}}, \quad (82)$$

where $(2l+1)!! \equiv (2l+1)(2l-1)\cdots 3 \cdot 1$.

If j_l and n_l are sin-like and cos-like, it will be convenient to define functions that resemble incoming and outgoing waves. These are the spherical Hankel functions of the first and second kind:

$$h_l^{(1)} = j_l + in_l \quad \text{and} \quad h_l^{(2)} = j_l - in_l \quad (83)$$

For large r , $h_l^{(1)}(kr) \rightarrow (-i)^{l+1} \frac{e^{ikr}}{kr}$, and so our scattered wave should be proportional to $h_l^{(1)}$. More precisely, $R_l(r)$ (i.e. the angular-momentum- l component) should be proportional to $h_l^{(1)}(kr)$. Putting this together we get

$$\psi(r, \theta) \stackrel{\text{when } V \approx 0}{=} e^{ikz} + \underbrace{\sum_{l \geq 0} c_l h_l^{(1)}(kr) P_l(\cos(\theta))}_{\psi_{\text{scat}}}, \quad (84)$$

for some coefficients c_l . It will be convenient to write the c_l in terms of new coefficients a_l as $c_l = k i^{l+1} (2l+1) a_l$, so that we have

$$\psi_{\text{scat}}(r, \theta) \stackrel{\text{when } V \approx 0}{=} k \sum_{l \geq 0} i^{l+1} (2l+1) a_l h_l^{(1)}(kr) P_l(\cos(\theta)) \quad (85)$$

$$\stackrel{\text{when } r \rightarrow \infty}{=} \underbrace{\sum_{l \geq 0} (2l+1) a_l P_l(\cos(\theta))}_{f(\theta)} \frac{e^{ikr}}{r} \quad (86)$$

We can then compute the differential cross-section in terms of the a_l

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left| \sum_l (2l+1) a_l P_l(\cos(\theta)) \right|^2. \quad (87)$$

Recall that the Legendre polynomials satisfy the orthogonality relation

$$\int_{-1}^1 dz P_l(z) P_{l'}(z) = \delta_{l,l'} \frac{2}{2l+1}. \quad (88)$$

Thus we can calculate

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi \sum_l (2l+1) |a_l|^2. \quad (89)$$

While the differential cross section involves interference between different values of l , the total cross section is simply given by an incoherent sum over l . Intuitively this is because we can think of l and θ as conjugate observables, analogous to momentum and position. If we measure the probability

of observing something at a particular position, we will see interference effects between different momenta, but if we integrate over all positions, these will go away.

The beauty of the partial-wave approach is that it reduces to a series of 1-d scattering problems, one for each value of l . We have written down the form of the scattered wave. For the incoming wave, we need to express e^{ikz} in the form of (76). From the arguments above we can see that e^{ikz} should have form $\sum_l (A_l j_l(kr) + B_l n_l(kr)) P_l(\cos \theta)$. The specific solution is given by *Rayleigh's formula* which we state without proof:

$$e^{ikz} = e^{ikr \cos \theta} = \sum_{l \geq 0} i^l (2l+1) j_l(kr) P_l(\cos \theta) \quad (90)$$

Plugging this in, we find that in the $V \approx 0$ region we have

$$\psi(r, \theta) \stackrel{\text{when } V \approx 0}{=} \sum_{l \geq 0} i^l (2l+1) P_l(\cos \theta) \left[\underbrace{j_l(kr)}_{\text{plane wave}} + \underbrace{ika_l h_l^{(1)}(kr)}_{\text{scattered}} \right] \quad (91)$$

$$= \frac{1}{2} \sum_{l \geq 0} i^l (2l+1) P_l(\cos \theta) \left[\underbrace{h_l^{(1)}(kr)}_{\text{outgoing}} (1 + 2ika_l) + \underbrace{h_l^{(2)}(kr)}_{\text{incoming}} \right] \quad (92)$$

Now we have really expressed this as a series of 1-d scattering problems. Here comes the crucial simplifying move. Because we are assuming that the collision is elastic, probability and angular-momentum conservation means that "what goes in must come out"; i.e.

$$|1 + 2ika_l| = 1. \quad (93)$$

The outgoing wave's amplitude must have the same absolute value as the incoming wave's amplitude. We can rewrite (93) by introducing the *phase shift* δ_l defined by

$$1 + 2ika_l = e^{2i\delta_l}. \quad (94)$$

The factor of 2 is conventional. We can rewrite (94) to solve for a_l as

$$a_l = \frac{2e^{i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l} \sin(\delta_l)}{k} = \frac{1}{k} \frac{1}{\cot(\delta_l) - i}. \quad (95)$$

Many equivalent expressions are also possible. In terms of the phase shifts, we can write

$$f(\theta) = \frac{1}{k} \sum_l (2l+1) P_l(\cos \theta) e^{i\delta_l} \sin(\delta_l) \quad (96)$$

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2(\delta_l). \quad (97)$$

As an application we can verify that this satisfies the optical theorem. Observe that $P_l(1) = 1$ for all l . Thus

$$\frac{4\pi}{k} \text{Im } f(0) = \frac{4\pi}{k} \frac{1}{k} \sum_l (2l+1) P_l(1) \sin^2(\delta_l) = \sigma. \quad (98)$$

Another easy application is *partial-wave unitarity*, which bounds the total amount of scattered wave with angular momentum l . Define $\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2(\delta_l)$, so that $\sigma = \sum_l \sigma_l$. Then using $\sin^2(\delta_l) \leq 1$ we have

$$\sigma_l \leq \frac{4\pi}{k^2} (2l+1). \quad (99)$$

This bound is called “partial-wave unitarity.”

How to compute phase shifts. Let us look again at the $r \rightarrow \infty$ solution. We can use the fact that overall phase and normalization don’t matter to obtain

$$R_l(r) = h_l^{(1)}(kr)e^{2i\delta_l} + h_l^{(2)}(kr) \quad (100a)$$

$$= (1 + e^{2i\delta_l})j_l(kr) + i(e^{2i\delta_l} - 1)n_l(kr) \quad (100b)$$

$$\propto \cos(\delta_l)j_l(kr) - \sin(\delta_l)n_l(kr) \quad (100c)$$

$$\propto j_l(kr) - \tan(\delta_l)n_l(kr) \quad (100d)$$

Suppose that we know the interior solution $R_l(r)$ for $r \leq b$ and that $V(r) \approx 0$ for $r > b$. Then we can compute the phase shift by matching $\frac{R_l'(r)}{R_l(r)}$ for $r = b \pm \epsilon$.

Here is a simple example. Consider a hard sphere of radius b . Then $R_l(r) = 0$ for $r \leq b$ and we have

$$j_l(kb) - \tan(\delta_l)n_l(kb) = 0 \implies \delta_l = \tan^{-1} \left(\frac{j_l(kb)}{n_l(kb)} \right). \quad (101)$$

One particularly simple case is when $l = 0$. Then

$$\delta_0 = \tan^{-1} \left(\frac{j_0(kb)}{n_0(kb)} \right) = \tan^{-1} \left(\frac{\frac{\sin(kb)}{kb}}{-\frac{\cos(kb)}{kb}} \right) = -\tan^{-1}(\tan(kb)) = -kb. \quad (102)$$

It turns out that in general repulsive potentials yield negative phase shifts.

What about larger values of l ? Suppose that $kb \ll 1$. Then using the $x \rightarrow 0$ approximations for $j_l(x), n_l(x)$, we obtain

$$\delta_l \xrightarrow{k \rightarrow 0} \tan^{-1} \left(\frac{(kb)^{2l+1}}{(2l+1)!!(2l-1)!!} \right) \approx \frac{(kb)^{2l+1}}{2l+1!!(2l-1)!!} \sim (kb)^{2l+1}. \quad (103)$$

Thus the $l = 0$ scattering dominates. In terms of cross-sections, we have

$$\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2(\delta_l) \approx \frac{4\pi}{(2l+1)((2l-1)!!)^4} (kb)^{4l} b^2. \quad (104)$$

For $l = 0$ this is $4\pi b^2$ which four times the classical value of πb^2 , and for higher value of l this drops exponentially (assuming $kb \ll 1$). Even if $kb > 1$ this drops exponentially once $l \gg kb$, which confirms our intuition that the angular momentum should be on the order of $\hbar kb$.

Another way to think about this reason to favor low values of l is because the $l(l+1)/r^2$ term in V_{eff} forms an angular momentum “barrier” that prevents low-energy incoming waves from penetrating to small enough r to see the potential $V(r)$.

The high-energy limit. The partial wave approximation is easiest to use in the low- k limit because then we can restrict our attention to a few values of l , or even just $l = 0$. But for the hard sphere we can also evaluate the $kb \gg 1$ limit. In this case we expect to find angular momenta up to $l_{\text{max}} \equiv kb$. Thus we approximate the total cross section by

$$\sigma \approx \frac{4\pi}{k^2} \sum_{l=0}^{l_{\text{max}}} (2l+1) \sin^2(\delta_l). \quad (105)$$

The phases δ_l will vary over the entire range from 0 to 2π so we simply approximate $\sin^2(\delta_l)$ by its average value of $1/2$. Thus we obtain

$$\sigma \approx \frac{2\pi}{k^2} \sum_{l=0}^{kb} (2l+1) = 2\pi b^2. \quad (106)$$

This is now *twice* the classical result. Even though the particles are moving quickly they still diffract like waves. One surprising consequence is that even though a hard sphere leaves a shadow, there is a small bright spot at the center of the shadow. Indeed the optical theorem predicts that $\text{Im } f(0) = \frac{k}{4\pi} \sigma \approx kb^2/2$. Thus $|f(0)|^2 \geq (kb)^2 b^2/4$. For a further discussion of this bright spot and the role it played in early 19th-century debates about whether light is a particle and/or a wave, look up “Arago spot” on wikipedia.

Phase shifts. As we have seen, scattering can be understood in terms of phase shifts. Now we describe a simple physical way of seeing this. If $V = 0$ then a plane wave has $u_0(r) = \sin(kr)$, due to the $u_0(0) = 0$ boundary condition. When there is scattering, the phase shift δ_0 will become nonzero and we will have

$$u_0(r) = \sin(kr + \delta_0).$$

If the potential is attractive then the phase will oscillate more rapidly in the scattering region and so we will have $\delta_0 > 0$ while if it is repulsive then the phase will oscillate more slowly and we will have $\delta_0 < 0$. See Fig. 2 for an illustration.

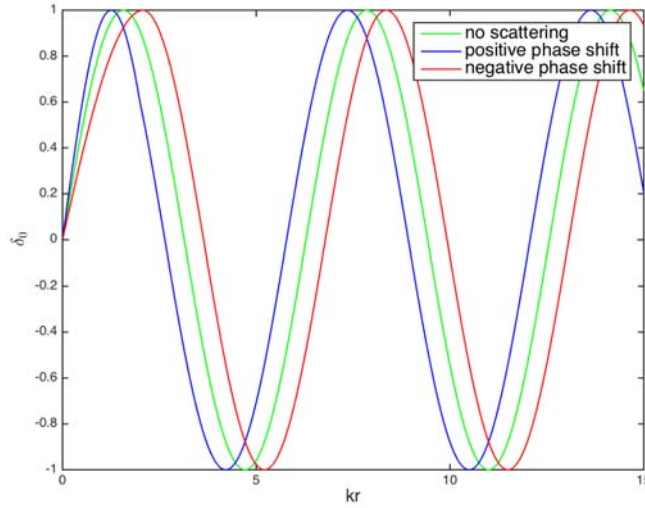


Figure 2: The phase shift δ_0 is positive for attractive potentials and negative for repulsive potentials.

Scattering length. In the regime of low k it turns out that many potentials behave qualitatively like what we have seen with the hard sphere, with a characteristic length scale called a “scattering length.” To derive this suppose there is some b such that $V(r) \approx 0$ for $r \geq b$. In this region we have $u_0(r) \approx \sin(kb + \delta_0)$ (neglecting normalization). In the vicinity of b we have

$$u_0(r) \approx u_0(b) + u'_0(b)(r - b).$$

If we extrapolate to smaller values of r our approximation hits 0 at $r = a$ where

$$a = b - \frac{u_0(b)}{u'_0(b)} = b - \frac{\tan(kb + \delta_0)}{k}.$$

Using the tan addition formula and taking the limit $k \rightarrow 0$ we find

$$a = b - \frac{1}{k} \frac{\tan(kb) + \tan(\delta_0)}{1 - \tan(kb)\tan(\delta_0)} \approx b - \frac{kb + \tan(\delta_0)}{k} = -\frac{\tan(\delta_0)}{k}. \quad (107)$$

Rearranging we have $\tan(\delta_0) = -ka$, and in the $ka \ll 1$ limit this yields

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2(\delta_0) \approx 4\pi a^2,$$

which is again the hard sphere result. Similar results hold for larger value of l . Thus the scattering length can be thought of as an effective size of a scattering target.

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8.06 Quantum Physics III
Spring 2016

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8.06 Spring 2016 Lecture Notes

3. Entanglement, density matrices and decoherence

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Last updated: May 18, 2016

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1 Axioms of Quantum Mechanics

We begin with a (very) quick review of some concepts from 8.04 and 8.05.

1.1 One system

States are given by unit vectors $|\psi\rangle \in V$ for some vector space V .

Observables are Hermitian operators $\hat{A} \in \mathcal{L}(V)$.

Measurements

Suppose $\hat{A} = \sum_{i=1}^d \lambda_i |v_i\rangle\langle v_i|$ for $\{|v_1\rangle \dots, |v_d\rangle\}$ an orthonormal basis of eigenvalues and (for simplicity) each λ_i distinct. If we measure observable \hat{A} on state $|\psi\rangle$ then the outcomes are distributed according to $\Pr[\lambda_i] = |\langle\psi|v_i\rangle|^2$.

Time evolution is given by Schrödinger's equation: $i\hbar \frac{\partial}{\partial t} |\psi\rangle = H|\psi\rangle$ where H is the Hamiltonian.

Heisenberg picture We can instead evolve operators in time using

$$i\hbar \frac{\partial}{\partial t} \hat{A}_H = [\hat{A}_H, H_H]. \quad (1)$$

Time-independent solution

If the Hamiltonian does not change in time, then the time evolution operator for time t is the unitary operator $\mathcal{U} = e^{-\frac{iHt}{\hbar}}$. The state evolves according to $|\psi(t)\rangle = \mathcal{U}|\psi(0)\rangle$ in the Schrödinger picture or the operator evolves according to $\hat{A}_H(t) = \mathcal{U}^\dagger \hat{A}_H(0) \mathcal{U}$ in the Heisenberg picture.

Systems are described by a pair (V, H) .

1.2 Two systems

Let's see how things change when we have two quantum systems: (V_1, H_1) and (V_2, H_2) .

States are given by unit vectors $|\psi\rangle \in V$ where

$$V = V_1 \otimes V_2 \equiv \text{span}\{|\psi_1\rangle \otimes |\psi_2\rangle : |\psi_1\rangle \in V_1, |\psi_2\rangle \in V_2\}.$$

A special case are the *product states* of the form $|\psi_1\rangle \otimes |\psi_2\rangle$. States that are not product are called *entangled*.

Observables are still Hermitian operators $\hat{A} \in \mathcal{L}(V)$. A general observable may involve interactions between the two systems. Local observables are of the form $\hat{A} \otimes I$, $I \otimes \hat{B}$ or more generally $\hat{A} \otimes I + I \otimes \hat{B}$, and correspond to properties that can be measured without interacting the two systems.

Measurements

The usual measurement rule still holds for collective measurements. But when only one system is measured, we need a way to explain what happens to the other system. Suppose we measure the first system using the orthonormal basis $\{|v_1\rangle, \dots, |v_d\rangle\}$. (Equivalently, we measure an operator with distinct eigenvalues and with eigenvectors $|v_1\rangle, \dots, |v_d\rangle$.) If the overall system is in state $|\psi\rangle$, then the first step is to write $|\psi\rangle$ as

$$|\psi\rangle = \sum_{i=1}^d \sqrt{p_i} |v_i\rangle \otimes |w_i\rangle,$$

for some unit vectors $|w_1\rangle, \dots, |w_d\rangle$ (not necessarily orthogonal) and some p_1, \dots, p_d such that $p_i \geq 0$ and $\sum_{i=1}^d p_i = 1$.

Then the probability of outcome i is p_i and the residual state in this case is $|v_i\rangle \otimes |w_i\rangle$.

Time evolution is still given by Schrödinger's equation, but now the joint Hamiltonian of two non-interacting systems is

$$H = H_1 \otimes I + I \otimes H_2. \quad (2)$$

Interactions can add more terms, such as the $\frac{q_1 q_2}{|\vec{r}_1 - \vec{r}_2|}$ Coulomb interaction, which generally cannot be written in this way. Note that a Hamiltonian term of the form $\hat{A}_1 \otimes \hat{A}_2$ *does* represent an interaction; e.g. $\sigma_z \otimes \sigma_z$ has energy ± 1 depending on whether the two spins have Z components pointing in the same or opposite directions.

Time-independent solution

For a Hamiltonian of the form in (2), the time evolution operator is

$$\mathcal{U} = e^{-\frac{iHt}{\hbar}} = e^{-\frac{iH_1 t}{\hbar}} \otimes e^{-\frac{iH_2 t}{\hbar}}.$$

You should convince yourself that this second equality is true. Of course if the Hamiltonian contains interactions then \mathcal{U} will generally not be of this form.

These principles are actually profoundly different from anything we have seen before. For example, consider the number of degrees of freedom. One d -level system needs d complex numbers to describe (neglecting normalization and the overall phase ambiguity) but N d -level systems need d^N complex numbers to describe, instead of dN . This exponential extravagance is behind the power of quantum computers, which will be discussed briefly at the end of the course, if time permits. It also seemed intuitively wrong to many physicists in the early 20th century, most notably including Einstein. The objections of EPR [A. Einstein, B. Podolsky and N. Rosen, *Physical Review*, **47** 777–780 (1935)] led to Bell's theorem, which we saw in 8.05 and will review on pset 6. Here, though, we will consider a simpler problem.

1.3 The problem of partial measurement

Let us revisit the scenario where we measure part of an entangled state. Suppose that Alice and Bob each have a spin-1/2 particle in the singlet state

$$|\psi\rangle = \frac{|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle}{\sqrt{2}} \quad (3)$$

(The singlet is an arbitrary but nice choice. The argument would be essentially the same for any entangled state.) Imagine that Alice and Bob are far apart so that they should not be able to quickly send messages to one another.

Now suppose that Alice decides to measure her state in the $\{|+\rangle, |-\rangle\}$ basis. Using the above rules we find that the outcomes are as described in Table 1.

Alice's outcome	joint state	Bob's state
$\text{Pr}[+] = \frac{1}{2}$	$ +\rangle \otimes -\rangle$	$ -\rangle$
$\text{Pr}[-] = \frac{1}{2}$	$ -\rangle \otimes +\rangle$	$ +\rangle$

Table 1: Outcomes when Alice measures her half of the singlet state (3) in the $\{|+\rangle, |-\rangle\}$ basis.

What can we say about Bob's state after such a measurement? It is not a deterministic object, but rather an *ensemble* of states, each with an associated probability. For this we use the notation

$$\{(p_1, |\psi_1\rangle), \dots, (p_m, |\psi_m\rangle)\} \quad (4)$$

to indicate that state $|\psi_i\rangle$ occurs with probability p_i . The numbers p_1, \dots, p_m should form a probability distribution, meaning that they are nonnegative reals that sum to one. The states $|\psi_i\rangle$ should be unit vectors but do not have to be orthogonal. In fact, the number m could be much larger than the dimension d , and could even be infinite; e.g. we could imagine a state with some coefficients that are given by a Gaussian distribution. We generally consider m to be finite because it keeps the notation simple and doesn't sacrifice any important generality.

In the example where Alice measures in the $\{|+\rangle, |-\rangle\}$ basis, Bob is left with the ensemble

$$\left\{ \left(\frac{1}{2}, |+\rangle \right), \left(\frac{1}{2}, |-\rangle \right) \right\}. \quad (5)$$

What if Alice chooses a different basis? Recall from 8.05 that if $\vec{n} \in \mathbb{R}^3$ is a unit vector then a spin-1/2 particle pointing in that direction has state

$$|\vec{n}\rangle \equiv |\mathbf{n}; +\rangle = \cos \frac{\theta}{2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi} |-\rangle. \quad (6)$$

Here $(1, \theta, \phi)$ are the polar coordinates for \vec{n} ; i.e. $n_x = \sin \theta \cos \phi$, $n_y = \sin \theta \sin \phi$, and $n_z = \cos \theta$. The notation $|\mathbf{n}; +\rangle$ was what we used in 8.05 and $|\vec{n}\rangle$ will be the notation used in 8.06 in contexts where it is clear that we are talking about spin states. The orthonormal basis $\{|\mathbf{n}; +\rangle, |\mathbf{n}; -\rangle\}$ in our new notation is denoted $\{|\vec{n}\rangle, |-\vec{n}\rangle\}$.

Suppose that Alice measures in the $\{|\vec{n}\rangle, |-\vec{n}\rangle\}$ basis. It can be shown (see 8.05 notes or Griffiths §12.2) that for any \vec{n} ,

$$|\psi\rangle = \frac{|\vec{n}\rangle \otimes |-\vec{n}\rangle - |-\vec{n}\rangle \otimes |\vec{n}\rangle}{\sqrt{2}}. \quad (7)$$

Thus, for any choice of \vec{n} , the two outcomes are equally likely and in each case Bob is left with a spin pointing in the opposite direction, as described in Table 2.

Alice's outcome	joint state	Bob's state
$\Pr[\vec{n}] = \frac{1}{2}$	$ \vec{n}\rangle \otimes -\vec{n}\rangle$	$ -\vec{n}\rangle$
$\Pr[-\vec{n}] = \frac{1}{2}$	$ -\vec{n}\rangle \otimes \vec{n}\rangle$	$ \vec{n}\rangle$

Table 2: Outcomes when Alice measures her half of the singlet state (3) in the $\{|\vec{n}\rangle, |-\vec{n}\rangle\}$ basis.

This leaves Bob with the ensemble

$$\left\{ \left(\frac{1}{2}, |\vec{n}\rangle \right), \left(\frac{1}{2}, |-\vec{n}\rangle \right) \right\}. \quad (8)$$

Uh-oh! At this point, our elegant theories of quantum mechanics have run into a number of problems.

- **Theory isn't closed.** When we combine two systems with tensor product we get a new system, meaning a new vector space and a new Hamiltonian. It still fits the definition of a quantum system. But when we look at the state of a subsystem, we do not get a single quantum state, we get an ensemble. Thus, if we start with states being represented by unit vectors, we are inevitably forced into having to use *ensembles* of vectors instead.
- **Ensembles aren't unique.** Any choice of \vec{n} will give Bob a different ensemble. We expect our physical theories to give us unique answers, but here we cannot uniquely determine which ensemble is the right one for Bob. Note that other choices of measurement can leave Bob with different ensembles as well; e.g. if Alice flips a coin and uses that to choose between two measurements settings, then Bob will have a distribution over four states, each occurring with probability 1/4.
- **Time travel?!** If Bob *could* distinguish between these different ensembles (including the case in which Alice does nothing and he still holds half of an entangled state), then Alice could instantaneously communicate to Bob with her choice of measurement basis (or perhaps her choice of whether to measure at all or not). According to special relativity, there is a different inertial frame in which this process looks like Alice sending a message backwards in time. This rapidly leads to trouble...

Fortunately density operators solve all three problems! As a bonus, they are far more elegant than ensembles.

2 Density operators

2.1 Introduction and definition

We would like to develop a theory of states that combines *randomness* and *quantum mechanics*. So it is worth reviewing how both randomness and quantum mechanics can be viewed as two different ways of generalizing classical states. For simplicity, consider a classical system which can be in d different states labelled $1, 2, \dots, d$. The quantum mechanical generalization of this would be to consider complex d -dimensional unit vectors while the probabilistic generalization would be nonnegative real d -dimensional vectors whose entries sum to one. These can be thought of as two incomparable generalizations of the classical picture. We are interested in considering both generalizations at once so that we consider state spaces that are both probabilistic and quantum. We summarize these different choices of state spaces in Table 3.

	classical	quantum
deterministic	$\{1, \dots, d\}$	$ \psi\rangle \in \mathbb{C}^d$ s.t. $\langle\psi \psi\rangle = 1$
probabilistic	$p_1, \dots, p_d \geq 0$ s.t. $p_1 + \dots + p_d = 1$	ensembles? density operators?

Table 3: Different theories yield different state spaces.

What do we put in the fourth box (probabilistic quantum) of Table 3? One possibility is to put ensembles of quantum states, as defined in (4). Besides the drawbacks mentioned in the previous section, these also have the flaw that of involving an unbounded number of degrees of freedom. For example, let's take a spin-1/2 particle (i.e. $d = 2$), so our quantum states are of the form $c_+|+\rangle + c_-|-\rangle$. Then one such probability distribution is $|+\rangle$ with probability 1/3, $|-\rangle$ with probability 1/2 and $\frac{|+\rangle - i|-\rangle}{\sqrt{2}}$ with probability 1/6. Another distribution is $\cos(\theta)|+\rangle + \sin(\theta)|-\rangle$ where θ is distributed according to a Gaussian with mean 0 and variance σ^2 .

This works, but there are an infinite number of degrees of freedom, even if we start with a single lousy electron spin! Surely nature would not be so cruel.

Another drawback with this approach is that different distributions can give the same measurement statistics for all possible measurements. As a result, many of these infinite degrees of freedom turn out to be simply redundant.

To see how this works, suppose that we have a discrete distribution where state $|\psi_a\rangle$ occurs with probability p_a , for $a = 1, \dots, m$. Consider an observable \hat{A} . The expectation of \hat{A} with respect to this ensemble is:

$$\begin{aligned}
\sum_{a=1}^m p_a \langle \psi_a | \hat{A} | \psi_a \rangle &= \sum_{a=1}^m p_a \text{tr}[\langle \psi_a | \hat{A} | \psi_a \rangle] && \text{since tr has no effect on } 1 \times 1 \text{ matrices} \\
&= \sum_{a=1}^m p_a \text{tr}[\hat{A} |\psi_a\rangle \langle \psi_a|] && \text{cyclic property of the trace} \\
&= \text{tr} \left[\hat{A} \underbrace{\sum_{a=1}^m p_a |\psi_a\rangle \langle \psi_a|}_{\text{density matrix } \rho} \right] && \text{linearity of the trace} \\
&= \text{tr}[\hat{A} \rho] && \text{nice simple formula} \\
&= \langle \hat{A}, \rho \rangle && \text{alternate interpretation}
\end{aligned}$$

We see that the measurement statistics are a function of the distribution only via the *density operator* $\rho = \sum_{a=1}^m p_a |\psi_a\rangle \langle \psi_a|$. This has about d^2 degrees of freedom, by contrast with $O(d)$ degrees of freedom for known quantum states and with the ∞ degrees of freedom associated with ensembles. This already solves one of the problems of ensembles, namely their use of unlimited amounts of redundant information.

This argument used only discrete distributions over \mathbb{C}^d but the extension to continuous distributions and/or infinite-dimensional states is straightforward.

Facts about traces: Let X be a matrix of dimension $m \times n$ and Y a matrix of dimension $n \times m$. In general these will not be square, but XY and YX both are, so their traces are well-defined. In fact, they are equal! A quick calculation shows

$$\text{tr}[XY] = \sum_{i=1}^m \sum_{j=1}^n X_{i,j} Y_{j,i} = \text{tr}[YX]. \quad (9)$$

This is called the *cyclic property of the trace* because it is often applied to traces of long strings of matrices. For example, we can repeatedly apply (9) (using curly braces to indicate which blocks of matrices we are calling X and Y) to obtain

$$\text{tr}[\underbrace{ABC}_X \underbrace{D}_Y] = \text{tr}[\underbrace{DAB}_X \underbrace{C}_Y] = \text{tr}[\underbrace{CDA}_X \underbrace{B}_Y] = \text{tr}[BCDA] \quad (10)$$

The trace can also be used to define an inner product on operators. Define

$$\langle X, Y \rangle \equiv \text{tr}[X^\dagger Y] = \sum_{i,j} X_{i,j}^* Y_{i,j}. \quad (11)$$

From this last expression we see that $\langle X, Y \rangle$ is equivalent to turning X and Y into vectors in the natural way (just listing all the elements in order) and taking the conventional inner product between those vectors.

2.2 Examples

2.2.1 Pure states

If we know the state is $|\psi\rangle$, then the density matrix is $|\psi\rangle\langle\psi|$. Observe that there is no phase ambiguity ($|\psi\rangle \mapsto e^{i\phi}|\psi\rangle$ leaves the density matrix unchanged) and each $|\psi\rangle$ gives rise to a distinct density matrix. Such density matrices are called *pure states*, and sometimes this terminology is also used when talking about wavefunctions, to justify not using the density matrix formalism. By contrast, all other density matrices are called *mixed states*.

2.2.2 Spin-1/2 pure states

Let us consider the special case of pure states when $d = 2$, corresponding to a spin-1/2 particle. If $|\vec{n}\rangle = \cos(\frac{\theta}{2})|+\rangle + \sin(\frac{\theta}{2})e^{i\phi}|-\rangle$ then

$$\begin{aligned} |\vec{n}\rangle\langle\vec{n}| &= \begin{pmatrix} \cos^2(\frac{\theta}{2}) & \cos(\frac{\theta}{2})\sin(\frac{\theta}{2})e^{-i\phi} \\ \cos(\frac{\theta}{2})\sin(\frac{\theta}{2})e^{i\phi} & \sin^2(\frac{\theta}{2}) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \cos^2(\frac{\theta}{2}) - \frac{1}{2} & 0 \\ 0 & \sin^2(\frac{\theta}{2}) - \frac{1}{2} \end{pmatrix} + \cos\frac{\theta}{2}\sin\frac{\theta}{2} \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \\ &= \frac{I}{2} + \frac{\cos(\theta)}{2}\sigma_z + \frac{\sin(\theta)}{2}(\cos(\phi)\sigma_x + \sin(\phi)\sigma_y) \\ &= \frac{I + \vec{n} \cdot \vec{\sigma}}{2} \end{aligned}$$

This result is beautiful enough to frame.

$$\boxed{|\vec{n}\rangle\langle\vec{n}| = \frac{I + \vec{n} \cdot \vec{\sigma}}{2}} \quad (12)$$

With this in hand we can return to the example of Alice measuring half of a singlet state. Whatever her choice of \vec{n} , Bob's density matrix is

$$\frac{1}{2}|\vec{n}\rangle\langle\vec{n}| + \frac{1}{2}|-\vec{n}\rangle\langle-\vec{n}| = \frac{1}{2} \frac{I + \vec{n} \cdot \vec{\sigma}}{2} + \frac{1}{2} \frac{I - \vec{n} \cdot \vec{\sigma}}{2} = \frac{I}{2}. \quad (13)$$

This rules out their earlier attempts at instantaneous signaling (and later we will prove this in more generality). Bob's density matrix fully determines the results of any measurement he makes, and it is independent of Alice's choice of \vec{n} .

2.2.3 The maximally mixed state

If $\{|v_1\rangle, \dots, |v_d\rangle\}$ are an orthonormal basis, and each occurs with probability $1/d$, then the resulting density matrix is

$$\rho = \frac{1}{d} \sum_{i=1}^d |v_i\rangle\langle v_i| = \frac{I}{d}, \quad (14)$$

independent of the choice of basis. This is called the *maximally mixed state*. The previous example was the $d = 2$ case of this: a $1/2$ probability of spin-up and $1/2$ probability of spin-down results in the same density matrix, *no matter which direction “up” refers to*.

The continuous distribution over all unit vectors in \mathbb{C}^d also yields the same density matrix, although this is a harder calculation.

2.2.4 Multiple decompositions

Consider the distribution where $|+\rangle$ occurs with probability $2/3$ and $|-\rangle$ with probability $1/3$. The density matrix is

$$\frac{2}{3}|+\rangle\langle+| + \frac{1}{3}|-\rangle\langle-| = \begin{pmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}. \quad (15)$$

Now consider the distribution

$$\begin{aligned} |\psi_1\rangle &\equiv \sqrt{\frac{2}{3}}|+\rangle + \sqrt{\frac{1}{3}}|-\rangle && \text{with probability } 1/2 \\ |\psi_2\rangle &\equiv \sqrt{\frac{2}{3}}|+\rangle - \sqrt{\frac{1}{3}}|-\rangle && \text{with probability } 1/2 \end{aligned}$$

The density matrix is now

$$\frac{1}{2}|\psi_+\rangle\langle\psi_+| + \frac{1}{2}|\psi_-\rangle\langle\psi_-| = \frac{1}{2} \begin{pmatrix} \frac{2}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{1}{3} \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \frac{2}{3} & -\frac{\sqrt{2}}{3} \\ -\frac{\sqrt{2}}{3} & \frac{1}{3} \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}. \quad (16)$$

One lesson is that we shouldn't take the probabilities p_a too seriously; i.e. they are not uniquely determined by the density matrix. Neither is the property of the states in the ensemble being orthogonal.

2.2.5 Thermal states

Introduce a Hamiltonian $H = \sum_{i=1}^d E_i |i\rangle\langle i|$. We can think of this classically, as saying that state i has energy E_i . In this case, the Boltzmann distribution at temperature T is $p_i = e^{-\beta E_i}/Z$, where $Z = \sum_{i=1}^d e^{-\beta E_i}$, $\beta = 1/k_B T$ and $k_B = 1.380688 \cdot 10^{-23} \text{ J/K}$ is Boltzmann's constant. In the quantum setting, “state i ” is replaced by $|i\rangle$. The resulting density matrix is

$$\rho = \sum_{i=1}^d p_i |i\rangle\langle i| = \frac{\sum_{i=1}^d e^{-\beta E_i} |i\rangle\langle i|}{Z} = \frac{e^{-\beta H}}{Z} = \frac{e^{-\beta H}}{\text{tr} e^{-\beta H}} \quad (17)$$

This is known as the *Gibbs state* or the *thermal state*. It describes the state of a quantum system at thermal equilibrium.

One specific example comes from NMR. Consider a proton spin in a magnetic field, say a 11.74 Tesla field in the \hat{z} direction. At this field strength, the proton spin will experience the Hamiltonian $H = -\omega_0 \sigma_z$ where $\omega_0 \approx 500$ MHz. (In fact, if you buy a 11.74T superconducting magnet, the vendor will probably call it a “500 MHz” magnet for this reason. It could also reasonably be called a 500K magnet because of its price.) The thermal state is

$$\begin{aligned}\rho &= \frac{e^{-\beta H}}{\text{tr} e^{-\beta H}} = \frac{e^{\beta \omega_0} |+\rangle\langle +| + e^{-\beta \omega_0} |-\rangle\langle -|}{e^{\beta \omega_0} + e^{-\beta \omega_0}} \\ &\approx \frac{(1 + \beta \omega_0) |+\rangle\langle +| + (1 - \beta \omega_0) |-\rangle\langle -|}{2} \\ &= \frac{I}{2} + \frac{\beta \omega_0}{2} \sigma_z.\end{aligned}$$

Let $T = 300$ K, which is close to room temperature. Then $1/\beta \approx 6.25$ THz and so $\beta \omega_0 \approx 10^{-4}$. This is the “polarization” of the state. In an NMR experiment we can think of a $\frac{1}{2} + 10^{-4}$ fraction of spins aligning with the external field and a $\frac{1}{2} - 10^{-4}$ fraction of the spins anti-aligning with the external field at thermal equilibrium. This means that observables are effectively attenuated by a factor of (in this case) 10^{-4} .

3 The general rule for density operators

We know what makes a vector a valid probability distribution or a valid quantum wave-vector. What makes an operator a valid density operator? One answer is “ ρ is a valid density operator if there exists $p_1, \dots, p_m, |\psi_1\rangle, \dots, |\psi_m\rangle$ such that $\rho = \sum_a p_a |\psi_a\rangle\langle \psi_a|$, $p_1, \dots, p_m \geq 0$, $p_1 + \dots + p_m = 1$ and $\langle \psi_a | = \langle \psi_i |$ for each i .” This is somewhat unsatisfactory if we want to build a theory where the density operators are the fundamental objects.

Fortunately, there is a simple answer.

Theorem 1. *If a $d \times d$ matrix ρ is a density matrix for some ensemble of quantum states then*

1. $\text{tr} \rho = 1$.
2. $\rho \succeq 0$.

Conversely, for any $d \times d$ matrix ρ satisfying these two conditions, there exists an ensemble $\{p_a, |\psi_a\rangle\}_{1 \leq a \leq m}$ such that $\rho = \sum_{a=1}^m p_a |\psi_a\rangle\langle \psi_a|$. Here m can be taken to be the rank of ρ .

The inequality $\rho \succeq 0$ means that ρ is *positive semidefinite*, which is defined to mean that $\langle \psi | \rho | \psi \rangle \geq 0$ for all $|\psi\rangle$. It is the matrix analogue of being nonnegative.

3.1 Positive semidefinite matrices

We say that a square matrix A is positive semidefinite if $\langle \psi | A | \psi \rangle \geq 0$ for all $|\psi\rangle$. Physically, A might be an observable that takes on only nonnegative values. Or it might be a density matrix. If furthermore A is Hermitian, then there are three equivalent ways to characterise the condition of being positive semidefinite.

Theorem 2. *If $A = A^\dagger$ then TFAE (the following are equivalent)*

1. For all $|\psi\rangle$, $\langle \psi | A | \psi \rangle \geq 0$.
2. All eigenvalues of A are nonnegative.

3. There exists a matrix B such that $A = B^\dagger B$. (This is called a Cholesky factorization.)

To get intuition for this last condition, observe that for 1×1 matrices, it is the statement that a real number $x \geq 0$ iff $x = z^* z$ for some complex z .

Proof of Theorem 2. Since A is Hermitian, we can write $A = \sum_{i=1}^d \lambda_i |e_i\rangle\langle e_i|$ for some orthonormal basis $\{|e_1\rangle, \dots, |e_d\rangle\}$ and some real $\lambda_1, \dots, \lambda_d$.

(1 \rightarrow 2): Take $|\psi\rangle = |e_i\rangle$. Then $0 \leq \langle \psi | A | \psi \rangle = \langle e_i | A | e_i \rangle = \lambda_i$.

(2 \rightarrow 3): Let $B = \sum_{i=1}^d \sqrt{\lambda_i} |e_i\rangle\langle e_i|$. As an aside, one can show that B satisfies $A = B^\dagger B$ if and only if $B = \sum_{i=1}^d \sqrt{\lambda_i} |e_i\rangle\langle f_i|$ for some orthonormal basis $\{|f_1\rangle, \dots, |f_d\rangle\}$. Sometimes we say that $B = \sqrt{A}$, by analogy to the scalar case.

(3 \rightarrow 1): For any $|\psi\rangle$, let $|\varphi\rangle = B|\psi\rangle$. Then $\langle \psi | A | \psi \rangle = \langle \psi | B^\dagger B | \psi \rangle = \langle \varphi | \varphi \rangle \geq 0$. \square

3.2 Proof of the density-matrix conditions

Here we prove Theorem 1. Start with an ensemble $\{p_i, |\psi_i\rangle\}_{1 \leq i \leq m}$. Define $\rho = \sum_{i=1}^m p_i |\psi_i\rangle\langle \psi_i|$.

- Then $\rho^\dagger = \sum_{i=1}^m p_i^* |\psi_i\rangle\langle \psi_i| = \rho$, since $p_i = p_i^*$. Thus ρ is Hermitian.
- Next, define $B = \sum_{i=1}^m \sqrt{p_i} |\psi_i\rangle\langle i|$. Then $\rho = B^\dagger B$, implying that $\rho \succeq 0$.
- Finally, $\text{tr} \rho = \sum_{i=1}^m p_i \text{tr} |\psi_i\rangle\langle \psi_i| = \sum_{i=1}^m p_i = 1$.

To prove the other direction, suppose that $\text{tr} \rho = 1$ and $\rho \succeq 0$. By Theorem 2, $\rho = \sum_{i=1}^d \lambda_i |e_i\rangle\langle e_i|$ for $\{|e_1\rangle, \dots, |e_d\rangle\}$ an orthonormal basis and each $\lambda_i \geq 0$. Additionally $\text{tr} \rho = \sum_{i=1}^d \lambda_i = 1$. Thus we can take $p_i = \lambda_i$ and now ρ is the density matrix corresponding to the ensemble $\{p_i, |e_i\rangle\}_{1 \leq i \leq d}$. If $\text{rank} \rho < d$, then the sum only needs $\text{rank} \rho$ terms.

3.3 Application to spin-1/2 particles: the Bloch ball

The geometry of the set of density matrices is unfortunately not quite as simple as the state spaces we have encountered previously. Pure quantum states form a ball (modulo the phase ambiguity) and probability distributions form a simplex. Intersections of planes (such as $\text{tr}[\rho] = 1$) with the set of positive semidefinite matrices are called *spectrahedra*, and apart from the wonderful name, I will not explore their general properties here.

However, the case of $d = 2$ is indeed simple and elegant. Given a Hermitian 2×2 matrix A , when is it a valid density matrix? First, if it is Hermitian then we can express it as

$$A = \frac{a_0 I + a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3}{2}$$

for some real numbers a_0, a_1, a_2, a_3 . The factor of 2 in the denominator is arbitrary, but we will see later that it simplifies things. If A is a density matrix, then $1 = \text{tr}[A] = a_0$. Thus, $A = \frac{I + \vec{a} \cdot \vec{\sigma}}{2}$ with $\vec{a} \equiv (a_1, a_2, a_3)$. We saw in 8.05 that $\text{eig}(\vec{a} \cdot \vec{\sigma}) = \pm |\vec{a}|$. Thus $\text{eig}(A) = \frac{1 \pm |\vec{a}|}{2}$. A is psd iff these are both nonnegative, which is true iff $|\vec{a}| \leq 1$.

This proves that the set of two-dimensional density matrices is precisely equal to the set

$$\frac{I + \vec{a} \cdot \vec{\sigma}}{2} : |\vec{a}| \leq 1 \quad . \quad (18)$$

Geometrically this looks like the unit ball in \mathbb{R}^3 . The pure states form the surface of the ball, corresponding to the case $|\vec{a}| = 1$. The maximally mixed state $I/2$ corresponds to $\vec{a} = 0$. In general, $|\vec{a}|$ can be thought of as the “purity” of a state.

This set is called the *Bloch ball*. The unit vectors at the surface are called the *Bloch sphere*. These have nothing to do with Bloch states or Bloch’s theorem (which arise in the solution of periodic potentials) except for the name of the inventor.

Beware also that for $d > 2$, the set of density matrices is no longer a ball and there is no longer a canonical way to quantify “purity.” However, notions of entropy do exist and are used in fields such as quantum statistical mechanics.

4 Dynamics of density matrices

4.1 Schrödinger equation

The Schrödinger equation states that

$$\frac{\partial}{\partial t}|\psi\rangle = -\frac{i}{\hbar}H|\psi\rangle \quad (19a)$$

$$\frac{\partial}{\partial t}\langle\psi| = \frac{i}{\hbar}\langle\psi|H \quad (19b)$$

$$\frac{\partial}{\partial t}|\psi\rangle\langle\psi| = -\frac{i}{\hbar}(H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H) = -\frac{i}{\hbar}[H, |\psi\rangle\langle\psi|] \quad (19c)$$

$$\frac{\partial}{\partial t} \sum_{a=1}^m p_a |\psi_a\rangle\langle\psi_a| = -\frac{i}{\hbar} [H, \sum_{a=1}^m p_a |\psi_a\rangle\langle\psi_a|] \quad (19d)$$

We conclude that the density matrix evolves in time according to

$$\boxed{i \hbar \frac{\partial}{\partial t} \rho = [H, \rho]}. \quad (20)$$

This is reminiscent of the Heisenberg equation of motion for operators, but with the opposite sign

$$i \hbar \frac{\partial}{\partial t} \hat{A}_H = [\hat{A}_H, H_H]. \quad (21)$$

One way to explain the different signs is that states and observables are dual to each other, in the sense that they appear in the expectation value as $\langle\hat{A}, \rho\rangle$.

Another way to talk about quantum dynamics is in terms of unitary transformations. If a system undergoes Hamiltonian evolution for a finite time then this evolution can be described by a unitary operator \mathcal{U} , so that state $|\psi\rangle$ gets mapped to $\mathcal{U}|\psi\rangle$. In this case $|\psi\rangle\langle\psi|$ is mapped to $\mathcal{U}|\psi\rangle\langle\psi|\mathcal{U}^\dagger$. By linearity, a general density matrix ρ is then mapped to $\mathcal{U}\rho\mathcal{U}^\dagger$.

4.2 Measurement

A similar argument shows that if we measure ρ in the orthonormal basis $\{|v_1\rangle, \dots, |v_d\rangle\}$, then the probability of outcome j is $\langle v_j | \rho | v_j \rangle$ and the post-measurement state is $|v_j\rangle\langle v_j|$. The fastest way to see this is to consider the observable $|v_j\rangle\langle v_j|$ which has eigenvalue 1 (corresponding to obtaining outcome $|v_j\rangle$) and eigenvalue 0 repeated $d - 1$ times (corresponding to the orthogonal outcomes). Then we use the fact that $\langle\hat{A}\rangle = \text{tr}[\hat{A}\rho]$ and set $\hat{A} = |v_j\rangle\langle v_j|$.

An alternate derivation is to decompose $\rho = \sum_{a=1}^m p_a |\psi_a\rangle\langle\psi_a|$. Then $\Pr[j|a] = |\langle v_j|\psi_a\rangle|^2$ and

$$\begin{aligned}\Pr[j] &= \sum_{a=1}^m p_a \Pr[j|a] \\ &= \sum_{a=1}^m p_a |\langle v_j|\psi_a\rangle|^2 \\ &= \sum_{a=1}^m p_a \langle v_j|\psi_a\rangle\langle\psi_a|v_j\rangle \\ &= \langle v_j| \left(\sum_{a=1}^m p_a |\psi_a\rangle\langle\psi_a| \right) |v_j\rangle \\ &= \langle v_j|\rho|v_j\rangle\end{aligned}$$

It should be reassuring that, even though we used the ensemble decomposition in this derivation, the final probability we obtained depends only on ρ .

What if we forget the measurement outcome, or never knew it (e.g. someone else measures the state while our back is turned)? Then ρ is mapped to

$$\sum_{j=1}^d \langle v_j|\rho|v_j\rangle |v_j\rangle\langle v_j| = \sum_{j=1}^d |v_j\rangle\langle v_j|\rho|v_j\rangle\langle v_j|. \quad (22)$$

Here it is important to note that density matrices, like probability distributions, represent not only objective states of the world but also subjective states; in other words, they describe our knowledge about a state. So subjective uncertainty (i.e. the state “really is” something definite but we don’t know what it is) will have implications for the density matrix.

If we now write ρ from (22) as a matrix in the $|v_1\rangle, \dots, |v_d\rangle$ basis, this looks like

$$\begin{pmatrix} \rho_{1,1} & 0 & \dots & 0 \\ 0 & \rho_{2,2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & \rho_{d,d} \end{pmatrix}$$

Can we unify measurement and unitary evolution the way that we have unified the probabilistic and quantum pictures of states? For example, how should we model an atom in an excited state undergoing fluorescence? We will return to this topic later when we discuss *open quantum systems* and *quantum operations*. However, already we are equipped to handle the phenomenon of decoherence, which is the monster lurking in the closet of every quantum mechanical experiment.

4.3 Decoherence

Unitary operators correspond to reversible operations: if U is a valid unitary time evolution then so is U^\dagger . In terms of Hamiltonians, evolution according to $-H$ will reverse evolution according to H . But other quantum processes cause an irreversible loss of information. Irreversible quantum processes are generally called “decoherence.” This somewhat imprecise term refers to the fact that this information loss is always associated with a loss of “coherence” and with quantum systems

becoming more like classical systems. In what follows we will illustrate it via a series of examples, but will not give a general definition.

Let's warm up with the concept of a *mixture*. If state $|\psi_a\rangle$ occurs with probability p_a , then the density matrix is $\sum_a p_a |\psi_a\rangle\langle\psi_a|$. But what if we have an ensemble of density matrices? e.g. $\{(p_1, \rho_1), \dots, (p_m, \rho_m)\}$ Then the “average” density matrix is

$$\rho = \sum_{a=1}^m p_a \rho_a. \quad (23)$$

We can use this to model *random unitary evolution*. Suppose that our state experiences a random Hamiltonian. Model this by saying that unitary \mathcal{U}_a occurs with probability p_a for $a = 1, \dots, m$. This corresponds to the map

$$\rho \mapsto \sum_{a=1}^m p_a \mathcal{U}_a \rho \mathcal{U}_a^\dagger. \quad (24)$$

Let's see how this can explain how coherence is lost in simple quantum systems. Suppose we start with the density matrix

$$\rho = \begin{pmatrix} \rho_{+,+} & \rho_{+,-} \\ \rho_{-,+} & \rho_{-,-} \end{pmatrix}$$

and choose a random unitary to perform as follows: with probability $1-p$ we do nothing and with probability p we perform a unitary transformation equal to σ_z . This corresponds to the ensemble of unitary transformations $\{(1-p, I), (p, \sigma_z)\}$. The density matrix is then mapped to

$$\begin{aligned} \rho' &\equiv (1-p)I\rho I^\dagger + p\sigma_z\rho\sigma_z^\dagger \\ &= (1-p) \begin{pmatrix} \rho_{+,+} & \rho_{+,-} \\ \rho_{-,+} & \rho_{-,-} \end{pmatrix} + p \begin{pmatrix} \rho_{+,+} & -\rho_{+,-} \\ -\rho_{-,+} & \rho_{-,-} \end{pmatrix} \\ &= \begin{pmatrix} \rho_{+,+} & (1-2p)\rho_{+,-} \\ (1-2p)\rho_{-,+} & \rho_{-,-} \end{pmatrix} \end{aligned}$$

If $p = 0$ then this of course corresponds to doing nothing, and if $p = 1$, we simply have $\rho' = \sigma_z\rho\sigma_z$. In between we see that the diagonal terms remain the same, but the off-diagonal terms are reduced in absolute value. The diagonal terms correspond to the probability of outcomes we would observe if we measured in the \hat{z} basis, and so it is not surprising that a \hat{z} rotation would not affect these. However, the off-diagonal terms reduce just as we would expect for a vector that is averaged with a rotated version of itself. If $p = 1/2$, then the off-diagonal terms are completely eliminated, meaning that all polarization in the \hat{x} and \hat{y} directions has been eliminated. One way to see this is that the \hat{x} and \hat{y} polarization of $\sigma_z\rho\sigma_z$ is opposite to that of ρ . Thus averaging ρ and $\sigma_z\rho\sigma_z$ leaves zero polarization in the \hat{x} - \hat{y} plane.

With a series of examples, I will illustrate that:

- Decoherence can be achieved in several ways that look different but have the same results.
- Decoherence destroys some quantum/wave-like effects, such as interference.
- This also involves the loss of information, often of phase information.

5 Examples of decoherence

5.1 Looking inside a Mach-Zehnder interferometer

This example is physically unrealistic (in one place) but makes the decoherence phenomenon clearest to see.

A Mach-Zehnder interferometer is depicted in Fig. 1.

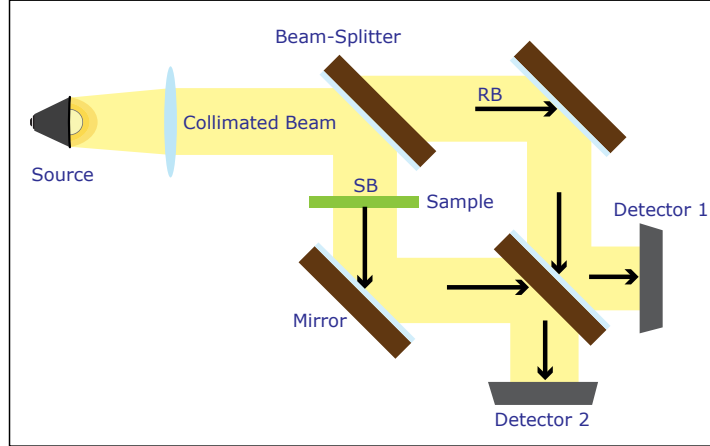


Image by MIT OpenCourseWare, adapted from the wikipedia article on [Mach-Zehnder](#) interferometers.

Figure 1: Mach-Zehnder interferometer. Image taken from the wikipedia article with this name.

At each point the photon can take one of two possible paths, which we denote by the states $|1\rangle$ and $|2\rangle$. Technically $|1\rangle$ means photon number in one mode and zero in the other modes, and similarly for $|2\rangle$. Also, we use $|1\rangle, |2\rangle$ to first denote the two inputs to the first beam splitter, then the two possible paths through the interferometer, and finally the two outputs of the second beam splitter leading to the detectors.

Each beam splitter can be modeled as a unitary operator. If they are “50-50” beam splitters, then this operator is

$$U_{\text{bs}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Thus, a photon entering in state $|1\rangle$ will go through the first beam splitter and be transformed into the state $\frac{|1\rangle + |2\rangle}{\sqrt{2}}$, corresponding to an even superposition of both paths. Assuming the paths have the same length and refractive index, it will have the same state when it reaches the second beam splitter. At this point the state will be mapped to

$$U_{\text{bs}} \frac{|1\rangle + |2\rangle}{\sqrt{2}} = \frac{|1\rangle + |2\rangle + |1\rangle - |2\rangle}{2} = |1\rangle$$

and the first detector will click with probability 1.

This is very different from what we’d observe if a particle entering a 50-50 beam splitter chose randomly which path to take. In that case, both detectors would click half the time.

The usual reason to build a Mach-Zehnder experiment, though, is not only to demonstrate the wave nature of light, but to measure something. Suppose we put some object in one of the paths so that light passing through it experiences a phase shift of θ . This corresponds to the unitary transformation

$$U_{\text{ph}} \equiv \begin{pmatrix} e^{i\theta} & 0 \\ 0 & 1 \end{pmatrix}. \quad (25)$$

Our modified experiment now corresponds to the sequence $U_{\text{bs}}U_{\text{ph}}U_{\text{bs}}$, which maps $|1\rangle$ to

$$U_{\text{bs}}U_{\text{ph}}U_{\text{bs}}|1\rangle = U_{\text{bs}}U_{\text{ph}}\frac{|1\rangle + |2\rangle}{\sqrt{2}} = U_{\text{bs}}\frac{e^{i\theta}|1\rangle + |2\rangle}{\sqrt{2}} = \frac{e^{i\theta}|1\rangle + e^{i\theta}|2\rangle + |1\rangle - |2\rangle}{2}.$$

The probability of the first detector clicking is now $|\frac{1+e^{i\theta}}{2}|^2 = \cos^2(\theta/2)$.

Now add decoherence. Suppose you find a way to look at which branch the photon is in without destroying the photon. (This part is a bit unrealistic, but if we use larger objects, then it becomes more reasonable. See the readings for a description of a two-slit experiment conducted with C_{60} molecules.) If we observe it then we will find that regardless of the phase shift θ :

- the photon is equally likely to be in each path; and
- each detector is equally likely to click.

Our measurement has caused decoherence that has destroyed the phase information in θ .

5.2 Spin rotations in NMR

Start with a spin-1/2 particle in the $|+\rangle$ state. Apply $H = S_y$ for time $t = \pi/2$, so that

$$U = e^{-\frac{iHt}{\hbar}} = e^{-i\frac{\pi}{4}\sigma_y} = \frac{I - i\sigma_y}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$$

Applying U once yields $U|+\rangle = \frac{|+\rangle + |-\rangle}{\sqrt{2}}$ and applying U a second time yields $|-\rangle$ (calculation omitted).

Suppose that we measure in the $\{|+\rangle, |-\rangle\}$ basis after applying the first U . Then each outcome occurs with probability 1/2 and the resulting density matrix is

$$\frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = \frac{I}{2}.$$

Applying U again leaves the density matrix unchanged. Decoherence has destroyed the polarization of the spin.

In actual NMR experiments, we have a test tube with 10^{20} water molecules at room temperature and we are not going to measure their individual spins. Instead, suppose that two nuclear spins get close to each other and interact briefly. Suppose that the first spin is in state ρ and the second spin is maximally mixed (i.e. density matrix $I/2$). Suppose that they interact for a time T according to the Hamiltonian

$$H = \frac{2}{\hbar}\lambda S_z \otimes S_z.$$

(Why not $\vec{S}^{(1)} \cdot \vec{S}^{(2)} \equiv \sum_{i=1}^3 S_i \otimes S_i$? This is a consequence of perturbation theory: if there is a large $S_z \otimes I + I \otimes S_z$ term in the Hamiltonian, then the $S_x \otimes S_x$ and $S_y \otimes S_y$ terms are suppressed but the $S_z \otimes S_z$ term is not.) This is equivalent to the first spin experiencing a Hamiltonian λS_z if the second spin is in a $|+\rangle$ state. and experiencing $-\lambda S_z$ if the second spin is in a $|-\rangle$ state.

Averaging over these, the first spin is mapped to the state

$$\begin{aligned}
\rho' &= \frac{1}{2} e^{-\frac{i}{\hbar} t \lambda S_z} \rho e^{\frac{i}{\hbar} t \lambda S_z} + \frac{1}{2} e^{\frac{i}{\hbar} t \lambda S_z} \rho e^{-\frac{i}{\hbar} t \lambda S_z} \\
&= \frac{1}{2} \begin{pmatrix} e^{-i\lambda t/2} & 0 \\ 0 & e^{i\lambda t/2} \end{pmatrix} \rho \begin{pmatrix} e^{i\lambda t/2} & 0 \\ 0 & e^{-i\lambda t/2} \end{pmatrix} + \frac{1}{2} \begin{pmatrix} e^{i\lambda t/2} & 0 \\ 0 & e^{-i\lambda t/2} \end{pmatrix} \rho \begin{pmatrix} e^{-i\lambda t/2} & 0 \\ 0 & e^{i\lambda t/2} \end{pmatrix} \\
&= \begin{pmatrix} \rho_{++} & \cos(\lambda t/2) \rho_{+-} \\ \cos(\lambda t/2) \rho_{-+} & \rho_{--} \end{pmatrix}
\end{aligned}$$

This doesn't completely destroy the off-diagonal terms, but attenuates them. Here we should think of λt as usually small.

If we average over many such interactions, then this might (skipping many steps, which you will explore on the pset) result in a process that looks like

$$\dot{\rho} = -\frac{1}{T_2} \begin{pmatrix} 0 & \rho_{+-} \\ \rho_{-+} & 0 \end{pmatrix}, \quad (26)$$

where T_2 is the *decoherence time*, sometime also called the *dephasing time* for this kind of decoherence.

If this is T_2 , then is there also a T_1 ? Yes, T_1 refers to a different kind of decoherence. In NMR, there is typically a static magnetic field in the \hat{z} direction, which gives rise to a Hamiltonian of the form $H = -\gamma B S_z$. From this (together with the temperature) we obtain a thermal state ρ_{thermal} described in Section 2.2.5. The process of thermalization is challenging to rigorously derive from the Schrödinger equation but it is usually sufficient to model it phenomenologically. Suppose that according to a Poisson process with rate $1/T_1$, the spin is discarded and replaced with a fresh spin in the state ρ_{thermal} . Then we would obtain the differential equation

$$\dot{\rho} = -\frac{1}{T_1} (\rho - \rho_{\text{thermal}}). \quad (27)$$

Of course, there is another source of dynamics, which is the natural time evolution from the Schrödinger equation: $\dot{\rho} = -\frac{i}{\hbar} [H, \rho]$. Putting this together, we obtain the *Bloch equation*:

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] - \frac{1}{T_1} (\rho - \rho_{\text{thermal}}) - \frac{1}{T_2} \begin{pmatrix} 0 & \rho_{+-} \\ \rho_{-+} & 0 \end{pmatrix}. \quad (28)$$

If we write $\rho = \frac{I + \vec{a} \cdot \vec{\sigma}}{2}$, then (28) becomes

$$\frac{\partial \vec{a}}{\partial t} = \hat{M} \vec{a} + \vec{b}, \quad (29)$$

for \hat{M}, \vec{b} to be determined on a pset.

(Why do I keep talking about NMR, and not ESR (electron spin resonance)? The electron's gyromagnetic ratio is about 657 times higher than the proton's so its room-temperature polarization is larger by about this amount, and signals from it are easier to detect. However, it also interacts more promiscuously and thus often decoheres quickly, with T_2 on the order of microseconds or worse in most cases. So when you get a knee injury, your diagnosis will be made via your nuclei and not your electrons.)

5.3 Spontaneous emission

Consider an atom with states $|g\rangle$ and $|e\rangle$, corresponding to “ground” and “excited.” We will also consider a photon mode, i.e. a harmonic oscillator. Suppose the initial state of the system is $|\psi\rangle_{\text{atom}} \otimes |0\rangle_{\text{photon}}$ with $|\psi\rangle = c_1|g\rangle + c_2|e\rangle$. These will interact via the Jaynes-Cummings Hamiltonian

$$H = \Omega(|g\rangle\langle e| \otimes \hat{a}^\dagger + |e\rangle\langle g| \otimes \hat{a}). \quad (30)$$

(For simplicity we have left out some terms that are usually in this Hamiltonian. This Hamiltonian can be derived using perturbation theory, as we discussed on a pset.) Suppose that the atom and photon field interact via this Hamiltonian for a time t . Assume that $\delta \equiv \Omega t$ is small and expand the state of the system in powers of δ :

$$e^{-\frac{iHt}{\hbar}} |\psi\rangle \otimes |0\rangle = (c_1|g\rangle + c_2|e\rangle) \otimes |0\rangle - i\delta c_2|g\rangle \otimes |1\rangle - \frac{\delta^2}{2} c_2|e\rangle \otimes |0\rangle + O(\delta^3). \quad (31)$$

Now measure and we see that with probability $|c_2|^2\delta^2$ the photon number is 1 and the atom is in the state $|g\rangle$. In this case, we observe an emitted photon and can conclude that the atom must currently be in the state $|g\rangle$. (It is tempting to conclude that we know it was previously in the state $|e\rangle$. This sort of reasoning about the past can be dangerous. In fact, all we can conclude is that c_2 must have been nonzero.)

With probability $|c_1|^2 + (1 - \delta^2)|c_2|^2 = 1 - |c_2|^2\delta^2$ we observe 0 photons and the state is

$$\frac{c_1|g\rangle + (1 - \delta^2)c_2|e\rangle}{\sqrt{1 - |c_2|^2\delta^2}},$$

again, up to $O(\delta^3)$ corrections. If we repeat this for long enough then we *also* end up in the state $|g\rangle$. This is because if we watch an atom for a long time and it never emits a photon we can conclude that it's probably in the ground state.

6 Multipartite density matrices

In Section 1.3 I complained that pure-state quantum mechanics is not closed under discarding subsystems. Here we will see that density matrices solve this problem. More generally we will extend the formalism of density matrices to handle composite quantum systems.

6.1 Product states

Suppose that we have two systems, called A and B , with density matrices ρ and σ respectively. I claim that their joint state is $\rho \otimes \sigma$.

One way to see this is by explicitly decomposing $\rho = \sum_i p_i |\alpha_i\rangle\langle\alpha_i|$, $\sigma = \sum_j q_j |\beta_j\rangle\langle\beta_j|$ and considering these as *independent* ensembles $\{(p_i, |\alpha_i\rangle)\}$ and $\{(q_j, |\beta_j\rangle)\}$. According to the rule for independent probability distributions the probability of finding system A in state $|\alpha_i\rangle$ and system B in state $|\beta_j\rangle$ is $p_i \cdot q_j$. In this case the joint state is $|\alpha_i\rangle \otimes |\beta_j\rangle$. This corresponds to the ensemble $\{(p_i q_j, |\alpha_i\rangle \otimes |\beta_j\rangle)\}$ which has density matrix

$$\sum_{i,j} p_i q_j (|\alpha_i\rangle \otimes |\beta_j\rangle)(\langle\alpha_i| \otimes \langle\beta_j|) = \sum_{i,j} p_i q_j |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_j\rangle\langle\beta_j| = \rho \otimes \sigma. \quad (32)$$

Therefore the product rule for density matrices can be inferred from the product rule for pure states.

We can also derive it from observables. If we measure observable \hat{A} on the first system then this corresponds to the observable $\hat{A} \otimes I$ on the composite system; likewise \hat{B} on the second system corresponds to $I \otimes \hat{B}$ on the joint system. Their product is $\hat{A} \otimes \hat{B}$. This arises for example when the dipole moments of two spins are coupled and the Hamiltonian gets a term proportional to $\vec{S}_1 \cdot \vec{S}_2 = S_x \otimes S_x + S_y \otimes S_y + S_z \otimes S_z$. Let ω be the joint state of a system where the first particle is in state ρ and the second is in state σ . The expectation of $\hat{A} \otimes \hat{B}$ with respect to ω should be

$$\text{tr}[\rho \hat{A}] \text{tr}[\sigma \hat{B}] = \text{tr}[(\rho \otimes \sigma)(\hat{A} \otimes \hat{B})]. \quad (33)$$

Since this is equal to $\text{tr}[\omega(\hat{A} \otimes \hat{B})]$ for all choices of \hat{A}, \hat{B} , we must have that $\omega = \rho \otimes \sigma$.

6.2 Partial measurement and partial trace

Density matrices were introduced by the fact that measuring one part of a larger system leaves the rest in a random state. As a result, pure-state quantum mechanics is not a closed theory; if the state of the joint system AB is pure, then it is possible that the states of A and B are not themselves pure. However, if there is a density matrix ρ^{AB} describing the joint state of systems A and B then we should be able to define density matrices for the individual systems. Indeed any observable X on system A should have a well-defined expectation value, and these can be used to define a *reduced density matrix* for system A . Mathematically we denote the density matrix of system A by ρ^A and define it to be the unique density matrix satisfying

$$\text{tr}[\rho^A X] = \text{tr}[\rho^{AB}(X \otimes I)], \quad (34)$$

for all observables X . (It is an instructive exercise to verify that there is always a solution to (34) and that it is unique.) Similarly we can define the state of system B to be ρ^B satisfying $\text{tr}[\rho^B X] = \text{tr}[\rho^{AB}(I \otimes X)]$.

Expanding (34) in terms of matrix elements yields

$$\sum_{a,a'} \rho_{a,a'}^A X_{a,a'} = \sum_{a,b,a',b'} \rho_{ab,a'b'}^{AB} X_{a,a'} \delta_{b,b'} = \sum_{a,a',b} \rho_{ab,a'b}^{AB} X_{a,a'}. \quad (35)$$

Since this must hold for any X , we have

$$\rho_{a,a'}^A = (\text{tr}_B[\rho])_{a,a'} = \sum_b \rho_{ab,a'b}^{AB}. \quad (36)$$

This looks like taking a trace over the B subsystem (i.e. summing over the $b = b'$ entries) while leaving the A system alone. For this reason we call the map from $\rho^{AB} \mapsto \rho^A$ the “partial trace” and denote it tr_B ; i.e. $\rho^A = \text{tr}_B[\rho^{AB}]$. The partial trace is the quantum analogue of the rule for marginals of probability distributions: $p^X(x) = \sum_y p^{XY}(x, y)$.

A similar equation holds for $\rho^B \equiv \text{tr}_A[\rho^{AB}]$ which can be expressed in terms of matrix elements as

$$\rho_{b,b'}^B = (\text{tr}_A[\rho])_{b,b'} = \sum_a \rho_{ab,ab'}^{AB}. \quad (37)$$

If A and B have dimensions d_A and d_B respectively and M_d denotes the set of $d \times d$ matrices, then $\text{tr}_A : M_{d_A d_B} \rightarrow M_{d_B}$ and $\text{tr}_B : M_{d_A d_B} \rightarrow M_{d_A}$ are linear maps defined by

$$\begin{aligned} \text{tr}_A[|\alpha\rangle\langle\beta| \otimes |\gamma\rangle\langle\delta|] &= \langle\alpha|\beta\rangle \cdot |\gamma\rangle\langle\delta| \\ \text{tr}_B[|\alpha\rangle\langle\beta| \otimes |\gamma\rangle\langle\delta|] &= \langle\gamma|\delta\rangle \cdot |\alpha\rangle\langle\beta| \end{aligned}$$

If $\{|a\rangle\}$ and $\{|b\rangle\}$ are orthonormal bases then $\text{tr}_A[|a\rangle\langle a'| \otimes |b\rangle\langle b'|] = \delta_{a,a'}|b\rangle\langle b'|$ and $\text{tr}_B[|a\rangle\langle a'| \otimes |b\rangle\langle b'|] = \delta_{b,b'}|a\rangle\langle a'|$.

Let's illustrate this by revisiting the example of spontaneous emission from Section 5.3. Suppose

$$|\psi\rangle = e^{-iHt/\hbar} \frac{|g\rangle + |e\rangle}{\sqrt{2}} \otimes |0\rangle,$$

where $H = \Omega(|g\rangle\langle e| \otimes a^\dagger + |e\rangle\langle g| \otimes a)$. $H|g, 0\rangle = 0$ and H acts on the $\{|e, 0\rangle, |g, 1\rangle\}$ subspace as a rotation. Thus

$$|\psi\rangle = \frac{1}{\sqrt{2}}|g, 0\rangle + \frac{1}{\sqrt{2}}(\cos(\theta)|e, 0\rangle - i\sin(\theta)|g, 1\rangle).$$

The corresponding density matrix is

$$|\psi\rangle\langle\psi| = \begin{matrix} & \begin{matrix} \langle g, 0| \\ \langle e, 0| \\ \langle g, 1| \\ \langle e, 1| \end{matrix} & \begin{matrix} \langle e, 0| \\ \langle g, 1| \\ \langle e, 1| \end{matrix} & \begin{matrix} \langle g, 1| \\ \langle e, 1| \end{matrix} \\ \begin{matrix} |g, 0\rangle \\ |e, 0\rangle \\ |g, 1\rangle \\ |e, 1\rangle \end{matrix} & \begin{pmatrix} \frac{1}{2} & \frac{1}{2}\cos(\theta) & \frac{i}{2}\sin(\theta) & 0 \\ \frac{1}{2}\cos(\theta) & \frac{1}{2}\cos^2(\theta) & \frac{i}{2}\cos(\theta)\sin(\theta) & 0 \\ \frac{-i}{2}\sin(\theta) & \frac{-i}{2}\sin(\theta)\cos(\theta) & \frac{1}{2}\sin^2(\theta) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix} \quad (38)$$

The reduced state of the atom is

$$\text{tr}_{\text{photon}}|\psi\rangle\langle\psi| = \begin{matrix} & \begin{matrix} \langle g| \\ \langle e| \end{matrix} \\ \begin{matrix} |g\rangle \\ |e\rangle \end{matrix} & \begin{pmatrix} \frac{1}{2} + \frac{1}{2}\sin^2(\theta) & \frac{1}{2}\cos(\theta) \\ \frac{1}{2}\cos(\theta) & \frac{1}{2}\cos^2(\theta) \end{pmatrix} \end{matrix} \quad (39)$$

and the reduced state of the photon is

$$\text{tr}_{\text{atom}}|\psi\rangle\langle\psi| = \begin{matrix} & \begin{matrix} \langle 0| \\ \langle 1| \end{matrix} \\ \begin{matrix} |0\rangle \\ |1\rangle \end{matrix} & \begin{pmatrix} \frac{1}{2} + \frac{1}{2}\cos^2(\theta) & \frac{i}{2}\sin(\theta) \\ \frac{-i}{2}\sin(\theta) & \frac{1}{2}\sin^2(\theta) \end{pmatrix} \end{matrix} \quad (40)$$

(The decorations surrounding the above matrices are meant as reminders of which basis elements the rows and columns correspond to.)

6.3 Purifications

One way density matrices can arise is via subjective uncertainty; i.e. we don't know what the state is, but it "really" is pure. If so, we might imagine that density matrices would be useful for a quantum theory of statistics or information, but are not essential to quantum physics. However, density matrices also arise in settings where the overall state is known exactly. We saw this earlier where Bob could not distinguish his half of a singlet from a uniformly random state. Conversely, a uniformly random state cannot be distinguished from half of a singlet, with the other half in an unknown location. This is in fact only a representative example of the general rule that *any* density matrix could arise by being part of an entangled state.

First, let $|\psi\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} \alpha_{i,j} |i\rangle \otimes |j\rangle$. If Bob measures his system, he obtains outcome j with probability $p_j \equiv \sum_i |\alpha_{i,j}|^2$ and the residual state for Alice is $\sum_i \alpha_{i,j} |i\rangle / \sqrt{p_j}$. Her density matrix is

$$\sum_{j=1}^{d_B} p_j \frac{\sum_{i=1}^{d_A} \alpha_{i,j} |i\rangle}{\sqrt{p_j}} \frac{\sum_{i'=1}^{d_A} \alpha_{i',j}^* \langle i'|}{\sqrt{p_j}} = \sum_{i=1}^{d_A} \sum_{i'=1}^{d_A} \underbrace{\sum_{j=1}^{d_B} \alpha_{i,j} \alpha_{i',j}^*}_{=(\alpha\alpha^\dagger)_{i,i'}} |i\rangle\langle i'| = \alpha\alpha^\dagger.$$

What if Alice measures? Working this out is a good exercise. The answer is $(\alpha^\dagger \alpha)^T$.

By Theorem 2 any density matrix ρ can be written as $\alpha \alpha^\dagger$ for some matrix α . It remains only to check the normalization to ensure that $|\psi\rangle$ is a valid state:

$$1 = \text{tr} \rho = \text{tr} \alpha \alpha^\dagger = \sum_{i,j} |\alpha_{i,j}|^2.$$

This means that if we produce ρ in the lab, we can never know whether the state is mixed because of uncertainty about which pure state it is, or because it is entangled with a particle that is out of our control.

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8.06 Quantum Physics III
Spring 2016

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8.06 Spring 2016 Lecture Notes

4. Identical particles

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Last updated: May 19, 2016

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1 Fermions and Bosons

1.1 Introduction and two-particle systems

Previously we have discussed multiple-particle systems using the tensor-product formalism (cf. Section 1.2 of Chapter 3 of these notes). But this applies only to distinguishable particles. In reality, all known particles are indistinguishable. In the coming lectures, we will explore the mathematical and physical consequences of this.

First, consider classical many-particle systems. If a single particle has state described by position and momentum (\vec{r}, \vec{p}) , then the state of N distinguishable particles can be written as $(\vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2, \dots, \vec{r}_N, \vec{p}_N)$. The notation $(\cdot, \cdot, \dots, \cdot)$ denotes an ordered list, in which different positions have different meanings; e.g. in general $(\vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2) \neq (\vec{r}_2, \vec{p}_2, \vec{r}_1, \vec{p}_1)$.

To describe indistinguishable particles, we can use set notation. For example, the sets $\{a, b, c\}$ and $\{c, a, b\}$ are equal. We can thus denote the state of N indistinguishable particles as

$$\{(\vec{r}_1, \vec{p}_1), (\vec{r}_2, \vec{p}_2), \dots, (\vec{r}_N, \vec{p}_N)\}. \quad (1)$$

(We can either forbid two particles from having exactly identical positions and momenta, or can let $\{\dots\}$ denote a multiset, meaning a set with the possibility of repeated elements.) This notation is meant to express that the particles do not have individual identities, and that there is no physical or mathematical difference between what we call particle 1, particle 2, etc.

In the quantum mechanical case, suppose we have N particles each with single-particle state space given by a vector space V . If the particles were distinguishable the composite space would be given by $V^{\otimes N} = V \otimes \dots \otimes V$. For example, the spins of N spin-1/2 particles have state space $(\mathbb{C}^2)^{\otimes N}$. The wavefunction of a N particles in 3-d is a function $\psi(\vec{r}_1, \dots, \vec{r}_N)$ that maps \mathbb{R}^{3N} to \mathbb{C} . If $S(\mathbb{R}^3)$ denotes well-behaved functions on \mathbb{R}^3 (formally called the Schwartz space), then this N -particle state space is equivalent to $S(\mathbb{R}^3)^{\otimes N}$. If this were a wavefunction of indistinguishable particles, then it is natural to guess that it should not change if we exchange the positions of the particles, e.g. swapping \vec{r}_1 and \vec{r}_2 . This turns out not to be quite true, since it may be that swapping two positions could result in an unobservable change, such as multiplying by an overall phase.

To be more concrete, consider the case of two indistinguishable particles. Then we should have $|\psi(\vec{r}_1, \vec{r}_2)| = |\psi(\vec{r}_2, \vec{r}_1)|$, or equivalently

$$\psi(\vec{r}_1, \vec{r}_2) = e^{i\theta} \psi(\vec{r}_2, \vec{r}_1) \quad (2)$$

for some phase $e^{i\theta}$. It is somewhat beyond the scope of this course to explain why the phase should be independent of \vec{r}_1, \vec{r}_2 , but I will mention that it relies on being in ≥ 3 spatial dimensions and that richer behavior exists in 1 and 2 dimensions. A more general way to express (2) is by defining the swap operator F by the relation

$$F(|\alpha\rangle \otimes |\beta\rangle) = |\beta\rangle \otimes |\alpha\rangle \quad (3)$$

for any single-particle states $|\alpha\rangle, |\beta\rangle$. Then (2) is equivalent to

$$F|\psi\rangle = e^{i\theta} |\psi\rangle. \quad (4)$$

Since $F^2 = I$, its eigenvalues can only be ± 1 , and so we must have $e^{i\theta} = \pm 1$. The corresponding eigenspaces are called the symmetric and antisymmetric subspaces, respectively, and are denoted

$$\text{Sym}^2 V = \{|\psi\rangle \in V \otimes V : F|\psi\rangle = |\psi\rangle\} \quad (5a)$$

$$\text{Anti}^2 V = \{|\psi\rangle \in V \otimes V : F|\psi\rangle = -|\psi\rangle\} \quad (5b)$$

Particles whose state space (for $N = 2$) is $\text{Sym}^2 V$ are called *bosons* and those with state space $\text{Anti}^2 V$ are called *fermions*. The *spin-statistics theorem* states that particles with half-integer spin ($1/2, 3/2$, etc.) are fermions and that particles with integer spin ($0, 1$, etc.) are bosons. The proof of this involves field theory (or at least the existence of antiparticles) and is beyond the scope of 8.06 (but could conceivably be a term-paper topic).

To find a basis for the symmetric and antisymmetric subspaces, we can construct projectors onto them, and apply them to a basis for $V \otimes V$. Since F has eigenvalues ± 1 , $P_{\text{sym}} \equiv \frac{I+F}{2}$ will project onto the $+1$ eigenspace (i.e. the symmetric subspace) and $P_{\text{anti}} \equiv \frac{I-F}{2}$ will project onto the -1 eigenspace (the antisymmetric subspace). The overall space $V \otimes V$ has a basis consisting of states

$|\alpha\rangle \otimes |\beta\rangle$. We can assume that $|\alpha\rangle, |\beta\rangle$ came from some orthonormal basis for V , so that in particular they are either equal or orthogonal. Applying P_{sym} we get $|\alpha\rangle \otimes |\alpha\rangle$ (if $|\alpha\rangle = |\beta\rangle$) or $\frac{|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle}{2}$ (if $|\alpha\rangle, |\beta\rangle$ are orthogonal). The latter state can be normalized to obtain $\frac{|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}}$. Similarly if we apply P_{anti} to $|\alpha\rangle \otimes |\beta\rangle$ we obtain 0 if $|\alpha\rangle = |\beta\rangle$ or $\frac{|\alpha\rangle \otimes |\beta\rangle - |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}}$ after normalizing if $|\alpha\rangle, |\beta\rangle$ are orthogonal. These states are all orthogonal to each other except for when we exchange $|\alpha\rangle$ and $|\beta\rangle$, in which case we get back either the same state (symmetric subspace) or the same state multiplied by -1 (antisymmetric subspace).

If V is d -dimensional and has basis $\{|1\rangle, \dots, |d\rangle\}$ then $V \otimes V$ is d^2 -dimensional and has basis $\{|1\rangle \otimes |1\rangle, |1\rangle \otimes |2\rangle, \dots, |d\rangle \otimes |d\rangle\}$. $\text{Sym}^2 V$ has basis

$$\{|\alpha\rangle \otimes |\alpha\rangle : 1 \leq \alpha \leq d\} \cup \left\{ \frac{|\alpha\rangle \otimes |\beta\rangle + |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}} : 1 \leq \alpha < \beta \leq d \right\}, \quad (6)$$

where we have arbitrarily assumed that $\alpha \leq \beta$. We could have equivalently chosen $\alpha \geq \beta$, but should not do both so that we do not double-count the same states. Similarly $\text{Anti}^2 V$ has basis

$$\left\{ \frac{|\alpha\rangle \otimes |\beta\rangle - |\beta\rangle \otimes |\alpha\rangle}{\sqrt{2}} : 1 \leq \alpha < \beta \leq d \right\}. \quad (7)$$

This has $\binom{d}{2} = \frac{d(d-1)}{2}$ elements, corresponding to the number of ways of choosing two elements from a d -element set. Similarly the basis for $\text{Sym}^2 V$ has $d + \binom{d}{2} = \frac{d(d+1)}{2}$ elements. We can check that the dimensions add up: $\frac{d(d+1)}{2} + \frac{d(d-1)}{2} = d^2$. (But beware that this situation is unique to $N = 2$. For $N > 2$, $V^{\otimes N}$ contains states that are neither completely symmetric nor completely antisymmetric. The situation then is beyond the scope of 8.06, but “Schur-Weyl duality” is the phrase to google to learn more.)

Example: spin-1/2 particles. The simplest case is when $d = 2$. In this case, we use spin notation and describe the single-particle basis with $\{|+\rangle, |-\rangle\}$. The resulting basis for $\text{Sym}^2 \mathbb{C}^2$ is $\{|++\rangle, \frac{|+-\rangle + |-+\rangle}{\sqrt{2}}, |--\rangle\}$ and the basis for $\text{Anti}^2 \mathbb{C}^2$ is $\{\frac{|+-\rangle - |-+\rangle}{\sqrt{2}}\}$. These are referred to as the triplet and singlet respectively.

1.2 N particles

Again if there are N distinguishable particles, then their joint state-space $V^{\otimes N}$, where V is the single-particle state space. A basis for this space is given by vectors of the form $|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle$. To define the symmetric and antisymmetric subspaces, define the operator $F^{i,j}$ to swap tensor positions i and j , i.e. if $i < j$ then

$$F^{i,j} |\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle = |\alpha_1\rangle \otimes \dots \otimes |\alpha_{i-1}\rangle \otimes |\alpha_j\rangle \otimes |\alpha_{i+1}\rangle \otimes \dots \otimes |\alpha_{j-1}\rangle \otimes |\alpha_i\rangle \otimes |\alpha_{j+1}\rangle \otimes \dots \otimes |\alpha_N\rangle \quad (8)$$

(and the definition is similar if $i > j$). While these operators do not commute, we can define the symmetric and antisymmetric subspaces to be their simultaneous +1 (resp. -1) eigenspaces:

$$\text{Sym}^N V \equiv \{|\psi\rangle \in V^{\otimes N} : F^{ij} |\psi\rangle = |\psi\rangle \forall i \neq j\} \quad (9a)$$

$$\text{Anti}^N V \equiv \{|\psi\rangle \in V^{\otimes N} : F^{ij} |\psi\rangle = -|\psi\rangle \forall i \neq j\} \quad (9b)$$

The corresponding wavefunctions are those satisfying

$$\psi(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots, \vec{r}_N) = \pm \psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots, \vec{r}_N) \quad (10)$$

To compute bases for the symmetric and antisymmetric subspaces, we need to repeat our exercise of defining the symmetric and antisymmetric projectors and then applying them to basis states. This will be more complicated than the $N = 2$ case. Define S_N to be the set of permutations of N objects, i.e. the set of 1-1 functions from $\{1, \dots, N\}$ to itself. $|S_N| = N!$ since there for $\pi \in S_N$ there are N ways to choose $\pi(1)$, $N - 1$ ways to choose $\pi(2)$ (i.e. any element of $\{1, \dots, N\}$ not equal to $\pi(1)$) $N - 2$ ways to choose $\pi(3)$ and so on for $\pi(4), \dots, \pi(N)$. For a permutation π define the operator F^π to the map sending each state $|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle$ to $|\alpha_{\pi^{-1}(1)}\rangle \otimes \dots \otimes |\alpha_{\pi^{-1}(N)}\rangle$. One particularly simple example of a permutation is a *transposition*, which exchanges two positions and leaves the other positions untouched. The F^{ij} operators above are the operators corresponding to transpositions.

One useful fact about S_N is that it is a *group*, meaning that it contains the identity permutation (denoted e) and is closed under multiplication and inverse. In other words if $\pi, \nu \in S_N$ then applying ν then π is another permutation (denoted $\pi\nu$) and there exists a permutation π^{-1} satisfying $\pi\pi^{-1} = \pi^{-1}\pi = e$. Additionally F^π is a *representation* meaning that $F^{\pi\nu} = F^\pi F^\nu$. Verifying these facts is a useful exercise. One consequence is that the sets $\{\pi : \pi \in S_N\}$ and $\{\nu\pi : \pi \in S_N\}$ are the same.

One can use these to show that the symmetric and antisymmetric projectors are given by

$$P_{\text{sym}} \equiv \frac{1}{N!} \sum_{\pi \in S_N} F^\pi \quad \text{and} \quad P_{\text{anti}} \equiv \frac{1}{N!} \sum_{\pi \in S_N} \text{sgn}(\pi) F^\pi. \quad (11)$$

To prove this, we need to argue that $\text{Im} P_{\text{sym}} \subseteq \text{Sym}^N V$ and that if $|\psi\rangle \in \text{Sym}^N V$ then $P_{\text{sym}}|\psi\rangle = |\psi\rangle$. For the former, an arbitrary element of $\text{Im} P_{\text{sym}}$ can be written as

$$P_{\text{sym}}|\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} F^\pi |\psi\rangle.$$

Applying F^ν yields

$$F^\nu P_{\text{sym}}|\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} F^\nu F^\pi |\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} F^{\nu\pi} |\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} F^\pi |\psi\rangle = P_{\text{sym}}|\psi\rangle.$$

The third equality used the fact that $\pi \mapsto \nu\pi$ is a 1-1 map. Next suppose that $|\psi\rangle \in \text{Sym}^N V$. Then

$$P_{\text{sym}}|\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} F^\pi |\psi\rangle = \frac{1}{N!} \sum_{\pi \in S_N} |\psi\rangle = |\psi\rangle,$$

where the second equality used the fact that $F^\pi |\psi\rangle = |\psi\rangle$ for all $|\psi\rangle \in \text{Sym}^N V$.

The argument for the antisymmetric projector is similar, but we first need to define $\text{sgn}(\pi)$, which is called the *sign* of a permutation. It is defined to be 1 if π can be written as a product of an even number of transpositions or -1 if π can be written as a product of an odd number of transpositions. For example, for $N = 3$, $\text{sgn}(\pi) = 1$ if π is the identity permutation, or a cycle of length 3, such as $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$; in fact, $\text{sgn}(\pi) = \epsilon_{\pi_1 \pi_2 \pi_3}$, where ϵ_{ijk} is familiar Levi-Civita symbol. It is not clear that $\text{sgn}(\pi)$ is well-defined: π can be written as a product of transpositions in an infinite number of ways, and what if some of them involve an even number of transpositions and some involve an odd number? It turns out that this never happens. To prove this, an alternate definition of $\text{sgn}(\pi)$ can shown to be

$$\text{sgn}(\pi) = \det \left(\sum_{i=1}^N |i\rangle \langle \pi(i)| \right), \quad (12)$$

which suffers from no such ambiguity. As an example of (12), the permutation which swaps 1 and 2 has sign -1 , which equals $\det \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Similarly any single transposition has sign -1 according to (12) and the multiplication rule for determinants ($\det(AB) = \det(A)\det(B)$) can be used to show that these two definitions of $\text{sgn}(\pi)$ are equivalent. Like the determinant, the sgn function obeys $\text{sgn}(\nu\pi) = \text{sgn}(\nu)\text{sgn}(\pi)$ for any permutations ν, π . This can be used to prove that P_{anti} is the projector onto the antisymmetric subspace, using an argument similar to the one used for P_{sym} and the symmetric subspace.

As a result, we can write a basis for $\text{Sym}^N V$ consisting of the states

$$|\psi_{\alpha_1, \dots, \alpha_N}^{\text{sym}}\rangle = \mathcal{N} \sum_{\pi \in S_N} |\alpha_{\pi(1)}\rangle \otimes \dots \otimes |\alpha_{\pi(N)}\rangle. \quad (13)$$

Here \mathcal{N} is a normalization term that is equal to $N!^{-1/2}$ if the $\alpha_1, \dots, \alpha_N$ are all distinct, equal to 1 if they are all the same, and in general will be somewhere between these two extremes. Similarly $\text{Anti}^N V$ has a basis consisting of the states

$$|\psi_{\alpha_1, \dots, \alpha_N}^{\text{anti}}\rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \text{sgn}(\pi) |\alpha_{\pi(1)}\rangle \otimes \dots \otimes |\alpha_{\pi(N)}\rangle. \quad (14)$$

Since these are always zero if any of the α_i 's are equal, the normalization is always $\frac{1}{\sqrt{N!}}$.

For spatial wavefunctions, there is a useful formula for $\langle \vec{r}_1, \dots, \vec{r}_N | \psi_{\alpha_1, \dots, \alpha_N}^{\text{anti}} \rangle$ derived by John Slater in 1929. First we recall a formula for the determinant of a matrix

$$\det(A) = \sum_{\pi \in S_N} \text{sgn}(\pi) A_{1, \pi(1)} A_{2, \pi(2)} \dots A_{N, \pi(N)}. \quad (15)$$

Using this and the notation $\psi_{\alpha}(\vec{r}) = \langle \vec{r} | \alpha \rangle$, it is straightforward to show that

$$\langle \vec{r}_1, \dots, \vec{r}_N | \psi_{\alpha_1, \dots, \alpha_N}^{\text{anti}} \rangle = \det \begin{pmatrix} \psi_{\alpha_1}(\vec{r}_1) & \dots & \psi_{\alpha_1}(\vec{r}_N) \\ \vdots & & \vdots \\ \psi_{\alpha_N}(\vec{r}_1) & \dots & \psi_{\alpha_N}(\vec{r}_N) \end{pmatrix}. \quad (16)$$

This is called a *Slater determinant*. For example when $N = 2$, the wavefunction is of the form

$$\frac{\psi_{\alpha_1}(\vec{r}_1)\psi_{\alpha_2}(\vec{r}_2) - \psi_{\alpha_2}(\vec{r}_1)\psi_{\alpha_1}(\vec{r}_2)}{\sqrt{2}}. \quad (17)$$

1.3 Non-interacting particles

So far we have described only the state spaces. Now we begin to consider Hamiltonians. If H is a single-particle Hamiltonian (i.e. a Hermitian operator on V) then define H_i to be H acting on system i (in an N -particle system):

$$H_i \equiv I^{\otimes i-1} \otimes H \otimes I^{\otimes N-i}. \quad (18)$$

If we have N particles each experiencing Hamiltonian H (e.g. N spins in the same magnetic field) then the total Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^N H_i. \quad (19)$$

Suppose that the eigenvalues and eigenstates of H are given by

$$H|\alpha\rangle = E_\alpha|\alpha\rangle$$

with $E_0 \leq E_1 \leq \dots$. Then what is the spectrum of \mathcal{H} ? There are three cases.

1.3.1 Distinguishable particles

The overall space is $V^{\otimes N}$ which has a basis consisting of all states $|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle$ that are tensor products of single-particle energy eigenstates. Since

$$H_i|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle = E_{\alpha_i}|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle,$$

it follows that

$$\mathcal{H}|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle = (E_{\alpha_1} + \dots + E_{\alpha_N})|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle. \quad (20)$$

Thus $\{|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle\}$ is an orthonormal basis of eigenstates of \mathcal{H} . The ground state is $|0\rangle^{\otimes N}$, which has energy NE_0 . The first excited subspace is N -fold degenerate and consists of all of the states of the form $|1, 0, 0, \dots, 0\rangle, |0, 1, 0, \dots, 0\rangle$, etc. It has energy $(N-1)E_0 + E_1$. A general energy level with all α_i distinct similarly has degeneracy $N!$, even aside from the possibility of obtaining the same total energy by adding up different collections of E_α 's.

1.3.2 Bosons

The ground state is still $|0\rangle^{\otimes N}$, or equivalently $|\psi_{0,0,\dots,0}^{\text{sym}}\rangle$, and the ground state energy is still NE_0 . Again the energy of the first excited state is $(N-1)E_0 + E_1$. But now there is no degeneracy. The first excited state is

$$|\psi_{1,0,\dots,0}^{\text{sym}}\rangle = \frac{|1, 0, 0, \dots, 0\rangle + |0, 1, 0, \dots, 0\rangle + \dots + |0, 0, 0, \dots, 1\rangle}{\sqrt{N}}. \quad (21)$$

We could write $|\psi_{0,1,\dots,0}^{\text{sym}}\rangle$ or any other subscript with $N-1$ 0's and one 1, but these all refer to exactly the same state. Similarly all the same energies $E_{\alpha_1} + \dots + E_{\alpha_N}$ still exist in the spectrum of \mathcal{H} restricted to $\text{Sym}^N V$, but the degeneracy of up to $N!$ is now gone. Specifically state $|\psi_{\alpha_1,\dots,\alpha_N}^{\text{sym}}\rangle$ has energy $E_{\alpha_1} + \dots + E_{\alpha_N}$. Since these are a basis for $\text{Sym}^N V$ we know we have thus accounted for the entire spectrum.

1.3.3 Fermions

Now things are substantially different. The state $|0\rangle^{\otimes N}$ is no longer legal, and so the ground state energy is going to be different. If we use the basis given by $\{|\psi_{\alpha_1,\dots,\alpha_N}^{\text{anti}}\rangle\}$, we see that this is already an eigenbasis with state $|\psi_{\alpha_1,\dots,\alpha_N}^{\text{anti}}\rangle$ having energy $E_{\alpha_1} + \dots + E_{\alpha_N}$. So far this is the same as in the boson case except that we must now have all the α_i distinct. Without loss of generality we can assume $\alpha_1 < \alpha_2 < \dots < \alpha_N$. As a result, $\alpha_i \geq i-1$ and the energy is $\geq E_0 + E_1 + \dots + E_{N-1}$. This energy is achieved by the state $|\psi_{0,1,\dots,N-1}^{\text{anti}}\rangle$ which must be the unique ground state. The first excited state is $|\psi_{0,1,\dots,N-2,N}^{\text{anti}}\rangle$ which has energy $E_0 + E_1 + \dots + E_{N-2} + E_N$. Both of these are non-degenerate unless there are degeneracies in the single-particle spectrum. One way to interpret the first excited state is that we have added a particle with state $|N\rangle$ and a "hole" (meaning the absence of a particle) with state $|N-1\rangle$. Higher excited states can be found by moving the particle to higher energies (e.g. $|\psi_{0,1,\dots,N-2,N+1}^{\text{anti}}\rangle$), moving the hole to lower energies (e.g. $|\psi_{0,1,\dots,N-3,N-1,N}^{\text{anti}}\rangle$) or creating additional particle-hole pairs (e.g. $|\psi_{0,1,\dots,N-3,N,N+1}^{\text{anti}}\rangle$). Holes are studied in solid-state physics, and were the way that Dirac originally explained positrons (although this explanation has now been superseded by modern field theory).

1.4 Non-zero temperature

Let us calculate the thermal state $e^{-\beta H}/Z$ for N non-interacting fermions or bosons.

The eigenstates can be labeled by occupation numbers n_0, n_1, n_2, \dots where n_i is the number of states with energy E_i . For fermions n_i can be 0 or 1, while for bosons, n_i can be any nonnegative integer.

Here it is easiest to work with the grand canonical ensemble. In this, the probability of a microstate with energy E and N particles is proportional to $e^{-\beta(E-\mu N)}$ where $\beta = 1/k_B T$ and μ is the chemical potential. We can think of this as resulting from the system being in thermal contact with a reservoir containing many particles each with energy μ . Alternatively, we can maximize entropy subject to energy and particle number constraints and then β, μ emerge as Lagrange multipliers.

For us, the benefit will be that the probability distribution factorizes. We find that the probability of observing occupation numbers n_0, n_1, \dots is

$$\Pr[n_0, n_1, \dots] = \frac{\exp(-\beta \sum_i n_i (E_i - \mu))}{Z} = \frac{\exp(-\beta \sum_i n_i (E_i - \mu))}{\sum_{n'_0, n'_1, \dots} \exp(-\beta \sum_i n'_i (E_i - \mu))}, \quad (22)$$

where in the sum each n'_i ranges over 0,1 (for fermions) or over all nonnegative integers (for bosons). Either way this factorizes as

$$\Pr[n_0, n_1, \dots] = \prod_{i \geq 0} \frac{e^{-\beta n_i (E_i - \mu)}}{\sum_{n'_i} e^{-\beta n'_i (E_i - \mu)}}. \quad (23)$$

In other words, each occupation number is an independent random variable.

For fermions this results in the *Fermi-Dirac distribution*.

$$\Pr[n_i = 0] = \frac{1}{1 + e^{-\beta(E_i - \mu)}} \quad \text{and} \quad \langle n_i \rangle = \Pr[n_i = 1] = \frac{e^{-\beta(E_i - \mu)}}{1 + e^{-\beta(E_i - \mu)}}, \quad (24)$$

while for bosons we obtain the *Bose-Einstein distribution*.

$$\Pr[n_i] = e^{-\beta n_i (E_i - \mu)} (1 - e^{-\beta(E_i - \mu)}) \quad (25)$$

$$\langle n_i \rangle = \frac{1}{e^{\beta(E_i - \mu)} - 1}. \quad (26)$$

Note that for bosons we require $\mu < E_i$ but for fermions this is not necessary.

The Fermi-Dirac occupation number can be rewritten as

$$\langle n_i \rangle = \frac{1}{1 + e^{\beta(E_i - \mu)}}. \quad (27)$$

As $\beta \rightarrow \infty$ this approaches a step function which is ≈ 1 for $E_i < \mu$ and ≈ 0 for $E_i > \mu$. Thus in the zero-temperature limit we will fill levels with energy up to some limit μ and no levels above this energy.

1.5 Composite particles

Usually particles have multiple attributes with distinct degrees of freedom, e.g. their positions and their spins. These are combined by tensor product, so we can write the state of a single electron as $|\psi_{\text{electron}}\rangle = |\psi_{\text{spatial}}\rangle \otimes |\psi_{\text{spin}}\rangle$. This division is often somewhat arbitrary, as in the case of

electrons in hydrogen-like atoms, where the state could be written either as $|n, l, m, s\rangle$ or (dividing into spatial and spin parts) as $|n, l, m\rangle \otimes |s\rangle$.

More generally, suppose the state space of a single particle is $V \otimes W$. Then the state of N distinguishable particles is

$$(V \otimes W)^{\otimes N} \cong V^{\otimes N} \otimes W^{\otimes N}. \quad (28)$$

This isomorphism is proved by simply rearranging the terms in the tensor product $V \otimes W \otimes V \otimes W \otimes \dots \otimes V \otimes W$ so that all the V 's precede all the W 's. For example, for N distinguishable particles in a $-1/r$ potential (e.g. imagine a proton surrounded by an electron, a muon, a tau particle, and, well, let's just take N to be 3) we could just as well use the basis

$$\{|n_1, l_1, m_1, s_1, \dots, n_N, l_N, m_N, s_N\rangle\} \quad (29)$$

corresponding to $(V \otimes W)^{\otimes N}$ or the basis

$$\{|n_1, l_1, m_1, \dots, n_N, l_N, m_N\rangle \otimes |s_1, \dots, s_N\rangle\} \quad (30)$$

corresponding to $V^{\otimes N} \otimes W^{\otimes N}$.

For fermions and bosons, the situation is not quite so simple since $\text{Sym}^N(V \otimes W) \not\cong \text{Sym}^N V \otimes \text{Sym}^N W$ and $\text{Anti}^N(V \otimes W) \not\cong \text{Anti}^N V \otimes \text{Anti}^N W$.

Let us focus for now on the case of $N = 2$. Then

$$\text{Anti}^2(V \otimes W) = \{|\psi\rangle \in V \otimes W \otimes V \otimes W : F^{12:34}|\psi\rangle = -|\psi\rangle\}, \quad (31)$$

where $F^{12:34}$ is the permutation that swaps positions 1,2 with positions 3,4. That is

$$F^{12:34}|\alpha_1, \alpha_2, \alpha_3, \alpha_4\rangle = |\alpha_3, \alpha_4, \alpha_1, \alpha_2\rangle. \quad (32)$$

What if we would like to understand $\text{Anti}^2(V \otimes W)$ in terms of the symmetric and antisymmetric subspaces of $V^{\otimes 2}$ and $W^{\otimes 2}$? Then it will be convenient to rearrange (31) and write (with some small abuse of notation)

$$\text{Anti}^2(V \otimes W) = \{|\psi\rangle \in V \otimes V \otimes W \otimes W : F^{13:24}|\psi\rangle = -|\psi\rangle\}, \quad (33)$$

where $F^{13:24}$ is the permutation that swaps positions 1,3 with positions 2,4, meaning

$$F^{13:24}|\alpha_1, \alpha_2, \alpha_3, \alpha_4\rangle = |\alpha_2, \alpha_1, \alpha_4, \alpha_3\rangle. \quad (34)$$

Since $F^{13:24}$ squared is the identity, its eigenvalues are again ± 1 . We can also write $F^{13:24} = F^{1:2}F^{3:4}$, where

$$F^{1:2}|\alpha_1, \alpha_2, \alpha_3, \alpha_4\rangle = |\alpha_2, \alpha_1, \alpha_3, \alpha_4\rangle. \quad (35a)$$

$$F^{3:4}|\alpha_1, \alpha_2, \alpha_3, \alpha_4\rangle = |\alpha_1, \alpha_2, \alpha_4, \alpha_3\rangle. \quad (35b)$$

Since $F^{1:2}$ and $F^{3:4}$ commute, the eigenvalues of their product are simply the product of their eigenvalues. The joint eigenspaces are as follows

$F^{12:34}$	$F^{1:2}$	$F^{3:4}$
+1	+1	+1
-1	+1	-1
-1	-1	+1
+1	-1	-1

Thus the -1 eigenspace of $F^{13:24}$ contains states in the $+1$ eigenspace of $F^{1:2}$ and the -1 eigenspace of $F^{3:4}$. It also contains states in the -1 eigenspace of $F^{1:2}$ and the $+1$ eigenspace of $F^{3:4}$, as well as superpositions states in these two spaces. Putting this together we have

$$\text{Anti}^2(V \otimes W) \cong (\text{Sym}^2 V \otimes \text{Anti}^2 W) \oplus (\text{Anti}^2 V \otimes \text{Sym}^2 W). \quad (36)$$

Similarly the symmetric subspace of two copies of $V \otimes W$ is

$$\text{Sym}^2(V \otimes W) \cong (\text{Sym}^2 V \otimes \text{Sym}^2 W) \oplus (\text{Anti}^2 V \otimes \text{Anti}^2 W). \quad (37)$$

As an application, a pair of electrons must have either a symmetric spatial wavefunction and an antisymmetric spin wavefunction (i.e. singlet), or vice versa, an antisymmetric spatial wavefunction and a symmetric spin wavefunction. This can lead to an effective spin-spin interaction, and is responsible for the phenomenon of ferromagnetism, which you will explore on your pset.

1.6 Emergence of distinguishability

Given that all types of particles are in fact either bosons or fermions, why do we talk about distinguishable particles? Do they ever occur in nature? It would seem that they do, since if we have N spatially well-localized electrons, we can treat their spins as distinguishable. In other words, we say that the wavefunction is

$$|\psi\rangle = \sum_{s_1, \dots, s_N \in \{+, -\}} c_{s_1, \dots, s_N} |s_1, \dots, s_N\rangle, \quad (38)$$

with no constraints on the amplitudes c_{s_1, \dots, s_N} apart from the usual normalization condition $\sum |c_{s_1, \dots, s_N}|^2 = 1$. A Hamiltonian that acts only on spin 2 (say) would be of the form $I \otimes H \otimes I^{\otimes N-2}$.

Let us examine carefully how this could be realized physically. Assume the electrons are in a potential that traps them in positions that are far from each other. Denote the resulting spatial vectors by $|1\rangle, |2\rangle, \dots, |N\rangle$ corresponding to wavefunctions $\psi_1(\vec{r}), \dots, \psi_N(\vec{r})$. If we had one electron in position $|1\rangle$ with spin in state $|s_1\rangle$, another electron in position $|2\rangle$ with spin in state $|s_2\rangle$, and so on, then the overall state would be

$$\frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \text{sgn}(\pi) |\pi(1)\rangle \otimes |s_{\pi(1)}\rangle \otimes |\pi(2)\rangle \otimes |s_{\pi(2)}\rangle \otimes \dots \otimes |\pi(N)\rangle \otimes |s_{\pi(N)}\rangle. \quad (39)$$

A general superposition of states of this form with different values of s_1, \dots, s_N would be

$$|\Psi\rangle = \sum_{s_1, \dots, s_N \in \{+, -\}} c_{s_1, \dots, s_N} \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \text{sgn}(\pi) |\pi(1)\rangle \otimes |s_{\pi(1)}\rangle \otimes |\pi(2)\rangle \otimes |s_{\pi(2)}\rangle \otimes \dots \otimes |\pi(N)\rangle \otimes |s_{\pi(N)}\rangle. \quad (40)$$

This wavefunction is manifestly antisymmetric under exchanges that swap the spatial and spin parts together.

To see how (38) emerges from (40) consider an experiment that would try to apply a Hamiltonian to, say, the spin of the 2nd particle. When we say “the second particle” what we mean is “the particle whose position in space corresponds to the wavefunction $\psi_2(\vec{r})$.” For example, if we want to apply a magnetic field that affects only this particle, we would apply a localized magnetic field that is nonzero only in the region where $\psi_2(\vec{r})$ is nonzero and $\psi_i(\vec{r}) = 0$ for $i \neq 2$. (Here we use the assumption that the electrons are well separated.) Suppose this field is $B_z \hat{z}$ in this region and zero elsewhere. This field would correspond to a single-particle Hamiltonian of the form $|2\rangle\langle 2| \otimes \omega_z S_z$

for $\omega_z = -\mu_e B_z$, where the $|2\rangle\langle 2|$ means that it affects only the part of the wavefunction in spatial state $|2\rangle$. The resulting N -particle Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^N (I \otimes I)^{\otimes i-1} \otimes (|2\rangle\langle 2| \otimes \omega_z S_z) \otimes (I \otimes I)^{\otimes N-i}. \quad (41)$$

Observe here that the tensor position has no physical significance, but that different particles are effectively labeled by their spatial positions. Imagine a law-school professor who calls on students by seat number instead of by name.

A similar argument could apply to N bosons. In each case, the states involved are not completely general states of N fermions/bosons. Returning to the case of electrons, we are considering states with exactly one electron per site. But states also exist with zero or two electrons in some sites (or superpositions thereof). If we have apply a magnetic field to a site where there is no electron, or bring a measuring device (say a coil to detect a changing magnetic field) nearby, then nothing will happen. What if there are *two* electrons on a site? Then again nothing will happen, but for a less obvious reason. This time is it because the spin singlet state is invariant under collective rotation, and will not be affected by a magnetic field. Overall it is possible to observe behavior that is more complicated than in the model of N distinguishable spins. Spatial position *can* be used to distinguish particles, but it does not have to in every case.

2 Degenerate Fermi gas

2.1 Electrons in a box

Consider N electrons in a box of size $L \times L \times L$ with periodic boundary conditions. (Griffiths discusses hard-wall boundary conditions and it is a good exercise to check that both yield the same answer.) Ignore interactions between electrons. Then the Hamiltonian is

$$H = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m}. \quad (42)$$

We will see that even without interactions, a good deal of interesting physics will result simply from the Pauli exclusion principle. This is because the N -electron ground state will occupy the lowest N levels of the single-electron Hamiltonian $\vec{p}^2/2m$.

To analyze this, we start with the one-particle states. The eigenstates and energies are given by

$$\psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{L^{3/2}} \quad \text{where} \quad \vec{k} = \frac{2\pi}{L}\vec{n}, \quad \vec{n} \in \mathbb{Z}^3. \quad (43)$$

$$E_{\vec{k}} = \frac{\hbar^2}{2m}\vec{k}^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \vec{n}^2. \quad (44)$$

The allowed values of \vec{k} form a lattice with a spacing of $2\pi/L$ between adjacent points. However, we will work in the limit where L and N are large; e.g. in macroscopic objects N will be on the order of 10^{23} . In this limit, we can neglect the details of the lattice and say instead that there is one allowed wavevector per $(2\pi/L)^3$ volume in \vec{k} -space (or two if we count spin). It is left as an exercise to make this intuition precise.

Because of the spin degree of freedom, N electrons in their ground state will fill up the lowest $N/2$ energies, corresponding to the \vec{k} with the lowest values of \vec{k}^2 . These \vec{k} vectors are contained in

a sphere of some radius which we call k_F (aka the Fermi wave vector). Since each wavevector can be thought of as taking up “volume” $(2\pi/L)^3$ in \vec{k} -space, we obtain the following equation for k_F :

$$\frac{4}{3}\pi k_F^3 \cdot \left(\frac{L}{2\pi}\right)^3 \cdot 2 = N \quad (45a)$$

$$k_F = \frac{(3\pi^2 N)^{1/3}}{L} = (3\pi^2)^{1/3} \left(\frac{N}{V}\right)^{1/3} = \boxed{(3\pi^2 n)^{1/3}} \quad (45b)$$

The fact that k_F (in this calculation) depends only on the density $n = N/V$ reflects the principle that k_F is independent of the shape of the material.

From this calculation we can immediately derive many physically relevant quantities. The chemical potential is the energy associated with adding one electron to the system, i.e. $\mu = E_{\text{gs}}(N+1) - E_{\text{gs}}(N)$. Since this new electron would have momentum $\approx \hbar k_F$, its energy (which is also the chemical potential) is

$$E_F = \frac{\hbar^2 k_F^2}{2m}. \quad (46)$$

This energy is also called the *Fermi energy*.

We can also calculate the ground-state energy. Here is a way to do this that is simple enough that you should be able to recreate it in your head. First recalculate the number of particles in terms of k_F as

$$N = \int_0^{k_F} 2 \cdot \left(\frac{L}{2\pi}\right)^3 (4\pi k^2 dk) = \int_0^{k_F} c k^2 dk = c \frac{k_F^3}{3}, \quad (47)$$

for some constant c . Similarly write E_{gs} as

$$E_{\text{gs}} = \int_0^{k_F} 2 \cdot \left(\frac{L}{2\pi}\right)^3 (4\pi k^2 dk) \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \int_0^{k_F} c k^4 dk = \frac{\hbar^2}{2m} c \frac{k_F^5}{5} = \frac{\hbar^2 k_F^2}{2m} N \frac{3}{5} = \frac{3}{5} N E_F. \quad (48)$$

In hindsight we should have guessed that E_{gs} would be some constant times $N E_F$. There are N electrons, each with energy somewhere between 0 and E_F depending on their position within the sphere. So the only nontrivial calculation was to get the constant $\frac{3}{5}$, which boils down to $\frac{\int k^4 dk}{\int k^2 dk}$.

Now consider the volume-dependence of the energy. The ground-state energy is proportional to E_F , which in turn scales like $n^{2/3}$, or equivalently, like $V^{-2/3}$. Thus there is pressure even from non-interacting fermions. This pressure has many equivalent forms

$$P = - \left. \frac{\partial E_{\text{gs}}}{\partial V} \right|_{N,T} = -N \frac{3}{5} \frac{\partial E_F}{\partial V} = -N \frac{3}{5} \left(-\frac{2}{3}\right) \frac{E_F}{V} = \frac{2}{5} n E_F = \frac{2}{3} \frac{E_{\text{gs}}}{V} = \frac{(3\pi^2)^{2/3}}{5m^{8/3}} \rho^{5/3}, \quad (49)$$

where in this last version we have defined the (mass) density $\rho = mn$.

Let's plug in some numbers for a realistic system. In copper, there is one free electron per atom. The density is about $6g/cm^3$ and the atomic weight is $63g/\text{mole}$, which corresponds to $n \approx 10^{23}/cm^3$. An electron has mass $511keV$ (working in units where $\hbar = 1$ and $c = 1$). In these units $1cm \approx 5 \cdot 10^4 eV^{-1}$. Putting this together we get $E_F = O(1)eV$.

This is $\gg k_B T$ for room-temperature T , justifying the assumption that the state is close to the ground state as room temperature, and corresponds to a $v_F = \sqrt{2E_F/m}$ that is $\ll c$, justifying a non-relativistic approximation.

Can we justify neglecting the Coulomb interaction? See the pset.

The Drude-Sommerfeld model. This model of a metal is simple but is already enough to derive the Drude-Sommerfeld model that explains thermal and electrical conductivity, heat capacity and thermal emission. On the other hand, adding a periodic potential (see below) will somewhat complicate this picture.

I will briefly describe the Drude-Sommerfeld model first. One goal is to explain Ohm's Law

$$\vec{J} = \sigma \vec{E}, \quad (50)$$

where \vec{E} is the electric field, \vec{J} is current and σ is conductivity. (Here σ will be a scalar but more generally it could be a 3×3 matrix.) Suppose that electrons accelerate ballistically for a typical time τ before a collision which randomizes their velocity. In the absence of a collision they will accelerate according to

$$m\dot{\vec{v}} = e\vec{E}, \quad (51)$$

so their mean velocity will be

$$\vec{v}_d = \frac{e}{m} \vec{E} \tau. \quad (52)$$

Here we write \vec{v}_d to mean the “drift” velocity of an electron. The actual velocity will include thermal motion as well but this averages to zero. The net current is $ne\vec{v}_d$, where n is the electron density. Putting this together we obtain

$$\sigma = \frac{ne^2\tau}{m}. \quad (53)$$

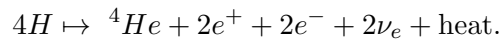
One unsatisfactory feature of this model is the presence of the phenomenological constant τ . On the other hand, a similar calculation (omitted) can express thermal conductivity κ in terms of τ , and predicts that the “Lorentz number” $\frac{\kappa}{\sigma T}$ should be a universal constant. Modeling electrons as a classical gas predicts that this number should be $\approx 1.1 \times 10^{-9} \frac{\text{watt} \cdot \text{ohm}}{\text{K}^2}$ and modeling them as a Fermi gas predicts $\approx 2.44 \times 10^{-8} \frac{\text{watt} \cdot \text{ohm}}{\text{K}^2}$. In real metals, this number is much closer to the Fermi gas prediction, which provides some support for the Drude-Sommerfeld theory.

There are some other aspects of the theory which are clearly too simplistic. The mean free path $\ell \equiv \tau v_F$ is hundreds of times larger than the spacing between atoms. Why aren't there more frequent collisions with the atomic lattice or the other electrons? There are qualitative problems as well. While (53) does not depend on the sign of the charge carriers, the Hall effect (discussed later) does. Observations show that most materials have negative charge carriers but some have positive charge carriers. Another strange empirical fact is that some crystals are conductors and others are semiconductors or insulators; overall, resistivity varies by more than a factor of 10^{20} . The conductance is also temperature dependent, but not always in the same direction: raising temperature will reduce the conductivity of metals but increase it for semiconductors such as silicon and germanium.

Explaining these facts will require understanding periodic potentials, which we will return to in Section 2.3.

2.2 White dwarves

Our sun is powered by fusion, primarily via the p - p process:



This creates thermal pressure outward which balances the inward gravitational pressure. When the hydrogen runs out, helium can further fuse and form carbon and oxygen. In larger stars

this will continue producing until iron is formed (heavier elements are also produced but do not create more energy), but eventually fusion will stop. At this point the heat will be radiated away, the temperature will drop and gravity will cause the star to dramatically shrink. This will not necessarily end in a black hole due to the degeneracy pressure of the electrons.

We will model the star by a collection of noninteracting nonrelativistic electrons in their ground state. There are a lot of assumptions here. The ground-state assumption is justified because photons will carry away most of the energy of the star. The non-interacting assumption will be discussed on the pset. We consider only electrons and not nuclei because degeneracy pressure scales with $E_F \propto 1/m$, although we will revisit this, as well as the nonrelativistic assumption, later in the lecture. We assume also a uniform density which is not really true, but does not change the qualitative picture.

For a given stellar mass M_* we would like to find the radius R_* that balances the gravitational pressure with the electron degeneracy pressure. We can find this by computing the total energy E_{tot} and setting $dE_{\text{tot}}/dR = 0$. The resulting value of R_* is a stable point if $d^2E_{\text{tot}}/dR^2 < 0$.

The free parameters are:

- N , the number of nucleons (protons and neutrons). These each have mass roughly $m_p \approx 10^9 eV/c^2$ and carry most of the mass of the star, so that $M_* \approx Nm_p$.
- f , the fraction of electrons per nucleon. Charge balance means that there are $N_e \equiv fN$ electrons, fN protons and $(1-f)N$ neutrons, and in particular that $0 \leq f \leq 1$.

Let's calculate the energy contribution from gravity. We will make use of the density $\rho \equiv \frac{M_*}{\frac{4}{3}\pi R^3}$.

$$\begin{aligned}
 E_{\text{grav}}(R) &= \int_0^R -\frac{G_N(\text{mass enclosed by radius } r)(\text{mass at distance } r)}{r} dr \\
 &= \int_0^R -\frac{G_N}{r} \frac{4}{3}\pi r^3 \rho 4\pi r^2 \rho dr \\
 &= \dots \\
 &= -\frac{3}{5}G_N \frac{M_*^2}{R} \\
 &\equiv -\frac{\kappa N^2}{R},
 \end{aligned}$$

where in the last step we have defined the universal constant $\kappa = \frac{3}{5}G_N m_p^2$.

On the other hand the energy from electron degeneracy is

$$\begin{aligned}
 E_{\text{degen}}(R) &= E_{\text{gs}} = \frac{3}{5}N_e E_F(R) \\
 &= \frac{3}{5}N_e \frac{\hbar^2}{2m_e} \left(\frac{3\pi^2 N_e}{V} \right)^{2/3} \\
 &= \underbrace{\left(\hbar^2 f^{5/3} \left(\frac{3}{10} \right) \left(\frac{9\pi}{4} \right)^{2/3} \right)}_{\equiv \lambda} \frac{N^{5/3}}{m_e R^2}, = \frac{\lambda N^{5/3}}{m_e R^2},
 \end{aligned}$$

where again λ is a universal constant. For $f = 0.6$ (as is the case for our sun) we have $\lambda \approx 1.1\hbar^2$.

Combining these we have

$$E_{\text{tot}}(R) = \frac{\lambda N^{5/3}}{m_e R^2} - \frac{\kappa N^2}{R}. \tag{54}$$

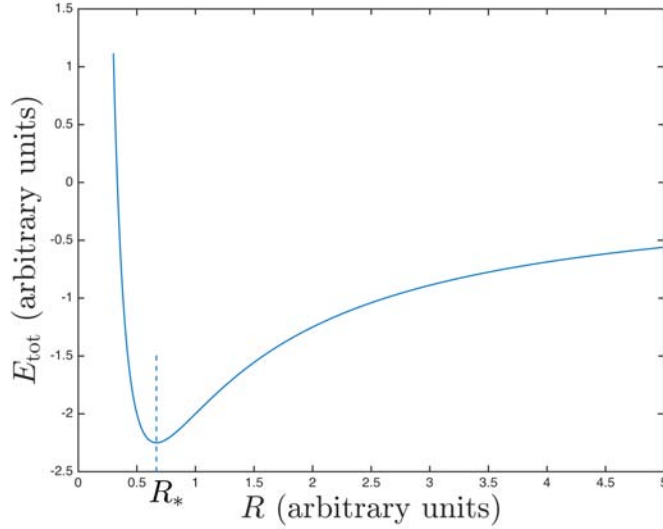


Figure 1: Plot of (54) showing energy from gravity and degeneracy pressure as a function of radius.

This is plotted in Fig. 1.

Setting $dE_{\text{tot}}(R)/dR = 0$ we find

$$R_* = \frac{2\lambda}{m_e \kappa} N^{-1/3}. \quad (55)$$

On the pset you will plug in numbers showing that for $M_* = M_{\text{Sun}}$ the radius is $R_* \approx R_{\text{Earth}}$. Thus, this predicts an enormous but finite density.

One strange feature of (55) is that as N increases (equiv. as M_* increases), the radius R_* decreases. This means as the star gets larger it approaches infinite density. This clearly cannot be valid indefinitely.

Let's revisit the non-relativistic assumption. This is valid if

$$1 \gg \frac{v_F}{c} = \frac{\hbar k_F}{m_e c} \sim \frac{\hbar n^{1/3}}{m_e c} \sim \frac{\hbar N^{1/3}}{m_e c R} \sim \frac{\hbar N^{1/3}}{m_e c \frac{\lambda}{m_e \kappa} N^{-1/3}} \sim \frac{G_N}{\hbar c} m_p^2 N^{2/3} = \frac{m_p^2}{m_{\text{Pl}}^2} N^{2/3}.$$

In the last step we have introduced the Planck mass m_{Pl} which is the unique mass scale associated with the fundamental constants G_N, \hbar, c . Thus the critical value of N at which the non-relativistic assumption breaks down is

$$N_{\text{crit}} \sim \left(\frac{m_{\text{Pl}}}{m_p} \right)^3 \approx 10^{57}.$$

The critical mass is $M_{\text{crit}} = N_{\text{crit}} m_p \approx 10^{66} \text{ eV}/c^2$. By contrast $M_{\text{Sun}} \approx 2 \cdot 10^{30} \text{ kg} \cdot 6 \cdot 10^{35} \frac{\text{eV}/c^2}{\text{kg}} \approx 10^{66} \text{ eV}/c^2$ which is right at the threshold where the non-relativistic assumption breaks down.

2.2.1 A relativistic free electron gas

We follow the same approach as before but instead of $E = \hbar^2 k^2 / 2m$ we have

$$E = \sqrt{m_e^2 c^4 + \hbar^2 \vec{k}^2 c^2} \approx \hbar c |\vec{k}|.$$

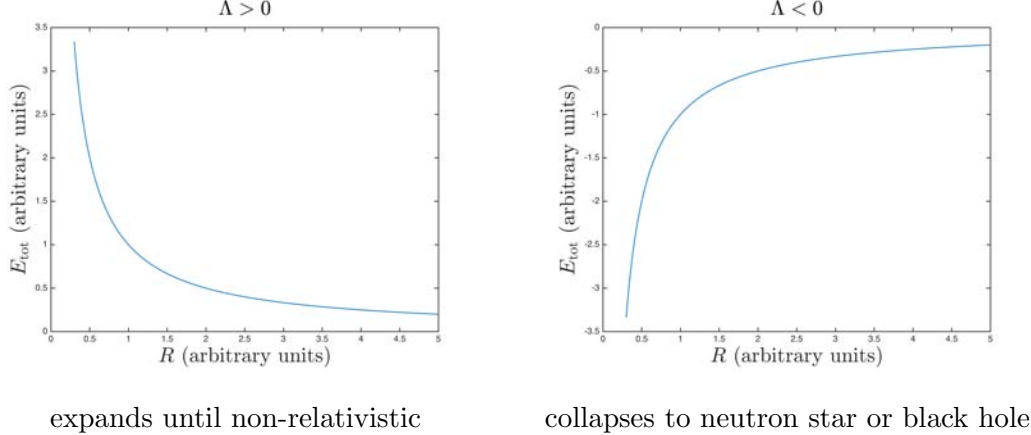


Figure 2: Plot of (56) showing the total energy from gravity and degeneracy pressure of a relativistic free electron gas.

The first expression is the exact energy valid for all \vec{k} and the latter is the ultra-relativistic limit which is relevant when $\hbar|\vec{k}| \gg m_e c$. In this case the lowest energy states are still those with $|\vec{k}| \leq k_F$ for some threshold k_F , but the modified form of E_F means we now have

$$\begin{aligned}
 E_{\text{gs}} &= \underbrace{\int_0^{k_F} 2 \left(\frac{L}{2\pi} \right)^3 4\pi k^2 dk \hbar c}_{N_e = \frac{V k_F^3}{3\pi^2}} \\
 &= \frac{V \hbar c}{4\pi^2} k_F^4 \\
 &= \kappa' \frac{N^{4/3}}{V^{1/3}}
 \end{aligned}$$

where $\kappa' \equiv \frac{3}{4} \left(\frac{9\pi}{4} \right)^{1/3} f^{4/3} \hbar c$. Now the total energy is

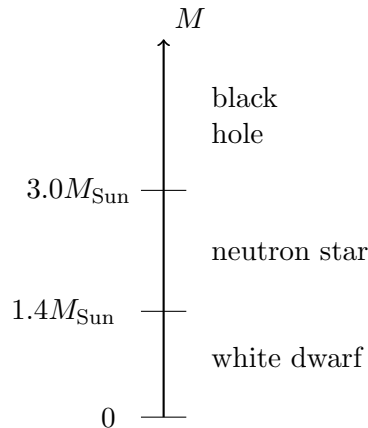
$$E_{\text{tot}} = -\frac{\kappa N^2}{R} + \frac{\kappa' N^{4/3}}{R} \equiv \frac{\Lambda}{R}. \quad (56)$$

The situation is now much simpler than in the non-relativistic case. If $\Lambda < 0$ then the star collapses and if $\Lambda > 0$ then the star expands until the electrons are no longer ultra-relativistic. See Fig. 2.

The critical value of N at which $\Lambda = 0$ occurs when $\kappa N^2 = \kappa' N^{4/3}$. Rearranging we find that this is at $N_c = (\kappa'/\kappa)^{3/2}$. The corresponding mass turns out (using $f = 0.6$ and $M_{\text{Sun}} = \frac{m_{\text{p1}}^3}{m_p^2}$) to be $M_c = m_p N_c \approx 1.4 M_{\text{Sun}}$. This bound is called the Chandrasekhar limit. (Actually the true bound drops some of the simplifying assumptions, such as constant density, but it is not far off from what we have estimated.)

We now can predict the fate of our sun: it will become a white dwarf. What happens when $\Lambda < 0$? In this case a white dwarf will collapse but not necessarily to a black hole. At high densities the reaction $e^- + p^+ \mapsto n + \nu$ will convert all the charged particles into neutrons. Neutrons are fermions and have their own degeneracy pressure. The analogue of a white dwarf is a neutron star, which is supported by this neutron degeneracy pressure. We now repeat the above calculation but with $f = 1$ and with m_e replaced by m_p . It turns out that neutron stars are stable up to masses of roughly $3.0 M_{\text{Sun}}$ (although this number is fairly uncertain in part because we don't know the

structure of matter in a neutron star; it may be that the quarks and gluons combine into more exotic nuclear matter). Above $3.0M_{\text{Sun}}$ there is no further way to prevent collapse into a black hole.



Besides our sun, some representative stars are Alpha Centauri A at 1.1 solar masses, destined to be a white dwarf, and Sirius A at 2.0 solar masses, destined to be a neutron star.

2.3 Electrons in a periodic potential

This lecture will explore how degenerate fermions can explain electrical properties of solids. In a solid, atomic nuclei are packed closely together in (roughly) fixed positions while some electrons are localized near these nuclei and some can be delocalized and move throughout the solid. We model this by grouping together the nuclei and localized electrons as a static potential $V(\vec{x})$, while assuming the delocalized electrons are subject to this potential but do not interact with each other. In other words, we add a potential but still do not consider interactions. This model is simple but already contains nontrivial physics. The resulting Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + V(\vec{x}_i).$$

We will see that this gives rise to band structure, which in turn can explain insulators, conductors and semiconductors all from the same underlying physics.

2.3.1 Bloch's theorem

Suppose at first that we have a single electron in a 1-d lattice with ions spaced regularly at distance a . The resulting potential is periodic and satisfies

$$V(x) = V(x + a) \tag{57}$$

for all x . We can express this equivalently in terms of the translation operator \hat{T}_a defined by $\hat{T}_a\psi(x) = \psi(x + a)$. Since $[\hat{T}_a, \hat{V}] = 0$ we have $[\hat{T}, \hat{H}] = 0$ and thus \hat{T}_a and \hat{H} can be simultaneously diagonalized. Bloch's theorem essentially states that we can take eigenstates of \hat{H} to be also eigenstates of \hat{T}_a .

To see what this means let's look more carefully at \hat{T}_a . We have seen this in 8.05 already:

$$\hat{T}_a = \exp\left(\frac{ia\hat{p}}{\hbar}\right) = \exp\left(a\frac{\partial}{\partial x}\right). \tag{58}$$

Our boundary conditions ensure that \hat{p} is Hermitian, and thus \hat{T}_a is unitary. Therefore its eigenvalues are of the form $e^{i\alpha}$ for $\alpha \in \mathbb{R}$. By convention we write the eigenvalues as e^{ika} for some $k \in \mathbb{R}$. The resulting eigenstates $\psi_{n,k}(x)$ thus satisfy

$$\hat{T}_a \psi_{n,k}(x) = \psi_{n,k}(x+a) = e^{ika} \psi_{n,k}(x). \quad (59)$$

Here n is a label for any additional degeneracy in the eigenstates of \hat{H} .

We can also write $\psi_{n,k}(x) = e^{ikx} u_{n,k}(x)$ with $u_{n,k}(x) = u_{n,k}(x+a)$. This form of Bloch's theorem is more conventionally used.

The probability density $|\psi_{n,k}(x)|^2 = |u_{n,k}(x)|^2$ is periodic but delocalized. In that sense it resembles plane waves, and implies that the electrons are generally free to move around, despite the presence of the ionic potential.

Range of k values? By definition if we add an integer multiple of 2π to k then the phase e^{ika} is the same. So we can WLOG restrict k to the “Brillouin zone” $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$.

Meaning of k . The value k is referred to as a “crystal momentum,” and even though it is only defined modulo $2\pi/a$, it has some momentum-like properties. To see this, first look at the eigenvalue equation satisfied by $u_{n,k}$.

$$(E_{n,k} - V(x))e^{ikx} u_{n,k}(x) = \frac{p^2}{2m} e^{ikx} u_{n,k}(x) = e^{ikx} \frac{(p + \hbar k)^2}{2m} u_{n,k}(x). \quad (60)$$

Rearranging we have

$$\underbrace{\left(\frac{(p + \hbar k)^2}{2m} + V \right)}_{H_k} |u_{n,k}\rangle = E_{n,k} |u_{n,k}\rangle. \quad (61)$$

By the Hellmann-Feynman theorem,

$$\frac{1}{\hbar} \frac{dE_{n,k}}{dk} = \langle u_{n,k} | \frac{dH_k}{dk} | u_{n,k} \rangle \quad (62)$$

$$= \langle u_{n,k} | \frac{p + \hbar k}{m} | u_{n,k} \rangle \quad (63)$$

$$= \langle \psi_{n,k} | \frac{p}{m} | \psi_{n,k} \rangle = \frac{\langle p \rangle}{m}. \quad (64)$$

If we interpret this last quantity as the velocity and define $\omega_{n,k} = E_{n,k}/\hbar$, then we find that the velocity is equal to $\frac{d\omega_{n,k}}{dk}$. This is the usual expression for the group velocity of a wave.

The 3-d case. We will not explore this in detail here, but here is a very rough treatment. If we have a cubic lattice with spacing a then we can write $\psi_{n,\vec{k}}(\vec{x}) = e^{i\vec{k} \cdot \vec{x}} u_{n,k}(\vec{x})$ for $u_{n,k}(\vec{x}) = u_{n,k}(\vec{x} + a\vec{e}_i)$ for $i = 1, 2, 3$. The resulting Brillouin zone is defined by $k_i \in [-\frac{\pi}{a}, \frac{\pi}{a}]$.

More generally suppose we have a lattice that is periodic under translation by $\vec{a}_1, \vec{a}_2, \vec{a}_3$. The theory of crystallographic groups includes a classification of possible values of $\vec{a}_1, \vec{a}_2, \vec{a}_3$. The “reciprocal lattice vectors” $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are defined by the relations

$$\vec{a}_i \cdot \vec{b}_j = \delta_{i,j}. \quad (65)$$

This is equivalent to the matrix equation

$$\begin{pmatrix} \vec{a}_1 \\ \vec{a}_2 \\ \vec{a}_3 \end{pmatrix} \cdot \begin{pmatrix} \vec{b}_1 & \vec{b}_2 & \vec{b}_3 \end{pmatrix} = I_3. \quad (66)$$

Similar arguments imply that \vec{k} lives in a space that is periodic modulo translations by $\vec{b}_1, \vec{b}_2, \vec{b}_3$. For more details, see a solid-state physics class, like 8.231, or a textbook like *Solid State Physics* by Ashcroft and Mermin.

The tight-binding model. On your pset you will consider some more general models, but for now let us consider a simple model that can be exactly solved. In the tight-binding model the potential consists of deep wells, each containing a single bound state with energy E_0 . Let $|n\rangle$ denote the state of an electron trapped at $x = na$ for $n = \dots, -2, -1, 0, 1, 2, \dots$. Suppose there is also a small tunneling term between adjacent sites, so that the Hamiltonian is

$$H = \sum_{n=-\infty}^{\infty} E_0 |n\rangle \langle n| - \Delta |n+1\rangle \langle n| - \Delta |n-1\rangle \langle n|.$$

This can be rewritten in terms of the translation operator $T = \sum_n |n+1\rangle \langle n|$ as

$$H = E_0 I - \Delta(T + T^\dagger). \quad (67)$$

By Bloch's theorem the eigenstates can be labeled by k , with

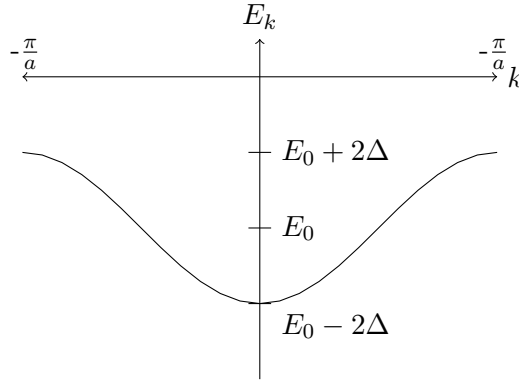
$$T|\psi_k\rangle = e^{ika}|\psi_k\rangle \quad (68)$$

$$H|\psi_k\rangle = E_k|\psi_k\rangle \quad (69)$$

From (67) we can calculate

$$E_k = E_0 - \Delta(e^{ika} + e^{-ika}) = E_0 - 2\Delta \cos(ka). \quad (70)$$

If $\Delta = 0$ then we have an infinite number of states with degenerate energy equal to E_0 . But when $\Delta \neq 0$ this broadens into a finite energy band $E_0 \pm 2\Delta$ (see plot).



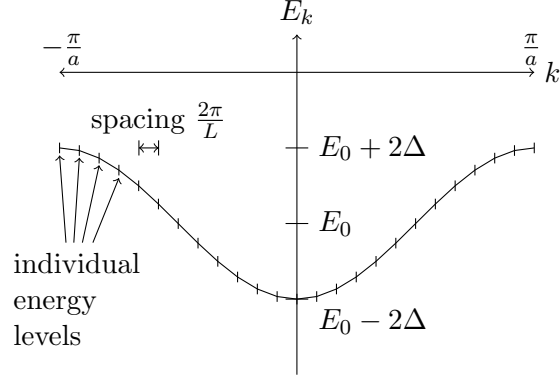
Real solids are not infinite. Suppose there are N sites with periodic boundary conditions, i.e. let $L = Na$ and suppose that $\psi(0) = \psi(L)$. This implies that $T^N|\psi\rangle = \psi$ and therefore for any eigenvalue e^{ika} we must have

$$e^{ikaN} = 1 \quad (71)$$

$$Nka = 2\pi n \quad \text{for some integer } n \quad (72)$$

$$k = \frac{2\pi n}{Na} = \frac{2\pi}{L}n \quad -\frac{N}{2} < n \leq \frac{N}{2} \quad (73)$$

The energy levels are along the same band as before but now the allowed values of k are integer multiples of $\frac{2\pi}{L}$.



Each one of these points corresponds to a delocalized state.

Band structure. Now suppose each site can support multiple bound states, say with energies $E_0 < E_1 < E_2$. Then tunneling opens up a band around each energy. If Δ is small enough then there will be a band gap between these.

Kronig-Penney model Another model that can be exactly solved is a periodic array of delta functions. We skip this because Griffiths has a good treatment in section 5.3.2.

Free electron. We now turn to a rather trivial example of a periodic potential, namely $V = 0$. This is periodic for any choice of a . Still it is instructive to apply Bloch's theorem, which implies that eigenstates can be written in the form

$$\psi_{n,k}(x) = e^{ikx} u_{n,k}(x), \quad (74)$$

where $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$ and $u_{n,k}(x) = u_{n,k}(x + a)$. One such choice of $u_{n,k}(x)$ is $e^{\frac{2\pi i n x}{a}}$. Plugging this into (74) we obtain

$$\psi_{n,k}(x) = e^{i(\frac{2\pi}{a}n + k)x} \quad \text{and} \quad E_{n,k} = \frac{\hbar^2}{2m} \left(\frac{2\pi}{a}n + k \right)^2. \quad (75)$$

This corresponds to a separation of scales into high and low frequency; the index n describes the rapid oscillations that occur within a unit cell of size a and the crystal momentum k describes the long-wavelength behavior that can only be seen by looking across many different cells.

If we did not use Bloch's theorem at all then the allowed energies would simply look like the parabola $E = p^2/2m$. Dividing momentum into k and n leads to a folded parabola; see Fig. 3.

Nearly-free electrons. Now suppose that V is nonzero but very weak. If $[T_a, V] = 0$ then V will be block diagonal when written in the eigenbasis of T_a . Recall that the eigenvalues of T_a are

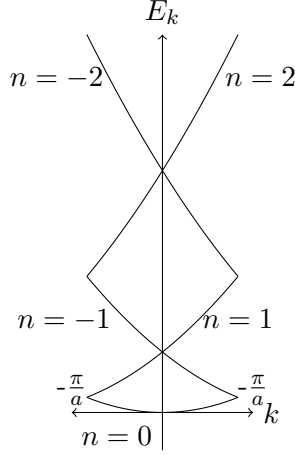


Figure 3: Band diagram for free electrons.

e^{ika} for k and integer multiple of $\frac{2\pi}{L}$. If we let $\phi := 2\pi a/L$ then there is a basis in which we have

$$T = \begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & 1 & \\ \hline & & e^{i\phi} & \\ & & & \ddots \\ & & & & e^{i\phi} \\ \hline & & & & e^{2i\phi} & \\ & & & & & \ddots \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} * & * & * & & & \\ * & * & * & & & \\ * & * & * & & & \\ \hline & & & * & * & * \\ & & & * & * & * \\ & & & * & * & * \\ \hline & & & & & * \\ & & & & & \ddots \end{pmatrix}$$

These blocks correspond to single values of k which are vertical lines in Fig. 3. Treat V as a perturbation. For a typical value of k the kinetic energy of these points is well-separated and so V does not significantly mix the free states. However, near $\pm\pi/a$, the kinetic energy term has a degeneracy, so there the addition of V will lead to a splitting, which will open up a gap between the bands (see figure drawn in class).

Conductors, semiconductors and insulators. A band with N sites can hold $2N$ electrons, once we take spin into account. Suppose that there are M delocalized electrons in this band. If $M < 2N$ then the band is partly filled. This means that it is possible for an electron at the edge of the filled region (see blackboard figure) to gain a small amount of momentum, perhaps in response to an applied electric field. In this situation we have a conductor. For example, in sodium there is 1 free electron per atom, so the band is half full. A crystal can also be a conductor if bands overlap (something more likely in three dimensions) resulting in multiple partially full bands.

Alternatively, suppose $M = 2N$, so the band is completely full. If there is a large band gap then there is no way for an electron to absorb a small amount of energy and accelerate. In this case the material is an insulator.

If the band gap is small then the material is a semiconductor. Call the band below the gap the

“valence band” and the band right above the gap the “conduction band.” At $T = 0$ the valence band is completely full and the conduction band is completely empty, but for $T > 0$ there are a few excited electrons in the conduction band and a few holes in the valence band. These are mobile and can carry current. The holes behave like particles with positive charge and negative mass.

The Fermi surface can also be pushed up or down by “doping” with impurities that either contribute or accept electrons. Adding a “donor” like phosphorus to silicon adds localized electrons right below the conduction band. A small electric field is enough to move this into the conduction band. The resulting material is called an “n-type semiconductor.” On the other hand, aluminum has one fewer electron than silicon, and so is an “acceptor.” Adding aluminum will increase the number of holes in the valence band and reduce the number of conduction electrons, resulting in a “p-type semiconductor.” An interface between n-type and p-type semiconductors is called a p-n junction, and is used for diodes (including LEDs), solar cells, transistors and other electronic devices.

3 Charged particles in a magnetic field

3.1 The Pauli Hamiltonian

Consider a particle with charge q and mass m . We will study its interactions with an electromagnetic field. To write down the Hamiltonian we will use not \vec{E} and \vec{B} but instead the vector potential \vec{A} and the scalar potential ϕ . Recall that their relation is

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad \text{and} \quad \vec{E} = -\vec{\nabla}\phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t}. \quad (76)$$

We have seen this already for the electric field, where the contribution to the Hamiltonian is $q\phi(\vec{x})$. The force from the magnetic field is velocity dependent (recall the classical EOM $m\ddot{\vec{x}} = q(\vec{E} + \frac{\vec{x}}{c} \times \vec{B})$ with $\vec{v} = \dot{\vec{x}}$), so its contribution to the Hamiltonian cannot be as a potential term.

To derive the correct quantum Hamiltonian we can start with the classical Hamiltonian and follow the prescription of canonical quantization (cf. “Supplementary Notes: Canonical Quantization and Application to the Quantum Mechanics of a Charged Particle in a Magnetic Field.”) or we can start with the Dirac equation and consider the nonrelativistic limit. Another option is to add a term $\frac{q}{c} \dot{\vec{x}} \cdot \vec{A}$ to the Lagrangian. Either way the magnetic field turns out to enter the Hamiltonian by replacing the kinetic energy term with $\frac{1}{2m}(\vec{p} - \frac{q}{c}\vec{A}(\vec{x}))^2$. We thus obtain the *Pauli Hamiltonian* (neglecting an additional spin term):

$$H = \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A}(\vec{x}) \right)^2 + q\phi(\vec{x}). \quad (77)$$

There are a few subtle features of (77). First, it contains a massive redundancy in that we are free to choose an arbitrary *gauge* for \vec{A} and ϕ without changing the physics. Specifically if we replace \vec{A}, ϕ with

$$\vec{A}' = \vec{A} + \vec{\nabla} f \quad \text{and} \quad \phi' = \phi - \frac{1}{c} \frac{\partial f}{\partial t}, \quad (78)$$

then all observable quantities will remain the same. This gauge-invariance will be explored more on your pset. For now observe that plugging (78) into (76) leaves \vec{E}, \vec{B} unchanged.

Also observe there are now two things we might call momentum: the original \vec{p} and the term appearing in the Hamiltonian $m\vec{v} \equiv \vec{p} - \frac{q}{c}\vec{A}(\vec{x})$. The operator \vec{p} still satisfies $[p_i, x_j] = -i\hbar\delta_{ij}$ and is called the *generalized momentum*. By contrast, $m\vec{v}$ is called the *kinetic momentum*. We will see on the pset that expectation values of one of these is gauge-invariant; this one can thus be physically

observed. (Sometimes an observable is said to be gauge invariant; this generally means not that the *operator* is gauge invariant but that its expectation values are. More concretely if \mathcal{O}' is the transformed version of \mathcal{O} then we say \mathcal{O} is gauge invariant if $\langle\psi'|\mathcal{O}'|\psi'\rangle = \langle\psi|\mathcal{O}|\psi\rangle$.)

Remark: This gauge freedom will appear many times in the coming lectures and often leads to seemingly strange results. It is worth remembering that we are already used to a simpler form of gauge invariance: that of replacing $H(t)$ with $H(t) + f(t)I$, and $|\psi(t)\rangle$ with $\exp(-i \int_{t_0}^t f(t') dt' / \hbar) |\psi(t)\rangle$. This change clearly describes the same physics and we have (often implicitly) restricted our attention to gauge-invariant observables. Specifically, we recognize that energies are arbitrary (here “non-gauge-invariant”) while differences in energies are physically observable (i.e. “gauge-invariant”). This also points to the difficulties in formulating an analogue of the Schrödinger equation in which there are no redundant degrees of freedom, such as the overall phase. If we tried to express Hamiltonians in terms of energy differences rather than energy levels then the differential equation would involve terms that were sums of many of these differences (e.g. $E_4 - E_1 = (E_4 - E_3) + (E_3 - E_2) + (E_2 - E_1)$), thus taking on a “non-local” character analogous to what would happen if we tried to express (77) in terms of \vec{E}, \vec{B} instead of \vec{A}, ϕ .

As a sanity check on (77) we will show that it reproduces the right classical equations of motion. Recall that Hamilton’s equations of motions are

$$\dot{x}_i = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}.$$

First we calculate

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{1}{m} \left(p_i - \frac{q}{c} A_i \right) \quad \implies \quad \vec{p} = m\dot{\vec{x}} + \frac{q}{c} \vec{A}, \quad (79)$$

obtaining a generalized momentum \vec{p} . Next we should remember that $\vec{A}(\vec{x}), \phi(\vec{x})$ depend on position so that

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} = -\sum_j \frac{q}{mc} \left(p_j - \frac{q}{c} A_j \right) \frac{\partial A_j}{\partial x_i} - q \frac{\partial \phi}{\partial x_i} = -\sum_j \frac{q}{c} \dot{x}_j \frac{\partial A_j}{\partial x_i} - q \frac{\partial \phi}{\partial x_i} \quad (80)$$

To evaluate the LHS, we apply d/dt to (79) and obtain

$$\dot{p}_i = \frac{d}{dt} \left(m\dot{x}_i + \frac{q}{c} A_i \right) = m\ddot{x}_i + \frac{q}{c} \left(\frac{\partial A_i}{\partial t} + \sum_j \frac{\partial A_i}{\partial x_j} \dot{x}_j \right). \quad (81)$$

Combining this with (80) and rearranging we obtain

$$m\ddot{x}_i = q \left(-\frac{\partial \phi}{\partial x_i} - \frac{1}{c} \frac{\partial A_i}{\partial t} \right) + \frac{q}{c} \left(\sum_j \dot{x}_j \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) \right). \quad (82)$$

To simplify the last term, observe that, for fixed i, j ,

$$\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} = \sum_k \epsilon_{ijk} (\vec{\nabla} \times \vec{A})_k = \sum_k \epsilon_{ijk} B_k$$

and thus

$$\sum_j \dot{x}_j \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) = \sum_{j,k} \epsilon_{ijk} \dot{x}_j B_k = (\dot{\vec{x}} \times \vec{B})_i.$$

We can now rewrite (82) in vector notation as

$$m\ddot{\vec{x}} = q \left(\underbrace{-\vec{\nabla}\phi - \frac{1}{c}\dot{\vec{A}}}_{\vec{E}} \right) + \frac{q}{c}\dot{\vec{x}} \times \vec{B}. \quad (83)$$

This recovers the familiar Lorentz force law. Phew!

3.2 Landau levels

For the rest of this section we consider particles with charge q and mass m confined to the x - y plane with $\vec{E} = 0$ and $\vec{B} = B\hat{z} = (0, 0, B)$.

The classical equations of motion are

$$\begin{aligned} m\ddot{\vec{x}} &= \frac{q}{c}\dot{\vec{x}} \times \vec{B} \\ \begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix} &= \frac{qB}{mc} \begin{pmatrix} \dot{y} \\ -\dot{x} \end{pmatrix} \end{aligned}$$

This corresponds to circular motion in the x - y plane with frequency $\omega_L \equiv \frac{qB}{mc}$, called the *Larmor frequency*. Circular motion is periodic and we might expect the quantum system to behave in part like a harmonic oscillator.

To solve the quantum case we need to choose a gauge. Here we face the sometimes conflicting priorities of making symmetries manifest and simplifying our calculations. We will choose the “Landau gauge” to make things simple, namely

$$\vec{A} = (-By, 0, 0), \quad \phi = 0. \quad (84)$$

Another variant of the Landau gauge is $\vec{A} = (0, Bx, 0)$. On the pset you will also explore the “symmetric gauge,” defined to be $\vec{A} = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$. It is nontrivial to show that these result in the same physics, but this too will be partially explored on the pset.

In the Landau gauge we have

$$H = \frac{1}{2m} \left(p_x + \frac{qB}{c}y \right)^2 + \frac{1}{2m}p_y^2. \quad (85)$$

(We might also add a $p_z^2/2m$ term if we do not assume the particles are confined in the x - y plane. This degree of freedom is in any case independent of the others and can be ignored.)

To diagonalize (85) the trick is to realize that $[H, p_x] = 0$. Thus all eigenstates of H are also eigenstates of p_x . Let us restrict to the $\hbar k_x$ eigenspace of p_x . Denote this restriction by H_{k_x} . Then

$$H_{k_x} = \frac{p_y^2}{2m} + \frac{1}{2m} \left(\hbar k_x + \frac{qB}{c}y \right)^2 = \frac{p_y^2}{2m} + \frac{1}{2}m \left(\frac{qB}{mc} \right)^2 \left(y - \frac{-\hbar k_x c}{qB} \right)^2. \quad (86)$$

This is just a harmonic oscillator! The frequency is

$$\omega \equiv \frac{qB}{mc} = \omega_L,$$

(i.e. the Larmor frequency) and the center of the oscillations is offset from the origin by

$$y_0 \equiv \frac{-\hbar k_x c}{qB} = -l_0^2 k_x.$$

In the last step we have defined l_0 to be characteristic length scale of the harmonic oscillator, i.e. $l_0 = \sqrt{\frac{\hbar}{m\omega_L}} = \sqrt{\frac{\hbar c}{qB}}$.

We can now diagonalize H from (85). The eigenstates are labeled by k_x and n_y , and have energies and wavefunctions given by

$$E_{k_x, n_y} = \hbar\omega_L(n_y + 1/2) \quad (87)$$

$$\psi_{k_x, n_y} = e^{ik_x x} l_0^{-1/4} \phi_{n_y} \left(\frac{y - y_0}{l_0} \right), \quad (88)$$

where $\phi_n(y)$ is the n^{th} eigenstate of the standard harmonic oscillator. As a reminder,

$$\phi_n(y) = \frac{(-1)^n}{\sqrt{2^n n!} \pi^{1/4}} e^{\frac{y^2}{2}} \frac{d^n}{dy^n} e^{-y^2}.$$

We refer to the different n_y as “Landau levels.” The lowest Landau level (LL) has $n_y = 0$, the next lowest has $n_y = 1$, etc. States within a LL are indexed by k_x . Since this can take on an infinite number of values (any real number), the LLs are infinitely degenerate.

These basis states look rather different from the small circular orbits that we observe classically. They are completely delocalized in the x direction, while in the y direction they oscillate over a band of size $O(l_0)$ centered around a position depending on k_x . Of course we could’ve chosen a different gauge and obtained eigenstates that are delocalized in the y direction and localized in the x direction. And on the pset you will see that the symmetric gauge yields something closer to the classical circular orbits. The reason these alternate pictures can be all simultaneously valid is the enormous degeneracy of the Landau levels. Changing from one set of eigenstates to another corresponds to a change of basis.

3.3 The de Haas-van Alphen effect

To make the above picture more realistic, let’s suppose our particle is confined to a finite region in the plane, say with dimensions $L \times W$. For simplicity we impose periodic boundary conditions. This means that

$$k_x = \frac{2\pi}{W} n_x, \quad n_x \in \mathbb{Z}.$$

We also have the constraint that y_0 should stay within the sample. (Assume that $l_0 \ll L, W$ so we can ignore boundary effects.) Then $0 < y_0 < L$, or equivalently

$$-\frac{WLqB}{2\pi\hbar c} < n_x < 0.$$

This implies that each LL has a finite degeneracy

$$D \equiv WL \frac{qB}{\hbar c} = \frac{A}{2\pi l_0^2} = \frac{BA}{\hbar c/q} = \frac{\Phi}{\Phi_0}. \quad (89)$$

Here $A = WL$ is the area of the sample, $\Phi = BA$ is the flux through it and $\Phi_0 = \hbar c/e$ is the fundamental flux quanta (specializing here to electrons so $q = -e$).

Let us now examine the induced magnetization. In general the induced magnetic moment $\vec{\mu}_I$ is given by $-\vec{\nabla}_{\vec{B}}E$. We can classify this response based on the sign of $\vec{\mu}_I \cdot \vec{B}$. If it is positive we say the material is paramagnetic and if it is negative we say it is diamagnetic. (Ferromagnetism can be thought of as a variant of paramagnetism in which there can be a nonzero dipole moment even with zero applied field. This “memory effect” is known as hysteresis and comes from an enhanced spin-spin interaction known as the exchange interaction; cf. pset 8.) The standard examples of para- and diamagnetism are spin and orbital angular momentum respectively. At finite temperature spins will prefer to align with an applied magnetic field, thus enhancing it, while induced current loops (e.g. orbital angular momentum) will oppose an applied field.

What is the induced magnetic moment for an electron in the n^{th} LL? The energy is

$$E = \hbar\omega_L(n + 1/2) = \frac{\hbar e B}{2m_e c}(2n + 1) \equiv \mu_B B(2n + 1) \quad \mu_B = \frac{e\hbar}{2m_e c}.$$

Thus the induced dipole moment is

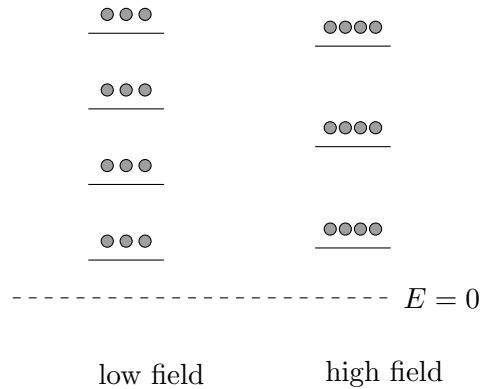
$$\mu_I = -\frac{\partial E}{\partial B} = -(2n + 1)\mu_B.$$

The minus sign means diamagnetism, corresponding to the fact that the circular orbits caused by a magnetic field will oppose that field. (We neglect here the contributions from spin.) The $2n + 1$ reflects the fact that higher LLs correspond to larger oscillations.

So it looks like the quantum effects do not change the basic diamagnetism predicted by Maxwell’s equations, right? Not so fast! That was for one electron. Now let’s look at N electrons. The *magnetism* of a material is the induced magnetic moment per unit area, i.e.

$$M \equiv -\frac{1}{A} \frac{\partial E_{\text{tot}}}{\partial B}.$$

To calculate this we need to combine the total energy as a function of B . This is nontrivial because the degeneracy of each LL grows with B . Thus as B increases each electron in a given LL gains energy, but each LL can hold more electrons, so in the ground state some electrons will move to a lower LL. The competition between these two effects will give rise to the *de Haas-van Alphen* effect. Below is a sketch of what this looks like.



Let $\nu = N/D$ be the number of filled LLs. Recall that $D = BA/\Phi_0$. (Neglect spin in part because the B field splits the two spin states.) Since B is the experimentally accessible parameter with the easiest knob to turn (as opposed to N, A), we can rewrite ν as

$$\nu = \frac{B_0}{B} \quad B_0 \equiv \frac{N\Phi_0}{A}.$$

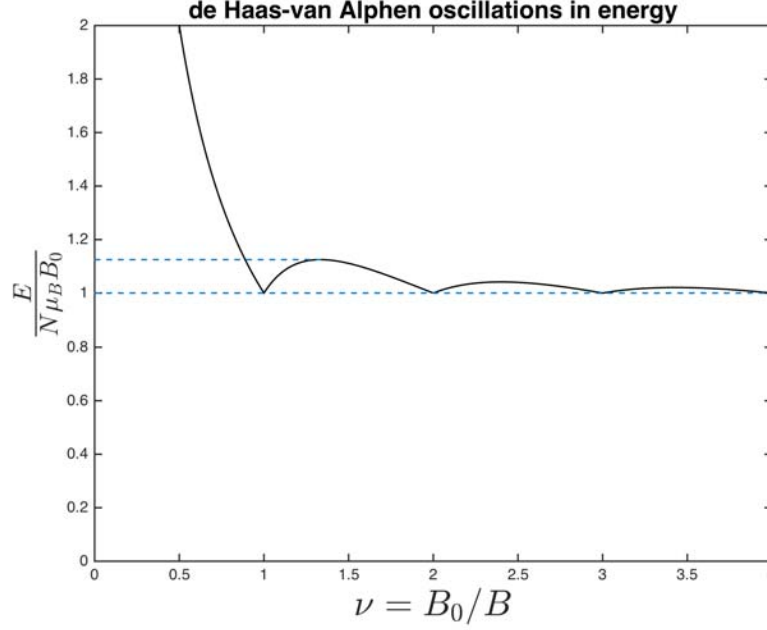


Figure 4: Ground-state energy E as a function of filling fraction, according to (90).

The number of fully filled LLs is $j \equiv \lfloor \nu \rfloor$, meaning the largest integer $\leq \nu$. Thus $j \leq \nu < j + 1$. The energy of the ground state is then

$$\begin{aligned}
 E &= \underbrace{\sum_{n=0}^{j-1} D \hbar \omega_L (n + 1/2)}_{\text{filled levels}} + \underbrace{(N - jD) \hbar \omega_L (j + 1/2)}_{\text{partially filled level}} \\
 &= N \frac{\hbar \omega_L}{2} \left(\sum_{n=0}^{j-1} \frac{1}{\nu} (2n + 1) + \left(1 - \frac{j}{\nu} \right) (2j + 1) \right).
 \end{aligned}$$

Using $\hbar \omega_L / 2 = \mu_B B = \mu_B B_0 / \nu$ and $\sum_{n=0}^{j-1} (2n + 1) = j^2$ we obtain

$$E = N \mu_B B_0 \left(\frac{2j + 1}{\nu} - \frac{j(j + 1)}{\nu^2} \right). \quad (90)$$

At integer points $E / N \mu_B B_0 = 1$. For $\nu < 1$ this equals $1/\nu$ and for $1 < \nu < 2$, we have $\frac{E}{N \mu_B B_0} = \frac{3}{\nu} - \frac{2}{\nu^2}$. In general there are oscillations at every integer value of ν . This is plotted in Fig. 4.

These oscillations mean that the magnetism M will oscillate between positive and negative. We calculate

$$M = -\frac{1}{A} \frac{\partial E}{\partial B} = -n \mu_B \left((2j + 1) - \frac{1}{\nu} 2j(j + 1) \right). \quad (91)$$

This is illustrated in Fig. 5. The key features are the oscillations between extrema of $M = \pm n \mu_B$ with discontinuities at integer values of ν . Also observe that for $\nu < 1$ all electrons are in a single LL, so we observe the simple classical prediction of diamagnetism, which we refer to here as “Landau diamagnetism” even though it is the only part of this diagram where the Landau levels do not really play an important role.

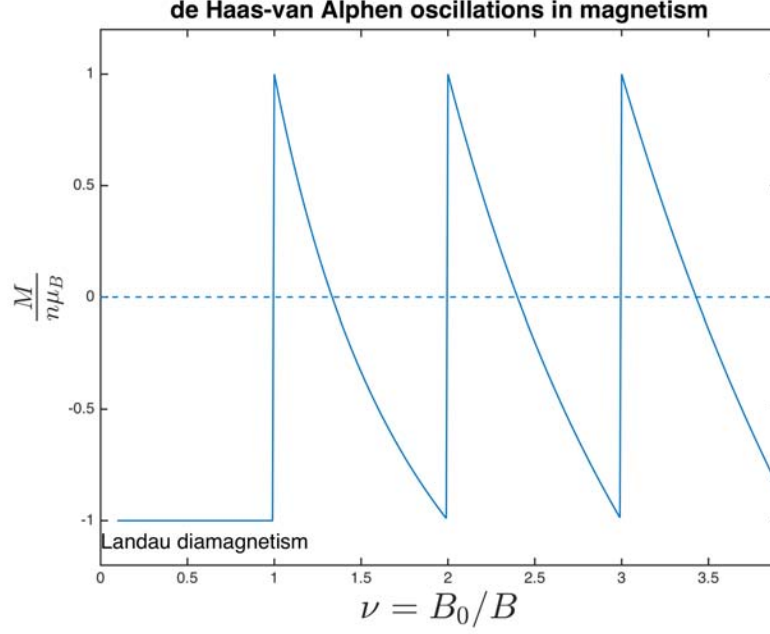


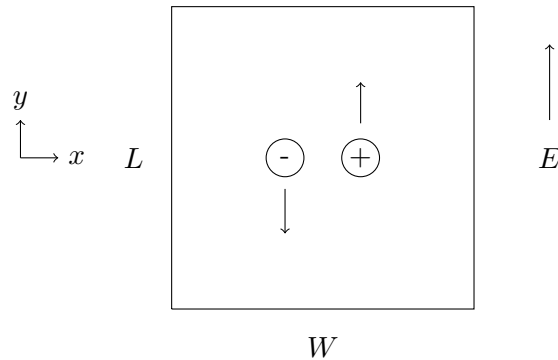
Figure 5: Magnetism M as a function of filling fraction, according to (91).

3.4 Integer Quantum Hall Effect

The IQHE (integer quantum Hall effect) is a rare example of quantization that can be observed at a macroscopic level. The Hall conductance (defined below) is found to be integer (or in some cases fractional) multiples of e^2/h to an accuracy of $\approx 10^{-9}$. This allows extremely precise measurements of fundamental constants such as e^2/h or (combined with other measurements) $\alpha = e^2/\hbar c$.

The quantum Hall effect also lets us determine the sign of the charge carriers.

The classical Hall effect. This was discovered by Edwin Hall in 1879. Consider a sheet of conducting material in the x - y plane with a constant electric field E in the y -direction.



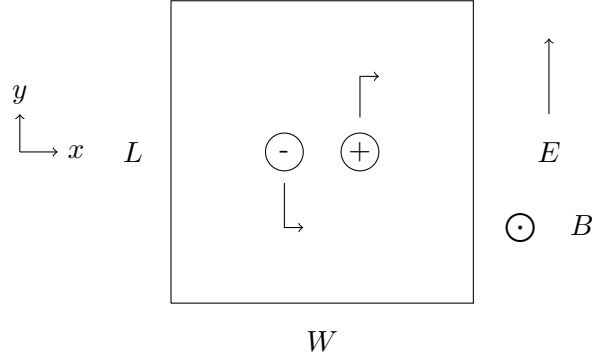
As discussed above, if the mean time between scattering events is τ_0 then there is a drift velocity $\vec{v}_d = \frac{q}{m} \tau_0 \vec{E}$ giving rise to a current density $\vec{j} = nq\vec{v}_d = \frac{nq^2\tau_0}{m} \vec{E}$. Thus the conductivity is $\sigma_0 = \frac{nq^2\tau_0}{m}$. We can also define the resistivity $\rho_0 = 1/\sigma_0$.

Now let's apply a magnetic field B in the \hat{z} direction. This causes the velocity-dependent force

$$\vec{F} = q\vec{E} + q\frac{\vec{v}}{c} \times \vec{B}. \quad (92)$$

This equation assumes that $v \ll c$, which we will see later is implied by the assumption $E \ll B$. To see that this assumption is reasonable, note that in units where $\hbar = 1, c = 1$ an electric field of $1V/cm$ is equal to $2.4 \cdot 10^{-4}eV^2$ while a magnetic field of 1 gauss is equal to $6.9 \cdot 10^{-2}eV^2$.

If the velocity is the one induced by the electric field then the magnetic field causes a drift in the positive \hat{x} direction, regardless of the sign of q . This means that the charge current *does* depend on the sign of q , which gave an early method of showing that the charge carriers in a conductor are negatively charged.



In general the \hat{x} velocity will build up until it cancels out the \hat{y} component of the velocity, and the velocity will oscillate between the x and y components. These oscillations will be centered around the value for which the RHS of (92) is zero, namely $\frac{E}{B}c\hat{x}$.

We will argue more rigorously below that there should be a net drift in the \hat{x} direction. Plugging $\vec{E} = E\hat{y}, \vec{B} = B\hat{z}$ into (92) we obtain

$$m\dot{v}_x = \frac{qB}{c}v_y \quad (93a)$$

$$m\dot{v}_y = qE - \frac{qB}{c}v_x \quad (93b)$$

Using $\omega_L = qB/mc$ we can rewrite this in matrix form as

$$\frac{d}{dt} \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \omega_L \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{qE}{m} \end{pmatrix}. \quad (94)$$

In general if A is an invertible matrix and we have a differential equation of the form

$$\frac{d}{dt}\vec{v} = A\vec{v} + \vec{b} = A(\vec{v} + A^{-1}\vec{b})$$

then we can rearrange as

$$\frac{d}{dt}(\vec{v} + A^{-1}\vec{b}) = A(\vec{v} + A^{-1}\vec{b}).$$

This has solution

$$\vec{v}(t) + A^{-1}\vec{b} = e^{At}(\vec{v}(0) + A^{-1}\vec{b}),$$

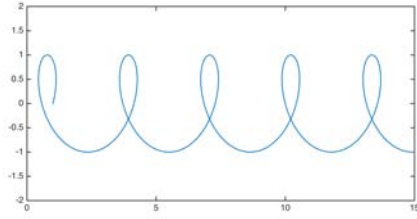


Figure 6: Motion of a charged particle subject to crossed electric and magnetic fields.

which we can rewrite as

$$\vec{v}(t) = \underbrace{e^{At}(\vec{v}(0) + A^{-1}\vec{b})}_{\text{oscillation}} - \underbrace{A^{-1}\vec{b}}_{\text{drift}}. \quad (95)$$

In our case

$$A = \omega_L \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad e^{At} = \begin{pmatrix} \cos(\omega_L t) & \sin(\omega_L t) \\ -\sin(\omega_L t) & \cos(\omega_L t) \end{pmatrix}, \quad A^{-1} = \omega_L \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 0 \\ \frac{qE}{m} \end{pmatrix} \quad (96)$$

We conclude that \vec{v} is a sum of an oscillatory term (which averages to zero) and a drift term equal to

$$v_H \hat{x} \equiv \frac{Ec}{B} \hat{x}.$$

Here $v_H = \frac{E}{B}c$ is the Hall velocity. (We see now why the $v \ll c$ and $E \ll B$ assumptions are related.)

A third and slicker derivation is as follows. Let us change to a reference frame that is moving at velocity $\vec{v} = v_H \hat{x}$. (Suppose for now that we do not know v_H .) To leading order in v/c the \vec{E}, \vec{B} fields transform as

$$\vec{E}' = \vec{E} + \frac{v}{c} \times \vec{B} = (E - \frac{v_H}{c} B) \hat{y} \quad (97a)$$

$$\vec{B}' = \vec{B} - \frac{v}{c} \times \vec{E} = (B - \frac{v_H}{c} E) \hat{z} \quad (97b)$$

To obtain $\vec{E}' = 0$ we should choose $v_H = \frac{E}{B}c$. This means that in the x', y' frame we have pure circular motion, and therefore in the original x, y frame we have circular motion superimposed on a drift with velocity $v_H \hat{x}$.

The resulting motion is depicted in Fig. 6.

This reasoning predicts a current in the \hat{x} direction known as the *Hall current*. The current density in the \hat{x} direction is

$$j_x = (e^- \text{ density})(e^- \text{ charge})(\text{velocity}) = nq \frac{E_y}{B} c \equiv \sigma_H E_y,$$

where $\sigma_H = nqc/B$ is the *Hall conductivity*.

More generally we should think of conductivity as a matrix $\vec{j} = \sigma E$. Thus $j_x = \sigma_H E_y$ but there may also be longitudinal conductivity which would yield a current $j_y = \sigma_L E_y$. Since there

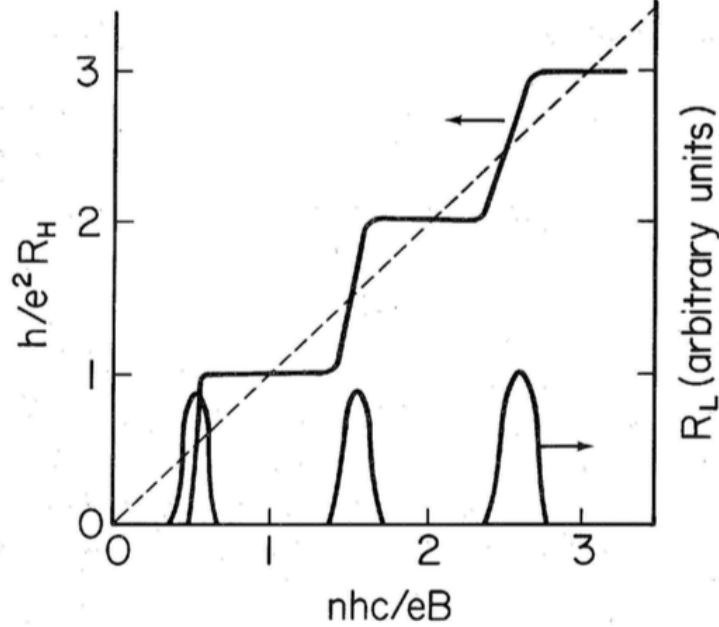


Figure 7: The dashed line is the classical prediction for the transverse resistance. We see instead that it rises quickly around integer values of ν but is nearly flat (in fact, flat to within a factor of 10^{-9}) in between. The longitudinal resistance (and also conductivity) is mostly zero but jumps to something nonzero around the integer values of ν .

is no drift in the y direction we have $\sigma_L = 0$. (In fact this conductivity is exponentially small.) We can also show that $j_y = -\sigma_H E_x$. We then conclude that

$$\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \sigma_H \\ -\sigma_H & 0 \end{pmatrix}}_{\sigma} \begin{pmatrix} E_x \\ E_y \end{pmatrix}.$$

(This matrix perspective is also useful when computing resistivity which is $\rho = \sigma^{-1}$.)

While the formula we have found is entirely classical, we can interpret in terms of various quantities from quantum mechanics. Recall that the filling fraction $\nu = \frac{B_0}{B} = \frac{nhc}{eB} = \frac{nec}{B} \frac{h}{e^2} = \frac{\sigma_H}{\sigma_0}$. Here we have used that $\sigma_0 = e^2/h$ is the fundamental unit of conductivity. We thus predict that

$$\sigma_H = \nu \sigma_0.$$

However, we find that the true picture is somewhat different.

The quantum Hall effect. We now examine this problem using quantum mechanics. The Hamiltonian is

$$H = \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 + q\phi. \quad (98)$$

Corresponding to our fields $\vec{B} = B\hat{z}$ and $\vec{E} = E\hat{y}$ we can choose $\vec{A} = -By\hat{x}$ and $\phi = -Ey$. We also neglect motion in the \hat{z} direction. This yields

$$H = \frac{1}{2m} \left(p_x - \frac{qBy}{c} \right)^2 + \frac{p_y^2}{2m} - qEy. \quad (99)$$

As with the dHvA effect we note that $[H, p_x] = 0$ and we restrict ourselves to the subspace of wavefunctions of the form $e^{ik_x x} f(y)$. Using $\omega_L = qB/mc$ and $l_0 = \sqrt{\hbar/m\omega_L} = \sqrt{\hbar c/qB}$, we then obtain

$$H|_{k_x} = \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2(y - y_0)^2 - qEy \quad y_0 \equiv -\ell_0^2 k_x \quad (100)$$

$$= \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2 \left(y^2 - 2yy_0 + y_0^2 - \frac{2qE}{m\omega_L^2} y \right) \quad (101)$$

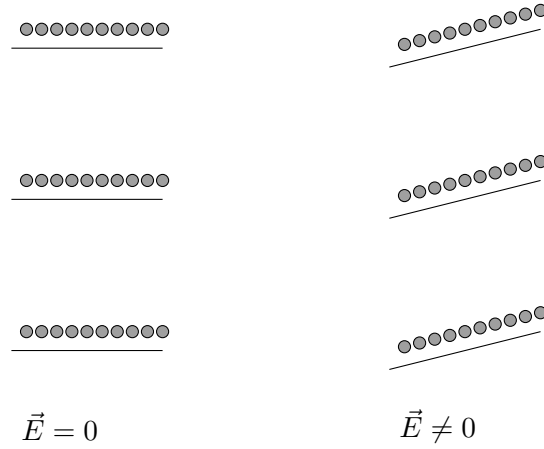
$$= \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2 (y - y_0 - y_1)^2 - \frac{1}{2}m\omega_L^2 (2y_0 y_1 + y_1^2) \quad y_1 \equiv \frac{qE}{m\omega_L^2} = \frac{qE}{m\omega_L \frac{qB}{mc}} = \frac{\frac{E}{B}c}{\omega_L} = \frac{v_H}{\omega_L} \quad (102)$$

This looks again like a shifted harmonic oscillator, now centered at $Y \equiv y_0 + y_1$. There is also an additional energy shift, which can be simplified a bit. The first term $-m\omega_L^2 y_0 y_1 = -m\omega_L^2 l_0^2 k_x \frac{v_H}{\omega_L} = m\omega_L \frac{\hbar}{m\omega_L} k_x v_H = \hbar k_x v_H$. The second term $\frac{1}{2}m\omega_L^2 y_1^2 = \frac{1}{2}mv_H^2$ is simply the kinetic energy corresponding to the Hall velocity, albeit with a negative sign.

We conclude that the energies are

$$E_{k_x, n_y} = \hbar\omega_L \left(n_y + \frac{1}{2} \right) + \hbar v_H k_x - \frac{1}{2}mv_H^2. \quad (103)$$

This first term labels the Landau levels and the last is simply an overall constant. The middle term, though, breaks the degeneracy in k_x . Thus the energy levels are no longer degenerate. We can think of the Landau levels as being “tilted” as follows.



Note that earlier we broke the symmetry between x and y somewhat arbitrarily, and using a different gauge would've resulted in wavefunctions that were plane waves in the y direction, or even localized states. This freedom was due to the extensive degeneracy of the Hamiltonian when $\vec{E} = 0$. Now that the degeneracy is broken we can really say that the energy eigenstates are plane waves in the x direction. There is a semi-classical explanation for this. Different values of y correspond to different value of the electric potential. Classically a particle in a potential experiencing a magnetic field will follow equipotential lines (i.e. contours resulting from making a contour plot of the potential). The quantum eigenstates are then superpositions corresponding to these orbits.

This picture can be useful when considering the situation with disorder. In this case the potential looks like a random landscape with many hills and valleys. Most orbits will be localized but (it turns out that) there will be one orbit going around the edges that wraps around the entire sample. We will, however, not discuss this more in 8.06.

We can rewrite (103) in a more intuitive way in terms of the center of mass $Y = y_0 + y_1$. A short calculation shows that

$$E_{k_x, n_y} = \hbar\omega_L \left(n_y + \frac{1}{2} \right) - qEY + \frac{1}{2}mv_H^2. \quad (104)$$

Here we see the energy from the LL, the energy from a particle with center of mass Y in an electric field and the kinetic energy corresponding to the Hall velocity.

We can also rewrite Y in a more intuitive way. Write $Y = y_0 + y_1 = -\frac{cp_x}{qB} + \frac{v_H}{\omega_L}$ and substitute

$$p_x = mv_x + \frac{q}{c}(-By) = mv_x - \frac{qB}{c}y$$

to obtain

$$Y = y - \frac{v_x - v_H}{\omega_L},$$

which is precisely the classical result we would expect from a particle undergoing oscillations with frequency ω_L on top of a drift with velocity v_H .

We can now calculate the group velocity $v_g = \frac{\partial\omega}{\partial k}$ of the eigenstates of H . From (103) we immediately obtain $v_g = v_H$, suggesting that each eigenstates moves with average velocity v_H .

Another way to measure the Hall current is to compute the probability current. On your pset you will show that this is $\vec{S} = \text{Re}\psi^* \vec{v} \psi$, where $\vec{v} = \frac{1}{m}(\vec{p} - \frac{q}{c}\vec{A})$. The charge current is then $\vec{j} = q\vec{S}$. Finally the wavefunction is

$$\psi(x, y) = \frac{e^{ikx}}{\sqrt{W}} \phi_{n_y}(y - y_0 - y_1), \quad (105)$$

where ϕ_n is the n^{th} eigenstate of the harmonic oscillator. For the average current density in the sample we average over a vertical strip to obtain $\vec{j}_{\text{avg}} = \frac{1}{L} \int_0^L \vec{j} dy$.

As a sanity check we first evaluate

$$S_y = \text{Re}\psi^* \frac{\hbar}{im} \frac{\partial}{\partial y} \psi = 0, \quad (106)$$

since $\phi_n(y - Y)$ is real. On the other hand

$$S_x = \text{Re}\psi^* \left(\frac{\hbar}{im} \frac{\partial}{\partial x} + \frac{qBy}{mc} \right) \psi \quad (107a)$$

$$= \frac{1}{W} |\phi_n(y - y_0 - y_1)|^2 \left(\frac{\hbar k_x}{m} + \omega_L y \right) \quad (107b)$$

$$= \frac{1}{W} |\phi_n(y - y_0 - y_1)|^2 \omega_L (y - y_0) \quad (107c)$$

To evaluate this last quantity observe that $|\phi_n(y - y_0 - y_1)|^2$ is an even function of $y - y_0 - y_1$ and

so we can write

$$\int_0^L S_x dy = \frac{\omega_L}{W} \int_0^L |\phi_n(y - y_0 - y_1)|^2 (y - y_0) dy \quad (108a)$$

$$\approx \frac{\omega_L}{W} \int_0^\infty |\phi_n(y - y_0 - y_1)|^2 (y - y_0) dy \quad (108b)$$

$$= \frac{\omega_L}{W} \int_0^\infty \underbrace{|\phi_n(y - y_0 - y_1)|^2}_{\text{even}} \underbrace{(y - y_0 - y_1 + y_1)}_{\text{odd}} dy \quad (108c)$$

$$= \frac{\omega_L}{W} y_1 \quad (108d)$$

We conclude that $\vec{j}_{\text{avg}} = q \frac{\omega_L}{LW} y_1 = q \frac{v_H}{A} = \frac{q}{A} \frac{E}{B} c$. Thus the Hall conductivity is

$$\sigma_H = \frac{j_x}{E_y} = \frac{qc}{AB} = \frac{qc}{\Phi} = \frac{hc}{e} \frac{e^2}{h} \frac{1}{\Phi} = \sigma_0 \frac{\Phi_0}{\Phi} = \nu \sigma_0. \quad (109)$$

This is the same as the classical result!

To see the quantized conductivity we will need some additional arguments. While some of these are beyond the scope of 8.06, we will sketch some of these arguments briefly here.

One argument that we can already make involves impurities/disorder. Thanks to impurities and disorder, many states are localized. We can think of the electron spectrum as containing not only Landau levels which are delocalized and can carry current but also many localized states which do not conduct. As we lower the B field the Landau levels move down and reduce their degeneracy. This has the same effect as raising the Fermi energy (see the wikipedia page on “Quantum Hall effect” for a nice animation). Sometimes the Fermi energy is between Landau levels and all we are doing is populating localized states, but when it sweeps through a LL then we rapidly fill a LL and the conductivity jumps up.

This explains the plateaus in the conductivity but not why the conductivity should be an integer multiple of σ_0 . We will return to this point later after discussing the Aharonov-Bohm effect.

3.5 Aharonov-Bohm Effect

To write down the Hamiltonian for a charged particle in electric and/or magnetic fields we seem to need the vector and scalar potentials \vec{A}, ϕ . But do these really have physical meaning? After all, they are only defined up to the gauge transform

$$\vec{A}' = \vec{A} + \vec{\nabla} f \quad (110a)$$

$$\phi' = \phi - \frac{1}{c} \frac{\partial f}{\partial t}. \quad (110b)$$

On the other hand, \vec{E} and \vec{B} are gauge-invariant. Are these all we need? Can we build any other gauge-invariant quantity from the \vec{E} and \vec{B} fields?

One attempt to construct a gauge-invariant quantity from the scalar potential \vec{A} is to consider performing a line integral. Fix some path with endpoints \vec{x}_1 and \vec{x}_2 and define the line integral

$$P \equiv \int_{\text{path}} \vec{A} \cdot d\vec{l}. \quad (111)$$

If we perform the transform in (110a) then we replace P with

$$P' = P + \int_{\text{path}} \vec{\nabla} f \cdot d\vec{l} = P + f(\vec{x}_2) - f(\vec{x}_1). \quad (112)$$

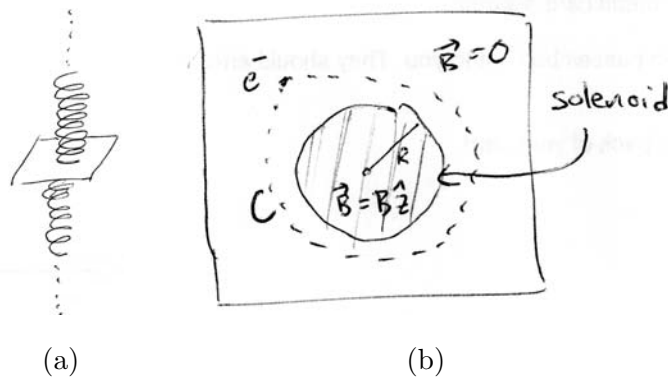


Figure 8: (a) An infinite solenoid of radius R intersects a plane. (b) A cross-section of that plane. The magnetic field inside the solenoid is $B\hat{z}$. An electron and the curve C are entirely outside the solenoid.

This is gauge invariant iff $\vec{x}_1 = \vec{x}_2$. In this case the path becomes a loop and

$$P = \oint_{\text{loop}} \vec{A} \cdot d\vec{\ell} \stackrel{\text{Stokes' thm}}{=} \int_{\text{surface}} (\vec{\nabla} \times \vec{A}) \cdot d\vec{a} = \int_{\text{surface}} \vec{B} \cdot d\vec{a} = \Phi. \quad (113)$$

In the last step we have defined Φ to be the magnetic flux through the surface. The last two quantities are manifestly gauge invariant. However, they are not local! In particular, P depends on \vec{A} along the loop but the enclosed magnetic field might be in a very distant region.

This is the fundamental tradeoff that we get with gauge theories. If we write our Hamiltonian in terms of gauge-covariant quantities like \vec{A}, ϕ then we have enormous redundancy thanks to the gauge freedom. But if we try to describe our physics in terms of gauge-invariant quantities like \vec{E}, \vec{B} then we give up locality, which is much worse.

The Aharonov-Bohm thought experiment. In 1959 Aharonov and Bohm proposed the following thought experiment in which an electron always stays within a region with $\vec{B} = 0$ but $\vec{A} \neq 0$ and this nonzero vector potential has an observable effect. (In fact, an equivalent experiment was proposed by Ehrenberg and Siday in 1949, and was arguably implicit in Dirac's 1931 arguments about magnetic monopoles.)

The idea is to have current running through solenoid going from $z = -\infty$ to $z = \infty$. The field inside the solenoid is $B\hat{z}$ and the field outside the solenoid is 0. (If the solenoid is finite the field outside would be small but nonzero.) An electron is confined to the $z = 0$ plane and always remains outside the solenoid. In particular it only moves through a region where $\vec{B} = 0$.

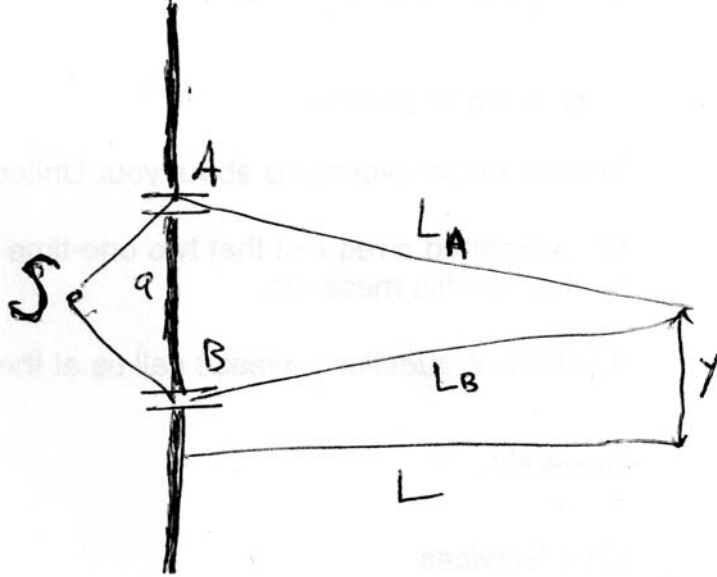
However, the vector potential cannot be zero outside the solenoid. Indeed consider a curve C enclosing the solenoid such as the dashed line in Fig. 8(b). The loop integral of \vec{A} around C is

$$\oint_C \vec{A} \cdot d\vec{\ell} = \pi R^2 B = \Phi \neq 0. \quad (114)$$

The two-slit experiment. First we recall the two-slit experiment first introduced in 8.04. A source S emits mass- m particles with energy $E = \frac{\hbar^2 k^2}{2m}$. They pass through a screen with two slits (labeled A and B) which are separated by a distance a before hitting a screen a distance L away. Suppose their position on the screen is y . (Let's just consider one dimension.) There are two paths:

one from S to A to y and one from S to B to y . Denote their lengths by L_A and L_B . If $L \gg a$ then a little trig will show that

$$L_B - L_A \approx \frac{ay}{L}. \quad (115)$$



The wavefunction at the screen will be the sum of the contributions from both paths. We write this somewhat informally as

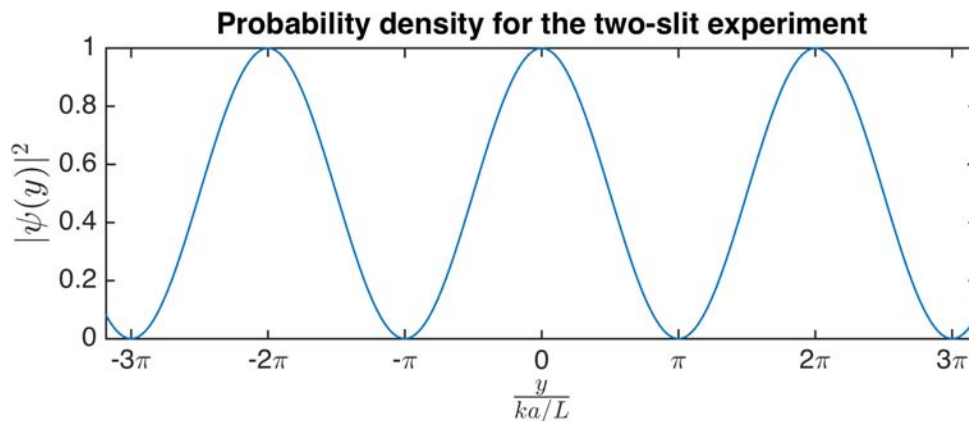
$$\psi(y) = \psi(S \rightarrow A \rightarrow y) + \psi(S \rightarrow B \rightarrow y). \quad (116)$$

Since a particle traveling a distance d picks up a phase of e^{ikd} , we find that

$$\psi(y) \propto e^{iL_A k} + e^{iL_B k}. \quad (117)$$

The probability of finding the particle at position y is then

$$|\psi(y)|^2 \propto \cos^2 \left(\frac{(L_B - L_A)k}{2} \right) = \cos^2 \left(\frac{kay}{2L} \right). \quad (118)$$



The two-slit experiment with non-zero vector potential. Suppose now that our particle has charge q . Suppose further that the two paths of the two-slit experiment go around an infinite solenoid, so that the particle experiences a nonzero vector potential but zero magnetic field.

We will need a prescription for solving the Schrödinger equation in a region where $\vec{B} = 0$ but \vec{A} may be nonzero. To do so, let us fix a point \vec{x}_0 , which in our scenario will be the location of the source S . Then given a curve C from \vec{x}_0 to \vec{x} , define

$$g(\vec{x}, C) \equiv \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x} \text{ along } C} \vec{A} \cdot d\vec{\ell}. \quad (119)$$

We claim that under some conditions $g(\vec{x}, C)$ is independent of C and can be expressed as a function only of \vec{x} . In other words

$$g(\vec{x}, C) = g(\vec{x}). \quad (120)$$

These conditions are that we restrict our curves C and our points \vec{x} to a simply-connected region of space in which $\vec{B} = 0$ everywhere. Here “simply connected” means that there is a path between any two points and any loop can be continuously contracted to a point. We will see in a minute where this requirement is used.

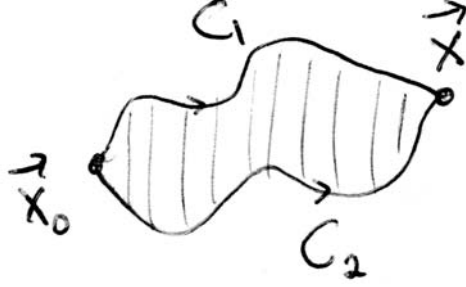


Figure 9: Two curves from \vec{x}_0 to \vec{x} and the region enclosed by them.

To prove (120), consider two curves C_1, C_2 with the same endpoint. Then

$$g(\vec{x}, C_1) - g(\vec{x}, C_2) = \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x} \text{ along } C_1} \vec{A} \cdot d\vec{\ell} - \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x} \text{ along } C_2} \vec{A} \cdot d\vec{\ell} \quad (121a)$$

$$= \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x} \text{ along } C_1} \vec{A} \cdot d\vec{\ell} + \frac{q}{\hbar c} \int_{\vec{x} \rightarrow \vec{x}_0 \text{ along } C_2} \vec{A} \cdot d\vec{\ell} \quad (121b)$$

$$= \frac{q}{\hbar c} \oint_{\vec{x}_0 \rightarrow \vec{x} \rightarrow \vec{x}_0 \text{ along } C_1 \text{ then } C_2} \vec{A} \cdot d\vec{\ell} \quad (121c)$$

$$= \frac{q}{\hbar c} \Phi \quad (121d)$$

In this last equation, Φ is the flux enclosed by the loop made up of C_1 and C_2 ; see Fig. 9.

Next we can use the function $g(\vec{x})$ to construct the solution of the Schrödinger equation in a simply connected region with $\vec{B} = 0$.

Claim 1. Let $\psi^{(0)}(\vec{x}, t)$ be a solution of the free Hamiltonian $H^{(0)} = p^2/2m$ and suppose that $\psi^{(0)}(\vec{x}, t)$ has support entirely in a simply connected region where $\vec{B} = 0$. Let $H = (p - \frac{q}{c}\vec{A})^2/2m$ and let $\psi(\vec{x}, t)$ be the solution of the Schrödinger equation $H\psi = i\hbar\partial_t\psi$.

$$\psi(\vec{x}, t) = e^{ig(\vec{x})}\psi^{(0)}(\vec{x}, t). \quad (122)$$

Note that the claim relies implicitly on the fact that we can write g solely as a function of \vec{x} .

Proof. Recall that for any $f(\vec{x})$ we have $[\vec{p}, f] = -i\hbar\vec{\nabla}f$. Then

$$[\vec{p}, e^{ig(\vec{x})}] = -i\hbar\vec{\nabla}e^{ig(\vec{x})} \quad (123a)$$

$$= \hbar e^{ig(\vec{x})}\vec{\nabla}g \quad (123b)$$

$$= \hbar e^{ig(\vec{x})} \frac{q}{\hbar c} \vec{A}(\vec{x}) \quad (123c)$$

$$= \frac{q}{c} \vec{A} e^{ig(\vec{x})} \quad (123d)$$

This means that when $\vec{p} - \frac{q}{c}\vec{A}$ “commutes past” e^{ig} it turns into simply \vec{p} . In other words

$$\left(\vec{p} - \frac{q}{c}\vec{A}\right) e^{ig} = e^{ig} \vec{p}. \quad (124)$$

This implies that

$$H e^{ig} = \frac{1}{2m} \left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 e^{ig} = e^{ig} \frac{\vec{p}^2}{2m} = e^{ig} H^{(0)}. \quad (125)$$

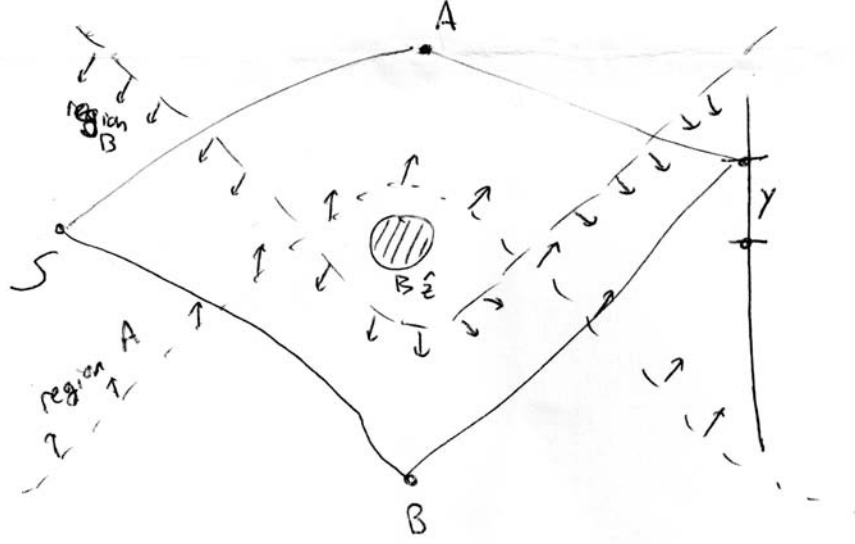


Figure 10: A two-slit experiment is conducted with a solenoid between the two paths. We define two simply connected regions A and B , both of which include the source and the screen where we observe interference. Region A contains paths $S \rightarrow A \rightarrow y$ and region B contains paths $S \rightarrow B \rightarrow y$.

Thus we have (using also the fact that $\partial_t g = 0$) that

$$H\psi = He^{ig}\psi^{(0)} = e^{ig}H^{(0)}\psi^{(0)} = e^{ig}i\hbar\partial_t\psi^{(0)} = i\hbar\partial_te^{ig}\psi^{(0)} = i\hbar\partial_t\psi. \quad (126)$$

□

We can now use Claim 1 to analyze the two-slit experiment in the presence of a magnetic field. Suppose that we add a solenoid in between the two paths, as depicted in Fig. 10. Then we can define regions A and B which (a) are both simply connected, (b) both contain the source S and the target y (for all values of y) and (c) region A contains point A and region B contains point B . This will allow us to use (122) separately in each region.

Let g_A and g_B denote the functions g restricted to regions A and B respectively, and let $\psi^{(0)}(S \rightarrow A \rightarrow y)$ and $\psi^{(0)}(S \rightarrow B \rightarrow y)$ be the solutions of the free Schrödinger equation in those regions. This means that

$$g_A(y) = \frac{q}{\hbar c} \int_{S \rightarrow A \rightarrow y} \vec{A} \cdot d\vec{\ell} \quad \text{and} \quad g_B(y) = \frac{q}{\hbar c} \int_{S \rightarrow B \rightarrow y} \vec{A} \cdot d\vec{\ell}. \quad (127)$$

Then from (122) we have

$$\psi(S \rightarrow A \rightarrow y) = \exp(ig_A(y))\psi^{(0)}(S \rightarrow A \rightarrow y) \quad (128a)$$

$$\psi(S \rightarrow B \rightarrow y) = \exp(ig_B(y))\psi^{(0)}(S \rightarrow B \rightarrow y) \quad (128b)$$

Again the total amplitude will have an interference term which is now shifted by $g_A - g_B$. Indeed

$$|\psi(y)|^2 \propto \left| e^{iL_A k} e^{ig_A} + e^{iL_B k} e^{ig_B} \right|^2 = \cos^2 \left(\frac{1}{2} \left(\frac{kay}{L} + (g_A - g_B) \right) \right). \quad (129)$$

This new phase shift is

$$g_A(y) - g_B(y) = \frac{q}{\hbar c} \oint_{S \rightarrow A \rightarrow y \rightarrow B \rightarrow S} \vec{A} d\vec{\ell} = \frac{q}{\hbar c} \Phi, \quad (130)$$

where $\Phi = \pi R^2 B$ is the enclosed flux. If $q = -e$ then $\frac{q}{\hbar c} = -2\pi\Phi_0$ and the phase shift is $-2\pi\frac{\Phi}{\Phi_0}$. The resulting interference pattern is then

$$|\psi(y)|^2 \propto \cos^2 \left(\frac{1}{2} \left(\frac{kay}{L} - 2\pi \frac{\Phi}{\Phi_0} \right) \right). \quad (131)$$

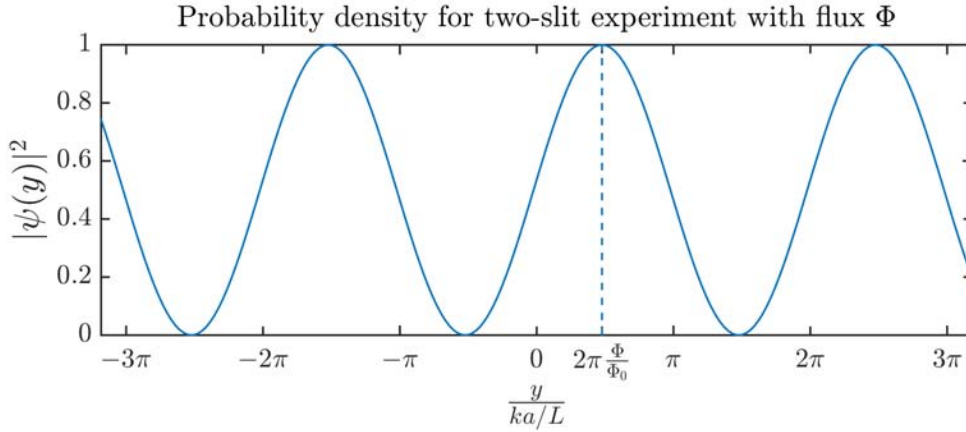


Figure 11: Observed interference pattern when performing the two-slit experiment with a magnetic flux Φ enclosed between the two paths.

The resulting interference pattern is depicted in Fig. 11. Observe that the experiment is only sensitive to the fractional part of Φ/Φ_0 . In that sense we find again a periodic dependence on the magnetic field.

On pset 10 you will explore a related phenomenon, this time for the energy levels of a time-independent Hamiltonian. A particle confined to a ring with a magnetic flux through the ring will have its energy eigenstates shifted by an amount that again depends only on the fractional part of Φ/Φ_0 . (This problem in turn is related to problem 2 on pset 5 which was a time-independent version of the Berry phase.)

In both cases, if Φ is an integer value of Φ_0 then this cannot be distinguished from there being no magnetic field. This is related to a deep property of electromagnetism, which is rather far beyond

the scope of 8.06. While we have presented \vec{A} and ϕ as real numbers, they can also be thought of as elements of the Lie algebra $u(1)$ which generates the Lie group $U(1)$. Electromagnetism is known as $U(1)$ gauge theory for this reason. Non-abelian gauge theories are also possible. Indeed the Standard Model is a $U(1) \times SU(2) \times SU(3)$ gauge theory, with the $U(1)$ part corresponding to electromagnetism, the $SU(2)$ part to the W and Z bosons in the weak force and the $SU(3)$ part to gluons in the strong force.

3.5.1 The IQHE revisited

Finally we review an argument by Laughlin and Halperin for explaining charge quantization in the IQHE.

First we need to review a concept known as the Thouless charge pump. Suppose we have a 1-d system containing some number of electrons. As $0 \leq t \leq T$ suppose we adiabatically change the Hamiltonian from $H(0)$ to $H(T)$, and suppose further that $H(T) = H(0)$. In other words we return to the Hamiltonian that we start with. Then the net flux of electrons from one end of the system to the other will be an integer. This is because, other than the endpoints, the state of the system should remain the same. We will see below how this applies to the IQHE.

In Section 3.4 we considered electrons on a sheet. Instead we will use an annulus geometry as depicted in Fig. 12.

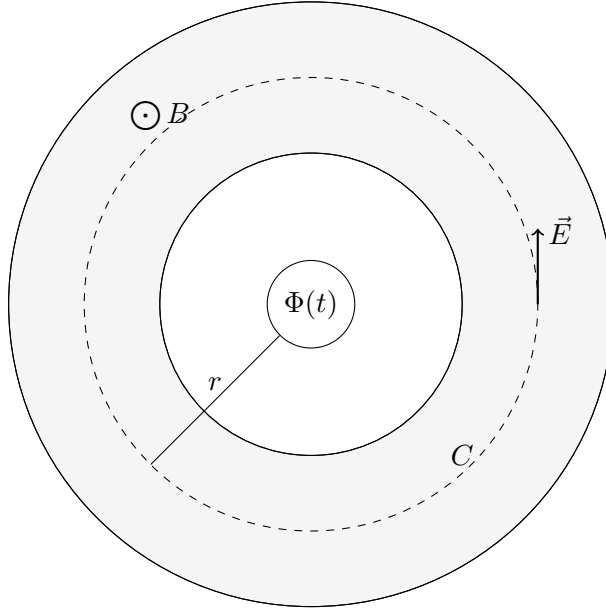


Figure 12: Hall effect on an annulus. There is still a B field in the \hat{z} direction, but now the electric field points in the $\hat{\phi}$ direction. We can think of it as being induced by a time-dependent flux in the center of the annulus. The Hall current now flows radially outward and can be measured by the amount of charge flowing across the contour C .

Suppose that the Hall conductivity is $\sigma_H = x\sigma_0$ for some unknown x . We would like to show that x is an integer.

To induce an electric field in the $\hat{\phi}$ direction we will apply a time-dependent flux in the center

of the annulus. If this flux is Φ then the vector potential at radius r is

$$\vec{A} = \frac{\Phi}{2\pi r} \hat{\phi}. \quad (132)$$

The electric field is then

$$\vec{E} = -\frac{1}{c} \frac{\partial A}{\partial t} = -\frac{1}{2\pi r c} \frac{\partial \Phi}{\partial t} \hat{\phi}. \quad (133)$$

The Hall current is then

$$j_H = \sigma \vec{E} = \frac{\sigma_H}{2\pi r c} \frac{\partial \Phi}{\partial t} \hat{r}. \quad (134)$$

Now suppose we adiabatically increase Φ from 0 to Φ_0 . By the results of the pset, the final Hamiltonian is the same as the initial Hamiltonian (up to a physically unobservable gauge transform), and by the Thouless charge pump argument, this means that an integer number of electrons must have flowed from the inner loop to the outer loop. (Note this integer could be zero or negative.)

Let ΔQ be the amount of charge transferred in this way. Then

$$\Delta Q = \int_0^T \frac{dQ}{dt} dt = \int_0^T 2\pi r j_H dt = 2\pi r \frac{\sigma_H}{2\pi r c} \Phi_0 = \frac{x \frac{e^2}{h}}{c} \frac{hc}{e} = x e. \quad (135)$$

We conclude that x is an integer, as desired.

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8.06 Quantum Physics III

Spring 2016

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8.06 Spring 2015 Lecture Notes

5. Quantum Computing

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Last updated: May 23, 2016

Quantum computing uses familiar principles of quantum mechanics, but with a different philosophy. The key differences are

- It looks at the information carried by quantum systems, and methods of manipulating it, in ways that are independent of the underlying physical realization (i.e. spins, photons, superconductors, etc.)
- Instead of attempting to describe the world around us, it asks what we can create. As a result, features of quantum mechanics that appear to be limitations, such as Heisenberg’s uncertainty principle, can be turned into new capabilities, such as secure quantum key distribution.

The approach is of course analogous to classical computing, where the principles of computing are the same whether your information is stored in magnetic spins (e.g. a hard drive) or electric circuits (e.g. RAM). After the modern notion of a computer was invented in the 1930s by Alan Turing, Alonzo Church, and others, many believed that all computing models (ranging from modern CPUs to DNA computers to clerks working with pencil and paper) were fundamentally equivalent. Specifically, the **Strong Church-Turing thesis** held that any reasonable computing model could simulate any other with modest overhead. Relativity turns out to still be compatible with this hypothesis, but as we will see, quantum mechanics is not.

1 Classical computing

Model a classical computer by a collection of m bits x_1, \dots, x_m upon which we perform *gates*, each acting on $O(1)$ bits. For example, the NOT gate acts on a single bit, maps 0 to 1, and 1 to 0. The NAND gate means “not-AND” is defined by

x	y	$x \text{ NAND } y$
0	0	1
0	1	1
1	0	1
1	1	0

The NAND gate is useful because it is *computationally universal*. Using only NAND gates, we can construct *any* function on n -bit strings.

Here, we can imagine the output of a gate overwriting an existing bit, but it is often simpler to work with *reversible* computers. The NOT gate is reversible. Another example of a reversible gate is the *controlled-NOT* or CNOT, which maps a pair of bits (x, y) to $(x, x \oplus y)$. Here \oplus denotes addition modulo 2.

x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

For reversible circuits, computational universality means the ability to implement any invertible function from $\{0,1\}^n$ (the set of n -bit strings) to $\{0,1\}^n$. It turns out that NOT and CNOT gates alone are not computationally universal (proving this is a nice exercise; as a hint, they generate only transformations that are linear mod 2). For computational universality in reversible circuits, we need some 3-bit gate. One convenient one is the Toffoli gate (named after its inventor, Tom Toffoli), which maps (x, y, z) to $(x, y, z \oplus xy)$. If we start with $(x, y, 1)$, then applying the Toffoli gate yields $(x, y, x \text{ NAND } y)$. Since the Toffoli gate can simulate the NAND gate, it is computationally universal.

There are not significant differences between the reversible and irreversible models, but the reversible one will be a more convenient way to discuss quantum computing.

1.1 Complexity

The complexity of a function is the minimum number of gates required to implement it. Since the exact number of gates is not very illuminating, and will in general depend on the details of the computational model, we often care instead about how the complexity scales with the input size n . For example, the time to multiply two n -bit numbers using the straightforward method requires time $O(n^2)$, since this is the number of pairs of bits that have to be considered. The true complexity is lower, since a more clever algorithm is known to multiply numbers in time $O(n \log(n))$. Factoring integers, on the other hand, is not something we know how to do quickly. The naive algorithm to factor an n -bit number x requires checking all primes $\leq \sqrt{x}$, which requires checking $\approx 2^{n/2}/n$ numbers. A much more complicated algorithm is known (the number field sieve) which requires time $O(2^{n^{1/3}})$, and modern cryptosystems are based on the assumption that nothing substantially faster is possible.

In general, we say that a problem can be solved efficiently if we can solve in time polynomial in the input size n , i.e. in time $\leq n^c$ for some constant $c > 0$. So multiplication can be solved efficiently, as well as many other problems, like inverting a matrix, minimizing a convex function, finding the shortest path in a graph, etc. On the other hand, many problems besides factoring are also not known to have any fast algorithms, of which one example is the “taxicab-ripoff problem”, namely finding the *longest* path in a graph without repeating any vertex.

The strong Church-Turing essentially states that modern computers (optionally equipped with true random number generators) can simulate any other model of computation with polynomial overhead. In other words “polynomial-time” means the same on any platform.

1.2 The complexity of quantum mechanics

Feynman observed in 1982 that quantum mechanics appeared to violate the strong Church-Turing thesis. Consider the state of n spin-1/2 particles. This state is a unit vector in $(\mathbb{C}^2)^{\otimes n} = \mathbb{C}^{2^n}$, so to describe it requires 2^n complex numbers. Similarly solving the Schrödinger equation on this system appears to require time exponential in n on a classical computer.

Already this suggests that the classical model of computing does not capture everything in the world. But Feynman then asked whether in this case a hypothetical *quantum computer* might be able to do better. On pset 10, you will have the option of exploring a technique by which quantum computers can simulate general quantum systems with overhead that is polynomial in the space and time of the region being simulated.

2 Quantum computers

2.1 Qubits and gates

A quantum computer can be thought of as n spin-1/2 particles whose Hamiltonian is under our control. A single spin-1/2 particle is called a *qubit* and we write its state as $a_0|0\rangle + a_1|1\rangle$ (think of $|0\rangle = |\uparrow\rangle$ and $|1\rangle = |\downarrow\rangle$ if you like, but $|0\rangle = |\text{ground}\rangle$, $|1\rangle = |\text{first excited}\rangle$ works equally well). The state of two qubits can be written as

$$a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle,$$

where we use $|x_1x_2\rangle$ as a shorthand for $|x_1\rangle \otimes |x_2\rangle$. And the state of n qubits can be written as

$$|\psi\rangle = \sum_{\vec{x} \in \{0,1\}^n} a_{\vec{x}} |\vec{x}\rangle.$$

The power of quantum computing comes from the fact that acting on one or two qubits is equivalent to applying a $2^n \times 2^n$ matrix to the state $|\psi\rangle$. Let's see concretely how this works.

If we have a single qubit and can apply any H we like for any time t , we can generate any unitary matrix $U = e^{-iHt}$. (Use units where $\hbar = 1$.) This is because any unitary matrix U can be diagonalized as $U = \sum_{j=1}^2 e^{i\theta_j} |v_j\rangle\langle v_j|$, and so applying the Hamiltonian $\sum_j -\theta_j |v_j\rangle\langle v_j|$ for time 1 will yield U .

What if we have two qubits? If we apply H to the first qubit then this is equivalent to the two-qubit Hamiltonian $H \otimes I_2$. The resulting unitary is

$$V = e^{-i(H \otimes I)} = e^{-iH} \otimes I = U \otimes I.$$

Similarly if we apply H to the second qubit, then this corresponds to the two-qubit Hamiltonian $I \otimes H$, which generates the unitary operation $I \otimes U$. If we instead apply a two-qubit Hamiltonian, then we can generate any two-qubit (i.e. 4×4) unitary.

This does not scale up to general n -qubit unitaries. Instead we perform these by stringing together sequences of one and two-qubit gates. Some important one-qubit gates (each of which is

both Hermitian and unitary, meaning their eigenvalues are 1, -1) are

$$\begin{aligned} X &= \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ Y &= \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ Z &= \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ H &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \sum_{x,y \in \{0,1\}} (-1)^{xy} |x\rangle\langle y| \end{aligned}$$

The last gate H is known as the Hadamard transform and plays an important role in quantum computing. It has the useful properties that $HXH = Z$ and $HZH = X$.

An important two-qubit is the controlled-NOT gate, which is discussed further on pset 10.

How do these look when acting on n qubits? If we apply a one-qubit (2×2) gate U to the j^{th} qubit, this results in the unitary

$$I_2^{\otimes j-1} \otimes U \otimes I_2^{\otimes n-j}.$$

If we apply a two-qubit gate V to qubits $j, j+1$, then we have the unitary

$$I_2^{\otimes j-1} \otimes V \otimes I_2^{\otimes n-j-1}.$$

There is no reason two-qubit gates cannot be applied to non-consecutive qubits, but it requires more notation, so we will avoid this.

One fact we will use later is that

$$\begin{aligned} H^{\otimes n} &= \frac{1}{\sqrt{2}} \sum_{x_1, y_1 \in \{0,1\}} (-1)^{x_1 y_1} |y_1\rangle\langle x_1| \otimes \frac{1}{\sqrt{2}} \sum_{x_2, y_2 \in \{0,1\}} (-1)^{x_2 y_2} |y_2\rangle\langle x_2| \otimes \cdots \otimes \frac{1}{\sqrt{2}} \sum_{x_n, y_n \in \{0,1\}} (-1)^{x_n y_n} |y_n\rangle\langle x_n| \\ &= \frac{1}{\sqrt{2^n}} \sum_{\vec{x}, \vec{y} \in \{0,1\}^n} (-1)^{x_1 y_1 + \cdots + x_n y_n} |\vec{y}\rangle\langle \vec{x}| \\ &= \frac{1}{\sqrt{2^n}} \sum_{\vec{x}, \vec{y} \in \{0,1\}^n} (-1)^{\vec{x} \cdot \vec{y}} |\vec{y}\rangle\langle \vec{x}| \end{aligned}$$

2.2 Quantum computing is at least as strong as classical computing

I claim that one and two-qubit gates can implement the quantum Toffoli gate. There is a construction with 6 CNOT gates and many single-qubit gates which I will not describe here. This means that given the ability to do arbitrary one- and two-qubit gates, a quantum computer can perform any *classical* reversible computation with asymptotically constant overhead.

This is good to know, but it is in going beyond classical computing that quantum computers become interesting. On the other hand, we may often want to use classical algorithms as a subroutine.

If $f : \{0,1\}^n \rightarrow \{0,1\}^n$ is a reversible (i.e. invertible) function, then the corresponding unitary is

$$U = \sum_{\vec{x} \in \{0,1\}^n} |f(\vec{x})\rangle\langle \vec{x}|.$$

3 Grover's algorithm

Grover's algorithm shows a quantum speedup for the simple problem of *unstructured search*. Suppose that f is a function from $\{0, \dots, N-1\} \rightarrow \{0, 1\}$ and our goal is to find some x for which $f(x) = 1$. How many times do we need to evaluate f to find such an x ? For simplicity, assume that there is a single w for which $f(w) = 1$. (w stands for "winner.") Evaluating $f(x)$ for random x will find w in an expected $N/2$ steps.

Remarkably, quantum computers can improve this by a quadratic factor, and can find w using $O(\sqrt{N})$ steps.

The algorithm has two ingredients. First, we need to be able to implement the unitary

$$A = \sum_{0 \leq x < N} (-1)^{f(x)} |x\rangle\langle x| = I - 2|w\rangle\langle w|.$$

An explanation of how to do this is on pset 10. The unitary A can be thought of as a reflection about the state $|w\rangle$.

Next, we will need to perform the reflection

$$B = 2|s\rangle\langle s| - I,$$

where $|s\rangle = \frac{1}{\sqrt{N}} \sum_{0 \leq x < N} |x\rangle$ is the uniform superposition state. This is closely related to the problem of preparing $|s\rangle$. If $N = 2^n$, then $H^{\otimes n}|0^n\rangle = |s\rangle$. (Here 0^n is the string of n zeroes.) Similarly $B = (H^{\otimes n})(2|0^n\rangle\langle 0^n| - I)(H^{\otimes n})$. Thus the problem of implementing B reduces to that of implementing $I - 2|0\rangle\langle 0|$. This in turn, reduces (again using pset 10) to the problem of detecting when a string is equal to the all-zeroes string, which is an easy classical computation.

Finally we can describe Grover's algorithm. It is

- Start with $|s\rangle$.
- Apply AB T times, where T will be determined later.
- Measure.

The key to analyzing Grover's algorithm is that we never leave the two-dimensional subspace spanned by $\{|w\rangle, |s\rangle\}$. These vectors are linearly independent, but not orthogonal. To construct an orthonormal basis from them, define

$$|v\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \neq w} |x\rangle,$$

so that $|s\rangle = \sqrt{\frac{N-1}{N}} |v\rangle + \frac{1}{\sqrt{N}} |w\rangle$.

In the $\{|v\rangle, |w\rangle\}$ basis we have

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

$$B = 2|s\rangle\langle s| - I = 2 \begin{pmatrix} \frac{N-1}{N} & \frac{\sqrt{N-1}}{N} \\ \frac{\sqrt{N-1}}{N} & \frac{1}{N} \end{pmatrix} - I = \begin{pmatrix} 1 - \frac{2}{N} & \frac{2\sqrt{N-1}}{N} \\ \frac{2\sqrt{N-1}}{N} & \frac{2}{N} - 1 \end{pmatrix}$$

$$AB = \begin{pmatrix} 1 - \frac{2}{N} & \frac{2\sqrt{N-1}}{N} \\ -\frac{2\sqrt{N-1}}{N} & 1 - \frac{2}{N} \end{pmatrix} = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}$$

If N is large, then $\theta = \sin^{-1}(2\sqrt{N-1}/N) \approx 2/\sqrt{N}$. Thus, after $T = \frac{\pi/2}{\theta} \approx \frac{\pi}{4}\sqrt{N}$ steps, we have rotated from $|s\rangle \approx |v\rangle$ to $\approx |w\rangle$, and measuring will have a high probability of returning the correct answer.

An alternate explanation of this rotation by $O(1/\sqrt{N})$ comes from the fact that we have reflected across two lines which are at an angle of $O(1/\sqrt{N})$ with each other. See the blackboard for a diagram.

4 Simon's algorithm

Grover's algorithm reduced $O(N)$ time to $O(\sqrt{N})$ for a very general problem. Shor's algorithm offers a more dramatic speedup for a more specialized problem: finding the prime factors of a large integer. As described above, the best known classical algorithms for factoring n -bit numbers require time slightly larger than $2^{n^{1/3}}$. By contrast, a quantum computers could factor an n -bit number using Shor's algorithm in time $O(n^3)$.

The key ingredient of Shor's algorithm is *period-finding*, meaning the problem of finding a given the ability to evaluate a function f for which $f(x) = f(x+a)$ for all x . This is straightforward, but takes time, so first I'll explain the algorithm which was one of the key pieces of inspiration for Shor's algorithm.

Let f be a function on $\{0,1\}^n$ with the promise that $f(\vec{x}) = f(\vec{y})$ if and only if $\vec{x} \oplus \vec{y} = \vec{a}$ for some secret $\vec{a} \in \{0,1\}^n$. The goal of the problem is to find \vec{a} .

Define $\mathbb{Z}_2 = \{0,1\}$ with $+$ meaning \oplus . We can check that $+, \cdot$ satisfy all the usual properties of addition and multiplication, and so $\mathbb{Z}_2^n \cong \{0,1\}^n$ is a vector space. We will see later why this is a useful move.

Consider the following algorithm.

- Start with the uniform superposition

$$H^{\otimes n}|0^n\rangle = \frac{1}{\sqrt{2^n}} \sum_{\vec{x} \in \mathbb{Z}_2^n} |\vec{x}\rangle.$$

- Compute f and store the answer in a second register.

$$\frac{1}{\sqrt{2^n}} \sum_{\vec{x} \in \mathbb{Z}_2^n} |\vec{x}\rangle \otimes |f(\vec{x})\rangle.$$

- Measure the second register. Suppose the answer is α . Then we are left with a superposition over all \vec{x} such that $f(\vec{x}) = \alpha$. By assumption, this state must have the form

$$\frac{|\vec{x}\rangle + |\vec{x} + \vec{a}\rangle}{\sqrt{2}}.$$

- Apply $H^{\otimes n}$ to obtain

$$\frac{1}{\sqrt{2^{n+1}}} \sum_{\vec{y} \in \mathbb{Z}_2^n} ((-1)^{\vec{x} \cdot \vec{y}} + (-1)^{(\vec{x} + \vec{a}) \cdot \vec{y}}) |\vec{y}\rangle.$$

- Measure, and obtain outcome y with probability

$$\Pr[y] = \frac{1}{2^{n+1}} (1 + (-1)^{\vec{a} \cdot \vec{y}})^2 = \begin{cases} \frac{1}{2^{n-1}} & \text{if } \vec{a} \cdot \vec{y} = 0 \\ 0 & \text{if } \vec{a} \cdot \vec{y} = 1 \end{cases}$$

Thus, this procedure gives us a random vector \vec{y} that is orthogonal to \vec{a} . After we have collected $n - 1$ linearly independent such \vec{y} we can determine \vec{a} using linear algebra on \mathbb{Z}_2^n . After we have collected $k \leq n - 2$ vectors $\vec{y}^{(1)}, \dots, \vec{y}^{(k)}$, the probability that a new \vec{y} is in the span of $\vec{y}^{(1)}, \dots, \vec{y}^{(k)}$ is $2^{n-k} \leq 1/4$. Thus we need to run this entire procedure $O(n)$ times in order to find \vec{a} with high probability.

By contrast, a classical algorithm would require $\geq 2^{n/2}$ evaluations of f in order to have a non-negligible chance of finding \vec{a} .

5 Shor's algorithm

Suppose we'd like to factor a large number N , say 2048 bits long. One approach is to try dividing by all primes up to \sqrt{N} . This takes a long time; on the order of 2^{1024} for our example. The best known classical algorithm is the General Number Field Sieve, which runs in time $\exp(\log(N)^{1/3} \cdot \text{poly}(\log \log(N)))$, and has not yet been used on numbers larger than 768 bits. By contrast, Shor's factoring algorithm runs in time $O(\log^3(N))$.

There are three main components to Shor's algorithm.

1. First factoring is reduced to "period-finding" which means finding an unknown period of a black-box function. This step uses number theory and not quantum mechanics.
2. A quantum algorithm for period-finding is given. It is similar to Simon's algorithm but instead of the Hadamard it uses a transform called the Quantum Fourier Transform (QFT).
3. Finally we describe an efficient circuit for the QFT.

We begin with the number theory part.

Euclid's Algorithm. Given two integers y and z you can quickly find the greatest common divisor $\text{gcd}(y, z)$.

Given N choose a random $1 < a < N$ and assume $\text{gcd}(a, N) = 1$. (If not, we have already found a nontrivial factor!) Define $\text{ord}(a)$ to be the least positive integer r such that $a^r \bmod N = 1$. Is there always such an r ? Yes, consider the sequence $a, a^2 \bmod N, a^3 \bmod N, \dots$. This sequence must eventually repeat. If $a^x \equiv a^y \bmod N$ and $y > x$ then $a^{y-x} \equiv 1 \bmod N$. (This is not obvious but can be proved using tools like the Chinese Remainder Theorem.)

Now suppose we have found $r = \text{ord}(a)$. This means that $a^r - 1 = mN$ for some integer m . Suppose that

- r is even, and
- $a^{r/2} + 1$ is not a multiple of N .

(If either of these fails, try another a . It turns out there is a reasonable probability that one of these holds.) Suppose even more concretely that $N = p_1^{k_1} \dots p_l^{k_l}$. Then

$$(a^{r/2} - 1)(a^{r/2} + 1) = mp_1^{k_1} \dots p_l^{k_l} \quad (1)$$

and since $a^{r/2} + 1$ is not a multiple of N there must be some p_j that divides $a^{r/2} - 1$. We can now compute $\text{gcd}(a^{r/2} - 1, N)$ using Euclid's algorithm and we will find a nontrivial factor of N .

That's it for the number theory. Now how do we find $\text{ord}(a)$? We use period finding! Define

$$f(x) = a^x \bmod N. \quad (2)$$

This has period r . Indeed

$$f(x+r) = a^{x+r} \bmod N = a^x a^r \bmod N = a^x \bmod N = f(x). \quad (3)$$

The intuition behind period finding is similar to what we did for Simon's algorithm, although now the Fourier transform is instead more like the traditional (i.e. $U(1)$) Fourier transform. Here's how this works. Choose n such that $N^2 \leq 2^n < 2N^2$. We will evaluate $f(x)$ on $x \in \{0, 1, \dots, 2^n - 1\}$.

Before describing Shor's algorithm we present a subroutine, the *Quantum Fourier Transform*.

$$U_{\text{QFT}}|x\rangle = \frac{1}{\sqrt{2^n}} \sum_{y=0}^{2^n-1} e^{2\pi i xy/2^n} |y\rangle. \quad (4)$$

This is a unitary transformation and I claim it can be performed using $O(n^2)$ gates. Let's see how we use it first and then show how to perform it next.

The quantum part of Shor's algorithm consists of these steps:

- Prepare the state $\frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle \otimes |0\rangle$.
- Calculate $f(x)$ in the second register to obtain

$$\frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle \otimes |f(x)\rangle.$$

- Discard the second register. (But we just calculated it!) We can think of this as measuring the register and ignoring the answer. The first register will be in a superposition of the form

$$C(|x_0\rangle + |x_0 + r\rangle + |x_0 + 2r\rangle + \dots).$$

for a random choice of x_0 . Let's make this more precise and say the state is

$$\frac{1}{\sqrt{m}} \sum_{k=0}^{m-1} |x_0 + kr\rangle, \quad (5)$$

with $m \approx 2^n/r$. At this point our superposition has period r . Think of this as a state with period r in time. If we Fourier transform we should get a peak in frequency proportional to $1/r$ (in fact $2^n/r$ for our discretized Fourier transform). Let's now do the math and see that this happens.

- Apply U_{QFT} . This yields

$$\frac{1}{\sqrt{m2^n}} \sum_{k=0}^{m-1} \sum_{y=0}^{2^n-1} e^{2\pi i x_0 y/2^n} e^{2\pi i k r y/2^n} |y\rangle. \quad (6)$$

- Measure y . We find

$$\Pr[y] = \frac{1}{m2^n} \left| \sum_{k=0}^{m-1} e^{\frac{2\pi i k r y}{2^n}} \right|^2. \quad (7)$$

To get some intuition for (7), suppose $y \approx 2^n j/r$ for some integer j . Then the phase will be ≈ 1 and we will get $\Pr[y] \approx m/2^n = 1/r$. Let's argue this more precisely. Observe that $\sum_{k=0}^{m-1} z^k = (1 - z^m)/(1 - z)$. Consider $y = 2^n j/r + \delta_j$ for $|\delta_j| \leq 1/2$. Then

$$\Pr[y] = \frac{1}{m2^n} \left| \frac{1 - \exp\left(\frac{2\pi i m r y}{2^n}\right)}{1 - \exp\left(\frac{2\pi i r y}{2^n}\right)} \right|^2 = \frac{1}{m2^n} \left| \frac{1 - \exp\left(\frac{2\pi i m r \delta_j}{2^n}\right)}{1 - \exp\left(\frac{2\pi i r \delta_j}{2^n}\right)} \right|^2 \quad (8)$$

Using $mr \approx 2^n$ and $|1 - e^{i\theta}| = 2 \sin(\theta/2)$ we have

$$\Pr[y] \approx \frac{1}{m2^n} \frac{\sin^2(\pi \delta_j)}{\sin^2(\pi \delta_j/m)} \geq \frac{1}{m2^n} \frac{(\pi \delta_j/(\pi/2))^2}{(\pi \delta_j/m)^2} = \frac{4}{\pi^2} \frac{1}{r}. \quad (9)$$

Therefore with probability $\geq 4/\pi^2$ we obtain $j2^n/r$ from which we can extract r .

- Extract r using more number theory. This part is a classical computation so I will not dwell on it. From the last step we obtain $\frac{y}{2^n} = \frac{j}{r} + \frac{\delta_j}{2^n}$ for an unknown integer j and unknown $|\delta_j| \leq 1/2$. Since $r < N$ and $N^2 \leq 2^n$, finding the best rational approximation with denominator $\leq N$ will do the job. This “best rational approximation” can be found by something called the continued fraction expansion, which we illustrate with an example.

$$\frac{49}{300} = \frac{1}{\frac{300}{49}} = \frac{1}{6 + \frac{6}{49}} = \frac{1}{6 + \frac{1}{\frac{49}{6}}} = \frac{1}{6 + \frac{1}{8 + \frac{1}{6}}}$$

Rational approximations are obtained by truncating this series, e.g. $1/(6 + 1/8) = 8/49 \approx 49/300$.

For the last twenty years there have been many attempts to generalize Shor's algorithm to other groups. In some cases these would break other cryptosystems. It is often possible to find efficient quantum Fourier transforms for other groups but finding analogues of the continued fraction expansion and the other ingredients has been elusive.

Finally let's talk about how to implement $U_{\text{QFT}}^{(n)}$. The superscript denotes the number of qubits. When $n = 1$ this is just our old friend the Hadamard transform.

$$U_{\text{QFT}}^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

When $n = 2$ we get fourth roots of unity, namely $\pm i$ in addition to ± 1 :

$$U_{\text{QFT}}^{(2)} = \frac{1}{\sqrt{4}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}$$

In general the matrix elements of $U_{\text{QFT}}^{(n)}$ look like $\exp(2\pi i xy/2^n)$. Let's see how this looks in terms of the bits of x and y . Write $x = x_0 + 2x_1 + 4x_2 + \dots + 2^{n-1}x_{n-1}$ and similarly $y = y_0 + \dots + 2^{n-1}y_{n-1}$. Then

$$xy \bmod 2^n = x_0 y_0 + 2(x_1 y_0 + x_0 y_1) + \dots + 2^{n-1}(x_0 y_{n-1} + \dots + x_{n-1} y_0).$$

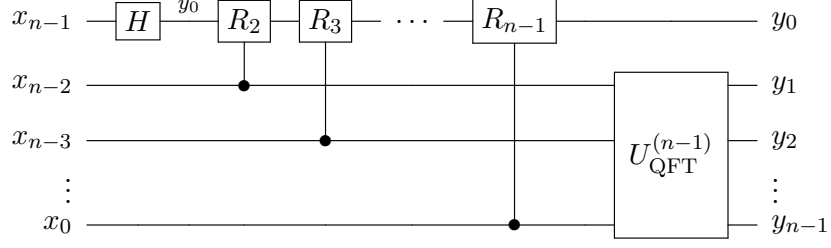


Figure 1: Quantum circuit implementing the quantum Fourier transform.

Write $x = 2^{n-1}x_{n-1} + \bar{x}$ and $y = 2\bar{y} + y_0$. Then

$$\frac{1}{\sqrt{2^n}} e^{\frac{2\pi i x y}{2^n}} = \frac{1}{\sqrt{2^n}} e^{\frac{2\pi i 2^{n-1} x_{n-1} y_0}{2^n}} e^{\frac{2\pi i \bar{x} y_0}{2^n}} \underbrace{e^{\frac{2\pi i 2^{n-1} x_{n-1} 2\bar{y}}{2^n}}}_1 e^{\frac{2\pi i \bar{x} 2\bar{y}}{2^n}} = \frac{(-1)^{x_{n-1} y_0}}{\sqrt{2}} e^{\frac{2\pi i \bar{x} y_0}{2^n}} \langle \bar{y} | U_{\text{QFT}}^{(n-1)} | \bar{x} \rangle.$$

This suggests a recursive algorithm for $U_{\text{QFT}}^{(n)}$ which we express as a circuit diagram. See Fig. 1. There we have defined the rotation gate

$$R_k \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i / 2^k} \end{pmatrix}. \quad (10)$$

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8.06 Quantum Physics III

Spring 2016

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MIT Quantum Theory Notes

Supplementary Notes for MIT's Quantum Theory Sequence

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February 8, 2007

Canonical Quantization and Application to the Quantum Mechanics of a Charged Particle in a Magnetic Field

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1 Introduction

Classical mechanics is internally consistent. No amount of examination of Newton's Laws as an abstract system will lead you to quantum mechanics. The quantum world forced itself upon us when physicists tried and failed to explain the results of experiments using the tools of classical mechanics. It took and still takes considerable guesswork to find the proper description of a new quantum system when first encountered. Notions like internal spin and the Pauli exclusion principle have no analog whatsoever in classical physics.

However, the equations of motion of quantum mechanics, looked at from a particular point of view, resemble the Hamiltonian formulation of classical mechanics. This similarity has led to a program for *guessing* the quantum description of systems with classical Hamiltonian formulations. The program is known as “canonical quantization” because it makes use of the “canonical” *i.e.* Hamiltonian, form of classical mechanics. Though it is very useful and quite powerful, it is important to remember that it provides only the first guess at the quantum formulation. The only way to figure out the complete quantum mechanical description of a system is through experiment. Also, recall from 8.05 that there are many quantum mechanical systems (like the spin-1/2 particle, for example) whose Hamiltonians cannot be obtained by canonically quantizing some classical Hamiltonian.

In lecture this week, we will apply the method of canonical quantization to describe the motion of a charged particle in a constant magnetic field. In so doing, we shall discover several beautiful, and essentially quantum mechanical, phenomena: Landau levels, the integer quantum Hall effect, and the Aharonov-Bohm effect. Our treatment will be self-contained, and thus of necessity will barely scratch the surface of the subject. We will, however, be able to grasp the essence of several key ideas and phenomena. This part of 8.059 serves as an introduction to the condensed matter physics of electrons in materials at low temperatures in high magnetic fields, which is a vast area of contemporary experimental and theoretical physics. The integer and fractional quantum hall effect (we shall not treat the fractional case) were both discovered in experiments done the 1980's, and were among the biggest surprises in physics of recent decades. They have been the subject of intense investigation ever since, including by many physicists here at MIT. Furthermore, understanding gauge invariance and phenomena like the Aharonov-Bohm effect are key aspects of the modern understanding of the theories that govern the interactions of all known elementary particles.

Section 1 describes the method of canonical quantization. We studied this in 8.05. I will not lecture on the material of Section 1; I am providing it here for you to read and review.

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2 Canonical Quantization

2.1 The canonical method

There is a haunting similarity between the equations of motion for operators in the Heisenberg picture and the *classical* Hamilton equations of motion in *Poisson bracket* form.

First let's summarize the quantum equations of motion. Consider a system with N degrees of freedom. These could be the coordinates of $N/3$ particles in three dimensions or of N particles in one dimension for example. Generically we label the coordinates $\{x_j\}$ and the momenta $\{p_j\}$, where $j = 1, 2, \dots, N$. We denote the Hamiltonian $\mathcal{H}(x, p)$, where we drop the subscripts on the x 's and p 's if no confusion results. From wave mechanics where p_j is represented by $-i\hbar\partial/\partial x_j$,

$$\begin{aligned} [x_j, x_k] &= 0 \\ [p_j, p_k] &= 0 \\ [x_j, p_k] &= i\hbar\delta_{jk} \end{aligned} \tag{1}$$

From Ehrenfest's equation (for a general operator), $\mathcal{A}_H(t)$, in the Heisenberg picture,

$$i\hbar\frac{\partial\mathcal{A}}{\partial t} = [\mathcal{A}, \mathcal{H}] \tag{2}$$

(where we suppress the subscript H on the operator) we can obtain equations of motion for the $\{x_j\}$ and $\{p_j\}$,

$$\begin{aligned} i\hbar\dot{x}_j &= [x_j, \mathcal{H}] \\ i\hbar\dot{p}_j &= [p_j, \mathcal{H}]. \end{aligned} \tag{3}$$

In the particular case where $\mathcal{H} = \sum_{j=1,N} (p_j^2/2m) + V(x)$, it is easy to extend the work we did in the case of the harmonic oscillator to obtain from (3)

$$\begin{aligned}\dot{p}_j &= -\frac{\partial \mathcal{H}}{\partial x_j} = -\frac{\partial V}{\partial x_j} \\ \dot{x}_j &= \frac{\partial \mathcal{H}}{\partial p_j} = \frac{p_j}{m}\end{aligned}\tag{4}$$

Equations (4) look exactly like Hamilton's equations. When the two lines are combined, we obtain Newton's second law, $m\ddot{x}_j = -\partial V/\partial x_j$. Of course, we have to remember that the *content* of these equations is very different in quantum mechanics than in classical mechanics: operator *matrix elements* between states are the observables, and the states cannot have sharp values of both x and p . Nevertheless (4) are identical in *form* to Hamilton's equations and the similarity has useful consequences.

In fact, it is the form of (2) and (3) that most usefully connects to classical mechanics. Let's now turn to the *Poisson Bracket* formulation of Hamilton's equations for classical mechanics. We have a set of N *canonical coordinates* $\{x_j\}$ and their *conjugate momenta* $\{p_j\}$. Suppose A and B are any two dynamical variables — that is, they are characteristics of the system depending on the x 's and the p 's. Examples of dynamical variables include the angular momentum, $\vec{L} = \vec{x} \times \vec{p}$, or the kinetic energy, $\sum_j p_j^2/2m$. Then the *Poisson Bracket* of A and B is defined by,

$$\{A, B\}_{\text{PB}} \equiv \sum_{j=1}^N \left\{ \frac{\partial A}{\partial x_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial x_j} \right\}.\tag{5}$$

Poisson Brackets are introduced into classical mechanics because of the remarkably simple form that Hamilton's equations take when expressed in terms of them,

$$\begin{aligned}\dot{x}_j &= \frac{\partial H}{\partial p_j} = \{x_j, H\}_{\text{PB}} \\ \dot{p}_j &= -\frac{\partial H}{\partial x_j} = \{p_j, H\}_{\text{PB}}\end{aligned}\tag{6}$$

as can easily be verified by using the definition of the PB on the dynamical variables x_j , p_j , and H . The time development of an arbitrary dynamical

variable can also be written simply in terms of Poisson Brackets. For simplicity we consider dynamical variables that do not depend explicitly on the time.¹ Then

$$\begin{aligned}\dot{A} \equiv \frac{dA}{dt} &= \sum_{j=1}^N \left\{ \frac{\partial A}{\partial x_j} \dot{x}_j + \frac{\partial A}{\partial p_j} \dot{p}_j \right\} \\ &= \{A, H\}_{\text{PB}}\end{aligned}\tag{7}$$

where the second line follows from the first by substituting from (6) for \dot{x} and \dot{p} .

Finally, to complete the analogy, note that the Poisson Brackets of the x 's and the p 's themselves are remarkably simple,

$$\begin{aligned}\{x_j, x_k\} &= 0 \\ \{p_j, p_k\} &= 0 \\ \{x_j, p_k\} &= \delta_{jk}\end{aligned}\tag{8}$$

because $\partial x_j / \partial p_k = 0$, $\partial x_j / \partial x_k = \delta_{jk}$, etc.

Now we can step back and compare the Poisson Bracket formulation of classical mechanics with the operator equations of motion of quantum mechanics. Compare (1) to (8), (2) to (7) and (3) to (6). It appears that a classical Hamiltonian theory can be transcribed into quantum mechanics by the simple rule,

$$\{A, B\}_{\text{PB}} \Rightarrow \frac{1}{i\hbar}[\mathcal{A}, \mathcal{B}].\tag{9}$$

where the quantum operators \mathcal{A} and \mathcal{B} are the same functions of the operators \hat{x}_j and \hat{p}_j as A and B are of x_j and p_j .

This remarkable rule tells us how to *guess* the quantum theory corresponding to a given classical dynamical system. The procedure is called “canonical quantization” because it follows from the canonical Hamiltonian description of the classical dynamics. In fact there are some important limitations of the canonical quantization method that will be discussed in a later subsection. First, however, let's summarize (and appreciate the elegance

¹A dynamical variable may or may not depend *explicitly* upon the time. Any dynamical variable will depend *implicitly* on the time through the variables x_j and p_j . Explicit time dependence arises when some agent external to the system varies explicitly with the time. An example is the time dependence of the magnetic interaction energy, $-\vec{\mu} \cdot \vec{B}(t)$, when an external magnetic field depends on time.

of) the simple steps necessary to find the quantum equivalent of a classical Hamiltonian system —

- Set up the classical Hamiltonian dynamics in terms of canonical coordinates $\{x_j\}$ and momenta $\{p_j\}$, with a Hamiltonian H .
- Write the equations of motion in Poisson Bracket form.
- Reinterpret the classical dynamical variables as quantum operators in a Hilbert space of states. The commutation properties of the quantum operators are determined by the rule (9).

Of course we cannot forget the difference between quantum and classical mechanics: Although the fundamental equations of motion can be placed in correspondence by the canonical quantization procedure, the different interpretation of classical and quantum variables leads to totally different pictures of phenomena.

2.2 Simple Examples

Here are some simple examples of the canonical quantization procedure. Later we will encounter a very important and non-trivial example in the problem of a charged particle moving in a magnetic field.

2.2.1 Bead on a Wire

Suppose a rigid wire is laid out in space along a curve $\vec{X}(s)$. We parameterize the wire by a single coordinate s which measures length along the wire. Let a bead slide without friction along the wire. This is a standard (easy) problem in Lagrangian mechanics. The energy of the bead is entirely kinetic and is given by $\frac{1}{2}mv^2 = \frac{1}{2}m\dot{s}^2$, because the bead is restricted to move only along the curve. So the Lagrangian is $L = \frac{1}{2}m\dot{s}^2$; the momentum conjugate to s is $p = \partial L / \partial \dot{s} = m\dot{s}$; the Hamiltonian is $H = p^2 / 2m$; and the quantum theory is defined by the operators \hat{s} , \hat{p} and $\mathcal{H} = \hat{p}^2 / 2m$. In short the bead behaves like a free particle on a line. It experiences no forces due to the curving of the wire.

We can dress up this problem a little by adding gravity. Suppose the wire is placed in a constant gravitational field $\vec{g} = -g\hat{y}$. Now there is a potential energy $V(s) = mgy(s)$. The canonical operators are still \hat{s} and \hat{p} , but now the Hamiltonian is $\mathcal{H} = \hat{p}^2 / 2m + mgy(\hat{s})$.

This is actually so oversimplified a problem that interesting physics has been lost. A real bead is held on a real wire by some force that prevents it moving in the directions transverse to the wire. A simple model of this would be to replace the wire by a *tube* whose center follows the track of the wire, but has a finite (say constant circular) cross section. Then the particle would be free to move in the tube, but unable to leave it. This is a more complicated problem, but it can be analyzed pretty simply in the limit that the transverse dimension of the tube, d , is small compared to the radius of curvature, $R(s)$, of the wire.^{2 3} The end result is the appearance of a new term in \mathcal{H} proportional to the inverse of the squared radius of curvature,

$$\mathcal{H} = \frac{p^2}{2m} - \frac{1}{4R(s)^2}. \quad (10)$$

So a real bead on a wire feels a force that *attracts* it to the regions where the wire is most curved ($R(s)$ is smallest).

2.2.2 Relative and Center of Mass Coordinates

Consider two particles moving in three dimensions and interacting with one another by a force that depends only on their relative separation. The classical Lagrangian is

$$L = \frac{1}{2}m_1\dot{\vec{r}}_1^2 + \frac{1}{2}m_2\dot{\vec{r}}_2^2 - V(\vec{r}_1 - \vec{r}_2). \quad (11)$$

We could quantize this canonically in this form and obtain a two particle Schroedinger equation. Instead let's make the transformation to relative and center of mass coordinates at the classical level and quantize from there. We define

$$\begin{aligned} \vec{r} &= \vec{r}_1 - \vec{r}_2 \\ \vec{R} &= \frac{1}{M}(m_1\vec{r}_1 + m_2\vec{r}_2) \end{aligned} \quad (12)$$

²The radius of curvature at some point $\vec{X}(s)$ is the radius of a circular disk that is adjusted to best approximate the wire at the point \vec{X} .

³This problem has attracted attention recently in connection with the propagation of electrons in “quantum wires”. If you're interested I can supply references.

where $M = m_1 + m_2$ is the total mass of the system. Substituting into (11) we find

$$L = \frac{1}{2}M\dot{\vec{R}}^2 + \frac{1}{2}\mu\dot{\vec{r}}^2 - V(\vec{r}). \quad (13)$$

where μ is the *reduced mass* of the two body system. Now is it easy to read off \vec{P} , the momentum canonically conjugate to \vec{R} , $\vec{P} = m\dot{\vec{R}}$, and \vec{p} , the momentum canonically conjugate to \vec{r} , $\vec{p} = \mu\dot{\vec{r}}$. The transition to quantum mechanics is accomplished by postulating the canonical commutators, $[\hat{R}_j, \hat{P}_k] = i\hbar\delta_{jk}$, $[\hat{r}_j, \hat{p}_k] = i\hbar\delta_{jk}$, etc. The Hamiltonian is

$$\mathcal{H} = \frac{1}{2M}\hat{\vec{P}}^2 + \frac{1}{2\mu}\hat{\vec{p}}^2 + V(\hat{\vec{r}}). \quad (14)$$

So just like classical mechanics, the center of mass moves like a free particle, and the interesting part of the dynamics is just like a single particle of mass μ moving in a potential $V(\vec{r})$.

These examples may seem overly elementary. If this were all canonical quantization was good for, it would not be necessary for us to spend much time on it. Moreover there are many mistakes to be made by applying the canonical method too naively (as we shall see below). In fact, canonical quantization helps us guess the quantum equivalent of some highly non-trivial classical systems like charged particles moving in electromagnetic fields, and the dynamics of the electromagnetic field itself.

2.3 Warnings

The canonical quantization method is not a *derivation* of quantum mechanics from classical mechanics. The substitution (9) cannot be motivated within classical mechanics. It represents a guess, or a leap of the imagination, forced on us by the bizarre phenomena that were observed by the early atomic physicists and that were inexplicable within the confines of classical mechanics. The canonical quantization method is simply a recognition that the quantum mechanics of a single particle that was developed from wave mechanics is in fact a representative of a class of systems — those described by traditional Hamiltonian mechanics — that all can be quantized by the same methods.

Many systems we are interested in quantizing differ from this norm. The attitude I would like to advocate is that we use canonical quantization as the first step toward a quantum equivalent of a classical theory, but that

we remain open minded about the need to augment or refine the quantum theory if phenomena force us. Some of the problems that arise on the road from classical to quantum mechanics are listed below in order of increasing severity (in my opinion).

2.3.1 Quantum variables without classical analogues

There are some systems that possesses quantum degrees of freedom that — for one reason or another — do not persist in the classical regime. The best known example is *spin*. When the quantum states of electrons were studied in the 1920's, it was soon discovered that the electron possesses other degrees of freedom that classical point particles don't have. Using guesswork and experimental information, physicists invented operators that describe the behavior of this innately quantum mechanical variable. Nature has forced us to postulate new quantum variables to augment the classical description of a system. This does not represent a failure of quantum mechanics. Quite the opposite — one of its great strengths is that phenomena *without classical analog* can be introduced relatively easily, without upsetting the basic framework of the theory.

Many great advances of 20th century physics (spin, color, internal symmetries, *etc.*) fall into the category of discovering and understanding quantum variables without classical analog. Physicists relish the possibility of such radical departures from classical dynamics.

2.3.2 Operator ordering ambiguities

Classical dynamical variables commute with one another, so the order in which they are written does not affect the dynamics. Not so in quantum mechanics. Suppose, our Lagrangian was $\frac{m}{2} \frac{\xi^2 \dot{\xi}^2}{R^2}$.⁴ Then the classical Hamiltonian would have been $H = \frac{1}{2m} \frac{p^2}{\xi^2}$. When p and ξ become operators, how is this to be interpreted? Is it $\frac{1}{\xi} p^2 \frac{1}{\xi}$? or $p \frac{1}{\xi^2} p$? or some other variant. Using $[\xi, p] = i\hbar$ it is easy to see that the different variants yield different Schroedinger wave equations and therefore different physics.

This problem is called an “operator ordering ambiguity”. More physics input is required to eliminate the ambiguity. Sometimes general principles

⁴This is the lagrangian of a point mass on a string wrapping around a spool of radius R . The coordinate ξ is the length of string (assumed straight) not wound up.

help: a Hamiltonian must be hermitian in order that probability be conserved. If the ambiguous term xp (note $xp \neq px$) occurred in a Hamiltonian, we could rather confidently replace it by the hermitian form $\frac{1}{2}(xp + px)$. Sometimes, hermiticity is not enough. General conservation laws, like conservation of momentum or angular momentum help. If all else fails, it is necessary to leave the ambiguity (parameterized by the relative strength of different hermitian combinations) and see which best describes experiment. In practice I am not aware of physically important examples where hermiticity and conservation laws fail to resolve operator ordering ambiguities.

2.3.3 Singular points

The canonical quantization method becomes complicated and subtle when one tries to apply it to coordinate systems that include singular points. A familiar example is spherical polar coordinates (r , θ , and ϕ). The origin, $r = 0$, is a singular point for spherical polar coordinates — for example, θ and ϕ are not defined at $r = 0$. If you follow the canonical formalism through from Lagrangian to canonical momenta (p_r , p_θ , and p_ϕ), to Hamiltonian, to canonical commutators, a host of difficulties arise. Although it is possible to sort them out by insisting that the canonical momenta be hermitian operators, it is considerably easier to quantize the system in Cartesian coordinates and make the change to spherical polar coordinates at the quantum level. This is the path taken in most elementary treatments of quantum mechanics in three dimensions: the operator $\vec{p}^2 = p_1^2 + p_2^2 + p_3^2$ is recognized as the Laplacian in coordinate representation ($p_j \leftrightarrow -i\hbar\partial/x_j \Rightarrow \vec{p}^2 \leftrightarrow -\hbar^2\vec{\nabla}^2$) and the transformation to polar coordinates is made by writing the Laplacian and the wavefunction in terms of r , θ , and ϕ . As a rule of thumb: the canonical approach becomes cumbersome when the classical coordinates and/or momenta do not range over the full interval from $-\infty$ to $+\infty$.

2.3.4 Constrained systems

Finally we must at least mention a complicated and rich variation of the canonical quantization method that has become an important focus for research in recent years. Sometimes the degrees of freedom of complicated systems are not all independent. For example, a particle may be constrained to move on a specified surface (in three dimensions). Then the coordinates and velocities that appear in the Lagrangian cannot be regarded as indepen-

dent variables. The changes in x , y and z must be correlated so that the particle remains on the surface. The canonical formalism can break down in several (related ways). Sometimes one (or more) of the canonical momenta is identically zero. If $p_k \equiv 0$, then the associated Hamilton's equation, $\partial H / \partial q_k = 0$ is not an equation of motion. Instead it is a constraint that must be satisfied by the canonical coordinates and momenta at each time. The constraint may not be consistent with canonical commutation relations. A simple, but not particularly interesting example, would be the constraint $x + y = 0$ imposed on motion in two dimensions. The constraint is not consistent with the canonical commutator $[x, p_y] = 0$ and $[y, p_y] = i\hbar$ because the commutators can be added to give $[x + y, p_y] = i\hbar$. This case is not serious because we could return to the original lagrangian, use the constraint to eliminate one dynamical variable from the problem, and then proceed without difficulty. In this case, we would write $\xi = x - y$ and $\eta = x + y$ and use the constraint to eliminate η from the problem. In more complicated cases it is not possible to remove the constraint in this fashion, either because it is too hard to solve the constraint equations for one or more variables, or because the problem has some deep underlying symmetry that would be broken by choosing to solve for and eliminate one variable as opposed to another. Dirac realized the importance of such problems and developed a method to handle quantization under constraints. Other powerful yet practical methods were developed by L. D. Faddeev and V. N. Popov in the 1960's. Quantum versions of electrodynamics, chromodynamics (the theory of the interactions of quarks and gluons) and gravity all make use of these modern extensions of the idea of canonical quantization.

3 Motion in a Constant Magnetic Field – “Landau Levels”

3.1 Introduction

A pretty and relatively simple application of canonical methods in quantum theory is to the motion of a charged particle in a constant magnetic field. This problem was first solved by the great Russian theoretical physicist, Lev Landau. In recent years condensed matter physicists have found interesting applications of Landau's problem to real physical systems.

Suppose a magnetic field \vec{B}_0 , constant in magnitude, direction, and time

fills a region of space. For definiteness we assume \vec{B}_0 points in the \hat{e}_3 direction. All points in the xy -plane are equivalent — a simple example of *translation invariance*. The classical motion of a charged particle in a constant magnetic field is determined by the Lorentz force law,

$$m\ddot{\vec{x}} = e\vec{E} + \frac{e}{c}\vec{v} \times \vec{B}. \quad (15)$$

When $\vec{E} = 0$ the force always acts at right angles to the velocity, so kinetic energy is conserved. For simplicity, we restrict the motion to the xy -plane. Then the particle moves in a circle at a constant angular velocity,

$$\begin{aligned} \frac{mv^2}{r} &= \frac{e}{c}vB_0 \\ \omega_L &\equiv \frac{v}{r} = \frac{eB_0}{mc} \end{aligned} \quad (16)$$

ω_L is known as the Larmor frequency. (You can also find it called the cyclotron frequency.)

Quantizing this system requires all the apparatus of the canonical quantization method we developed earlier in these notes. To analyze the problem quantum mechanically we must first find the classical Hamiltonian that describes the system. Then we will be able to go over to the quantum domain. This requires us to introduce the concept of a *vector potential*, \vec{A} , which determines the magnetic field by its *curl*,

$$\vec{B} = \vec{\nabla} \times \vec{A}, \quad (17)$$

in somewhat the same way that the electrostatic potential, Φ , determines the electric field, $\vec{E} = -\vec{\nabla}\Phi$. Once we have the Hamiltonian, we will solve the quantum problem, illustrate some of the subtleties, and apply what we have learned to the *Aharonov-Bohm* and *Integer Quantum Hall Effects*. A recurring theme in much of this study is how the system reflects the underlying translation invariance in the xy -plane. The magnetic field is independent of x and y . The Hamiltonian does not respect this symmetry, however, because the vector potential depends on x and y in an asymmetric manner. In the end the physics must be translation invariant but it will take some work to demonstrate this.

3.2 Lagrangian, Hamiltonian and Canonical Quantization

A velocity-dependent force like (15) requires a velocity-dependent Lagrangian. A detailed *derivation* of the Lagrangian is more appropriately the subject of a course in electrodynamics. Here I will tell you the answer and show that the Euler-Lagrange equations reduce to the Lorentz force law. The Lagrangian is

$$\mathcal{L}(\vec{x}, \dot{\vec{x}}) = \frac{1}{2}m\dot{\vec{x}}^2 + \frac{e}{c}\dot{\vec{x}} \cdot \vec{A}(\vec{x}). \quad (18)$$

First, the momentum canonically conjugate to x_j is,

$$p_j \equiv \frac{\partial \mathcal{L}}{\partial \dot{x}_j} = \frac{e}{c}A_j + m\dot{x}_j. \quad (19)$$

Notice that the momentum in this problem *is not* $m\vec{v}$. Next, the rest of the Euler-Lagrange equations,

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial x_j} &= \frac{e}{c} \sum_{k=1}^3 \dot{x}_k \frac{\partial A_k}{\partial x_j} \\ m\ddot{x}_j &= \frac{e}{c} \sum_{k=1}^3 \dot{x}_k \left(\frac{\partial A_k}{\partial x_j} - \frac{\partial A_j}{\partial x_k} \right) \end{aligned} \quad (20)$$

Notice that \vec{A} depends on the particle's position $\vec{x}(t)$ so that when we differentiate by t we obtain $\dot{A}_j = \sum_{k=1}^3 \dot{x}_k \partial A_j / \partial x_k$ by the chain rule. The two terms involving derivatives of \vec{A} combine to form its *curl*, $\frac{\partial A_k}{\partial x_j} - \frac{\partial A_j}{\partial x_k} = \epsilon_{jkl} B_l$. So (20) reproduces the Lorentz force law correctly provided the *curl* of \vec{A} gives the desired magnetic field as in (17).

Next form the Hamiltonian, $\mathcal{H}(\vec{x}, \vec{p}) = \dot{\vec{x}} \cdot \vec{p} - \mathcal{L}$, with the result,

$$\mathcal{H} = \frac{1}{2}m\dot{\vec{x}}^2 = \frac{1}{2m}(\vec{p} - \frac{e}{c}\vec{A})^2. \quad (21)$$

Notice that the energy is merely $\frac{1}{2}mv^2$ — since the magnetic field acts at right angles to the particle's velocity it does not contribute to the energy. *However the Hamiltonian must be regarded as a function of the canonical coordinates and momenta, \vec{x} and \vec{p} as in the last step of (21).*

To quantize, we postulate canonical commutation relations,

$$\begin{aligned}[x_j, p_k] &= i\hbar\delta_{jk} \\ [x_j, x_k] &= [p_j, p_k] = 0.\end{aligned}\tag{22}$$

Next we must prescribe a vector potential corresponding to $\vec{B}_0 = B_0\hat{e}_3$. We choose

$$\vec{A} = \frac{B_0}{2}(x_1\hat{e}_2 - x_2\hat{e}_1).\tag{23}$$

It is easy to verify that $\vec{\nabla} \times \vec{A} = B_0\hat{e}_3$, however other choices such as $\vec{A} = B_0x_1\hat{e}_2$ would do just as well. They all describe the same magnetic field. In classical mechanics we know that physics depends only on \vec{B} . The same is true here in the Landau problem, however at this moment we have only the Hamiltonian which appears to depend specifically on \vec{A} .

Substituting the explicit choice of \vec{A} into \mathcal{H} , we find

$$\begin{aligned}\mathcal{H} &= \frac{1}{2m}\left\{(p_1 + \frac{eB_0}{2c}x_2)^2 + (p_2 - \frac{eB_0}{2c}x_1)^2\right\} + \frac{1}{2m}p_3^2 \\ &= \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2) + \frac{1}{2}m\omega^2(x_1^2 + x_2^2) - \omega L_3\end{aligned}\tag{24}$$

where $\omega = \frac{1}{2}\omega_L = eB_0/2mc$, and $L_3 = x_1p_2 - x_2p_1$ is the angular momentum in the $x_1 - x_2$ plane. So the system looks like a particle in a two-dimensional harmonic oscillator with an additional potential $-\omega L_3$. Having solved the harmonic oscillator before, we can easily construct the energy eigenstates for this problem.

3.3 A solution to the quantum equations of motion

First consider conservation laws: Apparently angular momentum about the \hat{e}_3 - axis is conserved, $[L_3, \mathcal{H}] = 0$. So is momentum in the \hat{e}_3 direction, $[p_3, \mathcal{H}] = 0$. First, we dispose of the p_3 dependence by restricting the problem to motion in the $x_1 - x_2$ plane. Less formally we could equally well diagonalize p_3 , labeled our eigenstates by its eigenvalue, k_3 , and add $(1/2m)k_3^2$ to our eigenenergies.

The other components of momentum, however, are not conserved:

$$[p_j, \mathcal{H}] \neq 0\tag{25}$$

for $j = 1, 2$. This comes as a surprise: since the magnetic field is uniform in space we would expect the system to be translation invariant, and therefore to find momentum conserved. On the other hand, the classical motion is circular, so perhaps we should not be surprised that the usual concept of momentum has to be amended. Resurrecting momentum conservation will be a principal task in the following analysis.

To classify the eigenstates of (24) we introduce standard harmonic oscillator “creation” and “annihilation” operators (in the following we replace the coordinates x and y by x_1 and x_2),

$$x_k \equiv \sqrt{\frac{\hbar}{2m\omega}}(a_k + a_k^\dagger) \quad p_k \equiv -i\sqrt{\frac{\hbar m\omega}{2}}(a_k - a_k^\dagger), \quad (26)$$

and $a_\pm \equiv \frac{1}{\sqrt{2}}(a_1 \mp ia_2)$, with the usual commutation relations,

$$\begin{aligned} [a_j, a_k^\dagger] &= \delta_{jk}, \\ [a_j, a_k] &= [a_\pm, a_\pm] = [a_\mp, a_\pm] = 0 \\ [a_\pm, a_\pm^\dagger] &= 1, \end{aligned} \quad (27)$$

Substituting into \mathcal{H} and L_3 we obtain

$$\begin{aligned} L_3 &= \hbar(a_+^\dagger a_+ - a_-^\dagger a_-), \\ \mathcal{H} &= \hbar\omega(a_+^\dagger a_+ + a_-^\dagger a_- + 1) - \hbar\omega(a_+^\dagger a_+ - a_-^\dagger a_-) \\ &= \hbar\omega_L\left(a_-^\dagger a_- + \frac{1}{2}\right), \end{aligned} \quad (28)$$

which has a straightforward, though unusual interpretation. Eigenstates of \mathcal{H} and L_3 are labeled by the number of quanta of $+$ and $-$ excitation,

$$\begin{aligned} \mathcal{N}_\pm &\equiv a_\pm^\dagger a_\pm \\ \mathcal{N}_\pm |n_+, n_-\rangle &= n_\pm |n_+, n_-\rangle \end{aligned} \quad (29)$$

\pm quanta carry ± 1 unit of angular momentum, but *only n_- - quanta contribute to the energy*. So the energy eigenstates, known as *Landau levels*, are

each infinitely degenerate. After exploring some of the properties of Landau levels we will return and try to sort out this degeneracy.

To summarize:

- There are two physical conserved quantities, the energy E and z -component of angular momentum, L .
- Equivalently, the number of “oscillator quanta”, n_+ and n_- are conserved, with

$$\begin{aligned} - E(n_+, n_-) &= \hbar\omega_L(n_- + \tfrac{1}{2}), \text{ and} \\ - L(n_+, n_-) &= \hbar(n_+ - n_-). \end{aligned}$$

- E is independent of n_+ , and n_- can take on any non-negative integer value, so each Landau energy level is infinitely degenerate.
- For energy $(n_- + \frac{1}{2})\hbar\omega_L$ the *tower* of degenerate states begins at angular momentum $-n_-$ and grows in steps of \hbar to infinity.

3.4 Physical Interpretation of Landau Levels

The results of the last section are as puzzling as they are enlightening. Classically a particle moving in the x_1 - x_2 plane under the influence of a constant magnetic field, $B_0\hat{e}_3$, can have any energy and its (circular) orbit can be centered at any point (x_1, y_1) . In the quantum world the states are gathered into discrete energy levels separated by $\hbar\omega_L$. Each level is vastly degenerate. The Landau Hamiltonian, eq. (24), on the other hand, singles out a specific origin of coordinates about which the harmonic oscillator potential is centered. In this section we explore the meaning of the Landau degeneracy and (eventually) explain how the translational invariance so obvious at the classical level, is manifest in the quantum theory.

3.4.1 The location and size of Landau levels

Despite superficial appearances each energy eigenstate found in the previous section can be placed wherever we wish in the x_1 - x_1 plane. The simplest way to see this uses the coherent state formalism that was developed in 8.05. Since the energy depends only on n_- we can superpose states with different n_+ without leaving a fixed energy level. Define, then, the coherent state

$$|\alpha\rangle \equiv \exp \alpha a_+^\dagger |0, 0\rangle \quad (30)$$

where $|0, 0\rangle$ is the eigenstate of eq. (24) with $n_+ = n_- = 0$, and α is an arbitrary complex number. Eq. (30) creates a coherent state in the $+$ oscillator but leaves $n_- = 0$ untouched. Using eq. (26) and eq. (27) it is easy to show that

$$\begin{aligned}\langle x_1 \rangle &= \ell_0 \operatorname{Re} \alpha \\ \langle x_2 \rangle &= \ell_0 \operatorname{Im} \alpha,\end{aligned}\tag{31}$$

where $\ell_0 = \sqrt{\hbar/m\omega}$, so by choosing the real and imaginary parts of $\alpha = (x_1 - ix_2)/\ell_0$ we can center a state with energy $E_0 = \frac{1}{2}\hbar\omega_L$ wherever we wish.

Momentum and velocity are not directly proportional in this problem. The state $|\alpha\rangle$ provides a graphic example: The quantum equation of motion for x_k tells us,

$$\dot{x}_k = \frac{1}{i\hbar}[x_k, H]\tag{32}$$

so it is easy to show that the expectation value of the velocity is zero in the state $|\alpha\rangle$:

$$\begin{aligned}\langle \alpha | \dot{x}_k | \alpha \rangle &= \frac{1}{i\hbar} \langle \alpha | [x_k, H] | \alpha \rangle \\ &= \frac{1}{i\hbar} \langle \alpha | x_k E - E x_k | \alpha \rangle = 0.\end{aligned}\tag{33}$$

so the state centered at (x_1, x_2) does not wander away with time. On the other hand the components of the momenta p_1 , and p_2 do not vanish in the state $|\alpha\rangle$,

$$\begin{aligned}\langle p_1 \rangle &= \frac{\hbar}{\ell_0} \operatorname{Im} \alpha \\ \langle p_2 \rangle &= \frac{\hbar}{\ell_0} \operatorname{Re} \alpha,\end{aligned}\tag{34}$$

but this has no direct physical interpretation because the momenta not simply mv .⁵

In contrast to its position, the size of a Landau level is directly connected to its energy and to the strength of the external magnetic field. To see this we make a semiclassical estimate of the area, $\mathcal{A}(n_-)$. Since $v/r = \omega_L$, and

⁵We shall see in lecture that $\langle p_k \rangle$ is not gauge invariant, and therefore cannot correspond to a physical observable. $\langle mv_k \rangle = \langle p_k - (e/c)A_k \rangle$ is gauge invariant. KR.

classically $E = \frac{1}{2}mv^2$, we have $r^2 = E/2m\omega_L^2$. Now the quantum theory requires (28), so $r^2 = (\hbar/m\omega_L)(n_- + \frac{1}{2})$. This becomes more transparent if we multiply by πB_0 to form the *flux* through the orbit, $\Phi_L(n_-) \equiv \pi r^2 B_0$, and substitute for ω_L ,

$$\Phi_L(n_-) = \frac{hc}{e}(n_- + \frac{1}{2}) \quad (35)$$

It appears that the flux through the particle's orbit comes in units of a *fundamental quantum unit of flux*, $\Phi_0 \equiv hc/e$. In the next section, we shall see that something very close to this characterizes the full quantum treatment.

3.4.2 A more careful look at translation invariance

In this section we take a more sophisticated approach to the Landau problem that will clarify both the degeneracy of the Landau levels and the way in which the system manages to respect homogeneity in the xy -plane. We begin with a canonical transformation, trading x_j and p_j for new variables,

$$\begin{aligned} \Pi &= p_1 + m\omega x_2 \\ \phi &= \frac{1}{2}\left(x_1 - \frac{p_2}{m\omega}\right) \\ P_1 &= p_1 - m\omega x_2 \\ P_2 &= p_2 + m\omega x_1 \end{aligned} \quad (36)$$

It is easy to check that the Landau Hamiltonian, (21), can be written in terms of Π and ϕ alone,

$$\mathcal{H} = \frac{1}{2m}\Pi^2 + \frac{m}{2}\omega_L^2\phi^2, \quad (37)$$

with $[\phi, \Pi] = i\hbar$. Once again, we have a harmonic oscillator, with eigenenergies $E_n = (n + \frac{1}{2})\hbar\omega_L$.

The degeneracy formerly associated with n_- is now connected with the P_1 and P_2 . Since $[P_k, \phi] = [P_k, \Pi] = 0$ we see that P_1 and P_2 are candidate constants of the motion. To see what symmetry they generate consider the commutators of P_k with x_j , the spatial coordinates. A brief calculation yields

$$[x_j, P_k] = i\hbar\delta_{jk} \quad (38)$$

So the new “momenta”, P_k , generate translations of the coordinates in the usual sense. Thus the symmetry associated with the constants of the motion

(and the degeneracy of the Landau levels) is translation invariance. This is a welcome result. However, we cannot simply diagonalize P_1 and P_2 along with \mathcal{H} because *they do not commute with each other*,

$$[P_1, P_2] = -2im\omega\hbar. \quad (39)$$

Since the commutator of P_1 and P_2 is a c -number, perhaps we can construct *functions* of them which do commute. The simplest possibility is to look at finite translations of the form,

$$\begin{aligned} \mathcal{T}_1(b_1) &\equiv e^{-i\frac{P_1 b_1}{\hbar}} \\ \mathcal{T}_2(b_2) &\equiv e^{-i\frac{P_2 b_2}{\hbar}}. \end{aligned} \quad (40)$$

According to our study of translations, these operators should translate x_1 and x_2 by b_1 and b_2 respectively. Indeed, it is easy to show that on account of (38),

$$\begin{aligned} \mathcal{T}_1(b_1)^\dagger x_1 \mathcal{T}_1(b_1) &= x_1 + b_1 \\ \mathcal{T}_1(b_1)^\dagger x_2 \mathcal{T}_1(b_1) &= x_2 \end{aligned} \quad (41)$$

and so on.

The crucial question is whether we can choose b_1 and b_2 such that the finite translations commute, $[\mathcal{T}_1(b_1), \mathcal{T}_2(b_2)] = 0$. First, let's determine the effect of $\mathcal{T}_1(b_1)$ on P_2 ,

$$\begin{aligned} f_2(b_1) &\equiv \mathcal{T}_1(b_1)^\dagger P_2 \mathcal{T}_1(b_1) \\ \frac{df_2}{db_1} &= \frac{-i}{\hbar} \mathcal{T}_1(b_1)^\dagger [P_1, P_2] \mathcal{T}_1(b_1) \\ &= -2m\omega, \quad \text{so} \\ f_2(b_1) &= f_2(0) - 2m\omega b_1 \\ &= P_2 - 2m\omega b_1. \end{aligned} \quad (42)$$

This enables us to apply the operator $\mathcal{T}_1(b_1)$ to $\mathcal{T}_2(b_2)$,

$$\begin{aligned} \mathcal{T}_1^\dagger(b_1) \mathcal{T}_2(b_2) \mathcal{T}_1(b_1) &= e^{-2ib_1 b_2 m\omega/\hbar} \mathcal{T}_2(b_2), \quad \text{or} \\ \mathcal{T}_2(b_2) \mathcal{T}_1(b_1) &= e^{-2ib_1 b_2 m\omega/\hbar} \mathcal{T}_1(b_1) \mathcal{T}_2(b_2). \end{aligned} \quad (43)$$

So the finite translations fail to commute only by virtue of this multiplicative factor of unit magnitude. If (and only if) we choose the parameters b_1 and b_2 so that the phase is a multiple of 2π then the translations commute. This condition is

$$2m\omega b_1 b_2 / \hbar = 2\pi N \quad (44)$$

for an integer N . This defines a rectangle of area $b_1 b_2$ in the xy -plane. Let us find the flux through this rectangle,

$$\Phi(b_1, b_2) = b_1 b_2 B_0 = \frac{\pi \hbar}{m\omega} N = N \Phi_0 \quad (45)$$

So we have established a maximal set of commuting operators for the Landau problem: \mathcal{H} , $\mathcal{T}_1(b_1)$, and $\mathcal{T}_2(b_2)$, where b_1 and b_2 obey (45) completely characterize the states of a charged particle in a constant magnetic field.

Let's take some time to interpret this result...

Translations in the n_+, n_- basis Now that we know that $\mathcal{T}_1(b_1)$ and $\mathcal{T}_2(b_2)$, commute with \mathcal{H} when $\vec{b} \equiv (b_1, b_2)$ satisfies (45), we can use them to translate the states we found in §3.3 around the xy -plane. The motivation for this is to understand the degeneracy of the Landau levels associated with the n_- quantum number. Since the state with $n_+ = n_- = 0$ is localized at the origin, we anticipate that the translation by \vec{b} will produce a state localized around \vec{b} .

Consider, then, the state with $n_+ = n_- = 0$ — a harmonic oscillator ground state centered at $\vec{x} = 0$. Now translate this state to \vec{b} , where (b_1, b_2) satisfies the condition (45) with $N = 1$, so they represent the smallest translation that commutes with the Hamiltonian,

$$|\vec{b}, 0, 0\rangle \equiv \mathcal{T}_1(b_1)\mathcal{T}_2(b_2)|0, 0\rangle. \quad (46)$$

This state is normalized to unity because the operators \mathcal{T} are unitary. It has energy $E = \frac{1}{2}\hbar\omega_L$ and $\langle\vec{x}\rangle = \vec{b}$. What does it look like in terms of the original basis $|n_+, n_- \rangle$? To answer this we must express the translations in terms of the $\{a_k\}$. Using the Baker-Hausdorf Theorem, a short calculation gives:

$$|\vec{b}, 0, 0\rangle = \exp\left(-\frac{1}{2}\frac{|b|^2}{\ell_0^2}\right) \exp\left(\frac{b^* a_+^\dagger}{\ell_0}\right) |0, 0\rangle, \quad (47)$$

where $b \equiv b_1 - ib_2$ and $\ell_0 = \sqrt{\hbar/m\omega}$ is the natural scale of lengths associated with the Landau problem. This is an example of a “coherent state”, as we

discussed in §2, superposing an infinite series of degenerate states with differing values of n_+ . Note that $n_- = 0$ is preserved so, as promised, translation did not change the energy of the state. The prefactor is of particular interest because it determines the overlap of the translated state with the original state, $|0, 0\rangle$,

$$|\langle 0, 0 | \vec{b}, 0, 0 \rangle|^2 = \exp \left(-2\pi \frac{b_1^2 + b_2^2}{2b_1 b_2} \right). \quad (48)$$

The exponential is bounded by $e^{-2\pi}$. Thus the overlap of the original state and its translation to the next “cell” is very small. The same analysis applies to any of the eigenstates $|0, n_- \rangle$. We can translate each of these energy eigenstates to any point on rectangular lattice $(n_1 b_1, n_2 b_2)$ throughout the plane. Although these states are not orthonormal, they give us a qualitatively correct picture of the solutions of the Landau problem as towers of nearly localized energy eigenstates with $E = (n + \frac{1}{2})\hbar\omega_L$ situated in unit cells on a grid labeled by any pair of distances b_1 and b_2 satisfying (45).

Eigenstates of the finite translations Another, more conventional, approach is to study eigenstates of our maximal set of commuting operators, \mathcal{H} , $\mathcal{T}_1(b_1)$, and $\mathcal{T}_2(b_2)$. First we choose some b satisfying (45). Since \mathcal{T}_k is a unitary operator its eigenvalues are complex numbers of unit magnitude, which we parameterize by

$$\begin{aligned} \mathcal{T}_1(b_1)|\phi_1, \phi_2, n\rangle &= e^{i\phi_1}|\phi_1, \phi_2, n\rangle \\ \mathcal{T}_2(b_2)|\phi_1, \phi_2, n\rangle &= e^{i\phi_2}|\phi_1, \phi_2, n\rangle \\ \mathcal{H}|\phi_1, \phi_2, n\rangle &= (n + \frac{1}{2})\hbar\omega_L|\phi_1, \phi_2, n\rangle \end{aligned} \quad (49)$$

It is easy to see that the phase ϕ_j must be linear in b_j ($\mathcal{T}_1(2b_1) = [\mathcal{T}_1(b_1)]^2$), so we define $\phi_j \equiv k_j b_j$, where k_j is a real number in range $-\pi/b_j < k_j < \pi/b_j$ because the phase ϕ is only defined modulo 2π . This makes these states look very similar to plane waves even though they are not. If we construct the coordinate space wavefunction corresponding to $|\phi_1, \phi_2, n\rangle$,

$$\psi_{k_1 k_2 n}(x_1, x_2) \equiv \langle x_1, x_2 | \phi_1, \phi_2, n \rangle \quad (50)$$

then it is easy to see that the consequence of (49) is that

$$\psi_{k_1 k_2 n}(x_1 + b_1, x_2 + b_2) = e^{ik_1 b_1 + ik_2 b_2} \psi_{k_1 k_2 n}(x_1, x_2) \quad (51)$$

just like a plane wave, $\exp i(k_1 x_1 + k_2 x_2)$, would behave. The difference, of course is that ψ has this simple behavior only for the special translations we have discovered, not for an arbitrary translation, and as a consequence, the “momenta” (k_1, k_2) are not conserved.

States like these arise in many other situations where a system is invariant only under certain *finite* translations. The classic example is a crystal lattice which is invariant if we translate by the vectors that define a *unit cell* but not otherwise. In this way the Landau system resembles a two-dimensional crystal with a rectangular unit cell whose area is determined by the flux quantization condition (45). Wavefunctions that behave like (51) are known as Bloch waves in honor of Felix Bloch who first studied quantum mechanics in periodic structures. We will discuss them in detail when addressing the quantum theory of electrons in metals.

Note that the states $\psi_{k_1 k_2 n}(x_1, x_2)$ extend everywhere throughout the xy -plane. This is clear from (51) since their amplitude arbitrary distances away from some original location is only modulated by a phase. Thus this basis is very different from the quasi-localized basis we obtained by translating the state $|n_+ = 0, n_- = 0\rangle$ around the plane in the previous section. Of course they describe the same system and the same physics and are related through the marvelous power of the superposition principle.

4 The Aharonov Bohm Effect

The vector potential, $\vec{A}(\vec{x})$ makes a surprising appearance in the quantum description of a particle in a magnetic field. It all stems from the classical Hamiltonian,

$$\mathcal{H} = \frac{1}{2m}(\vec{p} - \frac{e}{c}\vec{A})^2. \quad (52)$$

Despite the appearance of \vec{A} in \mathcal{H} , we know that at the *classical* level, the dynamics depends only on \vec{E} and \vec{B} because only they appear in Newton’s Laws, eq. (15). In the classical domain \vec{A} and the electrostatic potential, ϕ can be regarded as merely useful, but inessential, abstractions.

In the quantum theory \mathcal{H} rather than $m\ddot{x}$ is fundamental, so the possibility exists that *physics* depends on \vec{A} . For the case we have studied in detail — motion in a constant magnetic field — $\vec{A} = \frac{1}{2}\vec{x} \times \vec{B}$ so we cannot even define dependence on \vec{A} independent of \vec{B} .

In 1959 Y. Aharonov and D. Bohm proposed a way to observe a direct effect of \vec{A} and established the quantum significance of \vec{A} .⁶ Although this may seem like a somewhat technical detail, it captures some of the unusual aspects of “reality” in the quantum world and has fascinated students ever since. Perhaps more important, vector potentials associated with generalizations of electromagnetism play a central role in our extraordinarily successful theories of subnuclear particle physics. In that arena observable consequences of the vector potentials abound.

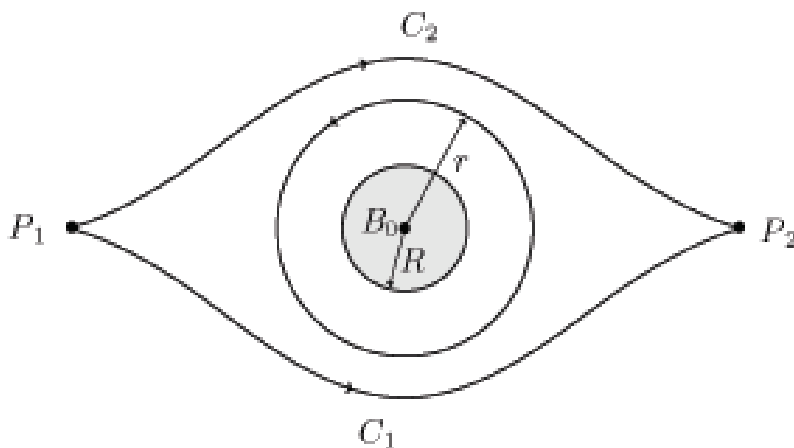


Figure 1: Paths for analysis of Aharonov-Bohm effect.

Aharonov and Bohm proposed to consider motion of a charged particle in the plane perpendicular to an idealized solenoid that produces a constant magnetic field, $\vec{B} = B_0 \hat{e}_3$, but *only within a circle of radius R* . For $r > R$, \vec{B} can be taken to vanish identically. This configuration is shown in Fig. 1 along with a couple of paths that will figure in the discussion. Even though $\vec{B} = 0$ for $r > R$, \vec{A} cannot vanish in this region because of Stokes' theorem. Consider the integral of the vector potential around the circle marked C (which is the boundary of a disk S) of radius r shown in the figure. Then

⁶Y. Aharonov and D. Bohm, *Phys. Rev.* **115** (1959) 485.

Stokes' theorem and the defining relation for \vec{A} , $\vec{B} = \vec{\nabla} \times \vec{A}$, give

$$\begin{aligned} \oint_C \vec{dl} \cdot \vec{A} &= \iint d^2S \hat{e}_3 \cdot \vec{\nabla} \times \vec{A} \\ &= \iint d^2S \hat{e}_3 \cdot \vec{B} = \pi r^2 B_0, \end{aligned} \quad (53)$$

so \vec{A} cannot vanish everywhere on the circle C . In fact symmetry requires that \vec{A} point in the azimuthal, $\hat{\phi}$, direction, so an elementary calculation gives,

$$\vec{A} = \frac{\Phi}{2\pi r} \hat{\phi} \quad \text{for } r > R \quad (54)$$

Of course the existence of a vector potential in the region outside R , where $\vec{B} = 0$, is a classical phenomenon no more surprising than the existence of an electrostatic potential inside a uniformly charged sphere where $\vec{E} = 0$. The question of interest is whether some physical phenomenon that takes place entirely in the region $r > R$, where $\vec{B} = 0$ can depend on \vec{A} . To study this, consider a charged particle described by a wave packet that moves on either of the two paths marked C_1 and C_2 in the figure. Of course a quantum particle cannot be constrained to a definite path, but we will see that the effect is the same along all paths close to C_1 or C_2 , so a diffuse path of the sort allowed in quantum mechanics will give the same result.

The particle's propagation through the vector potential is determined by the time dependent Schrödinger equation,

$$\frac{1}{2m} (\vec{p} - \frac{e}{c} \vec{A})^2 \psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t), \quad (55)$$

where $\vec{p} = -i\hbar \vec{\nabla}$. Define the Aharonov-Bohm phase factor,

$$g(\vec{r}, C) = \frac{e}{\hbar c} \int_C^{\vec{r}} \vec{dl} \cdot \vec{A} \quad (56)$$

where the line integral begins at the point P_1 , follows curve C and ends at a point \vec{r} . Note that

$$\vec{\nabla} g(\vec{r}, C) = \frac{e}{\hbar c} \vec{A}(\vec{r}) \quad (57)$$

independent of the curve C . Now factor the phase g out of the wavefunction,

$$\psi(\vec{r}, t) = \exp(ig) \chi(\vec{r}, t), \quad (58)$$

and substitute into eq. (55). The result is that χ obeys the free Schrödinger equation,

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\chi = i\hbar\dot{\chi}. \quad (59)$$

Thus all information about the vector potential is contained in the phase that multiplies χ .

With the form of eq. (58) in mind let us compare the phase accumulated by a well-localized charged particle wave packet that begins at point P_1 and propagates to P_2 along *either* path C_1 or C_2 . We start with $\psi(\vec{r}, t_1)$ concentrated at P_1 at $t = t_1$. Let us suppose, however, that ψ is a quantum mechanical superposition of two terms, $\psi(\vec{r}, t_1) = \psi_1(\vec{r}, t_1) + \psi_2(\vec{r}, t_1)$ such that $\psi_1(\vec{r}, t_1)$ and $\psi_2(\vec{r}, t_1)$ describe wave packets which subsequently (i.e. after t_1) follow the two different paths C_1 and C_2 . At time t_2 , the two wave packets both reach P_2 , and

$$\psi(\vec{r}, t_2) = \exp\left[\frac{ie}{\hbar c} \int_{C_1} \vec{dl} \cdot \vec{A}\right] \chi_1(\vec{r}, t_2) + \exp\left[\frac{ie}{\hbar c} \int_{C_2} \vec{dl} \cdot \vec{A}\right] \chi_2(\vec{r}, t_2) \quad (60)$$

with both $\chi_1(\vec{r}, t_2)$ and $\chi_2(\vec{r}, t_2)$ localized in the vicinity of the point P_2 . Whatever other (\vec{A} -independent) relative phase may have accumulated by the time the wave packets have reached P_2 , there is an \vec{A} -dependent *relative* phase,

$$\psi(\vec{r}, t_2) = \exp\left[\frac{ie}{\hbar c} \int_{C_1} \vec{dl} \cdot \vec{A}\right] \left\{ \chi_1(\vec{r}, t_2) + \exp\left[\frac{ie}{\hbar c} \oint_{\bar{C}} \vec{dl} \cdot \vec{A}\right] \chi_2(\vec{r}, t_2) \right\}. \quad (61)$$

Note that the relative phase is given by the loop integral over the closed path $\bar{C} = C_2 - C_1$.

The relative phase in eq. (61) is measureable, for example by watching the interference pattern on a detector at P_2 as the magnetic field, \vec{B} is slowly changed. The phase depends only on the loop integral of \vec{A} , which in turn depends only on the total magnetic field enclosed within the path \bar{C} ,

$$\begin{aligned} g(\bar{C}) &\equiv \frac{e}{\hbar c} \oint_{\bar{C}} \vec{dl} \cdot \vec{A} \\ &= e\pi R^2 B_0 / \hbar c = e\Phi / \hbar c \end{aligned} \quad (62)$$

where $\Phi = \pi R^2 B_0$ is the magnetic flux contained within \bar{C} .

We have been fairly careful in this discussion to make it clear that the particle moves entirely in a region where $\vec{B} = 0$, so the only source of the phase is the vector potential \vec{A} . The result does not depend on the details of the path followed by the particle. For example, if we replace the path C_2 by a nearby path C'_2 on the same side of the solenoid, then the resulting phase, $g(\bar{C}')$, where $\bar{C}' = C'_2 - C_1$ is unchanged because $g(\bar{C}')$ depends only on the magnetic flux enclosed by \bar{C}' , which is the same as that enclosed by \bar{C} . Thus it does not matter that the quantum particle cannot follow a sharp trajectory. The Aharonov-Bohm phase is a global property of the motion, not a property of the particle's exact path. A similar argument shows that $g(\bar{C})$ does not depend on the gauge we choose to describe the vector potential. If we change gauge, from \vec{A} to \vec{A}' , with

$$\vec{A}' = \vec{A} - \vec{\nabla}\Lambda,$$

then

$$g(\bar{C}) \rightarrow g'(\bar{C}) = g(\bar{C}) - \frac{e}{\hbar c} \oint_{\bar{C}} d\vec{l} \cdot \vec{\nabla}\Lambda = g(\bar{C}) \quad (63)$$

because the integral of the gradient of any continuous function around a closed path is zero.

So Aharonov and Bohm have shown in this simple example, that the vector potential has physical manifestations in quantum mechanics. Although the phase $g(\bar{C})$ depends on the magnetic flux enclosed by the path, \bar{C} , the path itself lies entirely in a region of space in which $\vec{B} = 0$ and $\vec{A} \neq 0$.

To quote Griffiths, page 349, “What are we to make of the Aharonov-Bohm effect? Evidently our classical preconceptions are simply *mistaken*. There *can* be electromagnetic effects in regions where the fields [\vec{B} and \vec{E}] are zero. Note, however, that this does not make \vec{A} itself measurable — only the enclosed *flux* comes into the final answer, and the theory remains gauge invariant.” You should read Griffiths, section 10.2.4, but should for now ignore the connection to Berry's phase.

The Aharonov-Bohm effect does not only manifest itself as shifts in interference patterns. See pages 344-345 in Griffiths for a description of how the Aharonov-Bohm effect leads to shifts in the *energy levels* for a “bead on a loop of string” if the string is everywhere in a region with $\vec{B} = 0$ but encircles a flux carrying solenoid.

5 Integer Quantum Hall Effect

The Hall Effect is an elementary electromagnetic phenomenon where a conducting strip carrying a current along its length develops a current across its width when placed in a magnetic field. The direction of the induced current is sensitive to the *sign* of the electric charge of mobile species in the material and can be used to show that conventional currents are carried by electrons (negative charge) and that certain semiconductors contain positive mobile charges. In 1980, von Klitzing discovered that the relation between the external electric potential and the Hall current is quantized in strong magnetic fields — the conductance, I_{Hall}/V , comes in units of e^2/h . Von Klitzing was awarded the 1985 Nobel Prize for his discovery of the Quantum Hall Effect (QHE). There has been a tremendous amount of work on this subject over the past 20 years. New effects — including the *fractional* QHE — have been discovered, and a decent treatment of the subject would fill a course. In Quantum Physics III I would like to explain the origins of the effect — as an extension of the Landau problem — under ideal circumstances. First I will review the ordinary Hall Effect (though I will not assume you have seen it before). Next I will solve an idealized quantum problem: the Schrödinger equation for electrons propagating in the xy -plane with a magnetic field normal to the plane and an electric field in the y direction. This will lead to quantization of the Hall conductance provided we make some simplifying assumptions about the structure of the material in which the electrons propagate. As usual in condensed matter physics, after solving an idealized problem I will have to return to the real world of actual materials and explain why the results of the idealized analysis survive unscathed. Much of my presentation relies heavily on the introductory sections of the review *The Quantum Hall Effect*, by R. E. Prange and S. M. Girvin (Springer-Verlag, Berlin, 1987).

5.1 The ordinary Hall effect and the relevant variables

First let us review the ordinary Hall effect. A strip of conductor lies in the xy -plane. A constant and uniform electric field, \vec{E} , points in the y -direction. A constant and uniform magnetic field, \vec{B} , is oriented normal to the xy -plane.

First consider the case where $\vec{B} = 0$. Mobile charge carriers⁷ with charge

⁷Electrons, for our case, but to keep track of signs we consider the charge carriers

q accelerate in response to \vec{E} , but suffer random, redirecting collisions with ions. An elementary argument (presented in 8.02?) leads to the conclusion that the electrons develop a *drift velocity* $\vec{v} = q\vec{E}\tau_0/m$, where τ_0 is the average time between collisions. These drifting charges generate a current density (charge per unit time per unit length in the xy -plane), $\vec{j} = qn\vec{v}$, where n is the density of charge carriers (per unit area). The result is a current density linearly proportional to the impressed electric field,

$$\vec{j} = \frac{nq^2\tau_0}{m}\vec{E}. \quad (64)$$

The constant of proportionality relating \vec{j} and \vec{E} is the *conductivity*, and has units (in two dimensions) $[j]/[E] = \ell/t = [\text{velocity}]$. This is simply Ohm's law with conductivity, $\sigma_0 = nq^2\tau_0/m$. It is useful to define the resistivity by the relation $\vec{E} = \rho\vec{j}$ (which is the local analog of $V = IR$), in which case $\rho_0 = 1/\sigma_0$. It is also useful to think of the resistivity (and conductivity) as a matrix relating the vector \vec{j} to the vector \vec{E} . In this simple case, the matrix is diagonal,

$$\rho = \begin{pmatrix} \rho_0 & 0 \\ 0 & \rho_0 \end{pmatrix}. \quad (65)$$

When the magnetic field is turned on, the mobile charges respond to the an “effective” electric field arising from the combined electric and magnetic fields according to the Lorentz force law,

$$\vec{F} \equiv q\vec{E}_{\text{eff}} = q\vec{E} + q\frac{\vec{v}}{c} \times \vec{B}. \quad (66)$$

The current comes from the charge carriers drift in response to \vec{E}_{eff} and is therefore given by $\vec{j} = \sigma_0\vec{E}_{\text{eff}}$. Also, $\vec{v} = \vec{j}/nq$, so (66) can be rewritten as

$$\vec{j} = \sigma_0\vec{E} + \frac{\sigma_0}{nqc}\vec{j} \times \vec{B}. \quad (67)$$

The current is no longer only parallel to \vec{E} : Because of the second term in (67) it develops a component perpendicular to \vec{E} . This is most conveniently summarized in terms of a resistivity matrix, $\vec{E} = \rho\vec{j}$, which is no longer diagonal. From eq. (67) we have

$$\vec{E} = \frac{1}{\sigma_0}\vec{j} + \frac{1}{nqc}\vec{B} \times \vec{j}. \quad (68)$$

arbitrary with charge q .

We take the magnetic field $\vec{B} = -\hat{e}_3$ and obtain,

$$\rho = \begin{pmatrix} \rho_0 & -\frac{B}{nqc} \\ \frac{B}{nqc} & \rho_0 \end{pmatrix}. \quad (69)$$

Note that an electric field in the y -direction gives rise to a current density in the x -direction (and vice versa). This *Hall current* is easy to observe and depends on the sign of the charge carriers, because the off diagonal elements of the matrix ρ depend on the sign of q . In contrast, the normal resistivity depends only on q^2 . This is the stuff of undergraduate physics labs. This *Hall resistivity* describes the behavior of realistic conductors over a wide range of conditions. Surprisingly the behavior of a system of electrons described by Schroedinger's equation subject to the same external fields is very different.

5.2 Electrons in crossed electric and magnetic fields

5.2.1 Setting up the problem

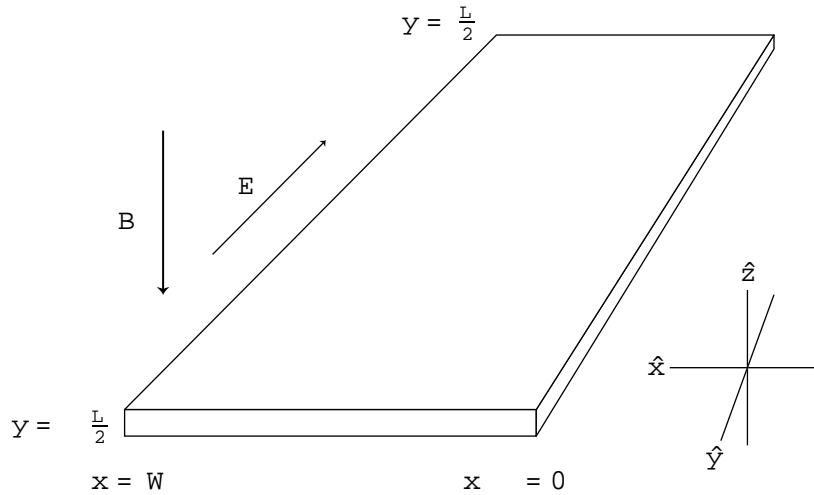


Figure 2: Idealized Hall effect system

In this section we ignore all the complexities of a physical conductor — electron ion interactions, thermal effects, impurities, and so forth — and

consider the idealized problem of a gas of electrons moving in the xy -plane subject to an electric field, $\vec{E} = -E_0\hat{e}_2$, in the negative y -direction, and a magnetic field, $\vec{B} = -B_0\hat{e}_3$ in the negative z -direction. We assume that the conductor forms a strip with $0 < x < W$ and study a section between $y = -L/2$ and $y = L/2$. (See Figure 2.) We assume that the magnetic field is sufficiently strong that only one of the two electron spin states is of interest. The other is promoted to higher energy by the dipole interaction energy, μB_0 .

To construct the Hamiltonian we need an electrostatic potential to produce \vec{E} — $\Phi = E_0y$ — will do; and a vector potential to produce \vec{B} — $\vec{A} = B_0y\hat{e}_1$. Note that we have chosen a different vector potential than we used in our solution to the Landau problem. This choice is more convenient here, but the physics cannot depend on it. The Hamiltonian is given by,

$$\mathcal{H} = \frac{1}{2m} \left[\left(-i\hbar \frac{\partial}{\partial x} - \frac{eB_0y}{c} \right)^2 - \hbar^2 \frac{\partial^2}{\partial y^2} \right] + eE_0y. \quad (70)$$

As usual, it is convenient to introduce some scaled variables. We define the Larmor frequency $\omega_L = eB_0/mc$ as usual, and introduce the natural length scale of the Landau problem, $\ell_0 \equiv \sqrt{\hbar c/eB_0}$. If we now scale the dimensional factors out of (70) we obtain,

$$\mathcal{H} = \frac{\hbar\omega_L}{2} \left[\left(-i \frac{\partial}{\partial \xi} - \eta \right)^2 - \frac{\partial^2}{\partial \eta^2} + 2\alpha\eta \right], \quad (71)$$

where

$$\begin{aligned} \xi &= x/\ell_0 \\ \eta &= y/\ell_0 \\ \alpha &= eE_0\ell_0/\hbar\omega_L. \end{aligned} \quad (72)$$

ξ and η are scaled coordinates and α measures the energy scale of electric relative to magnetic effects.

We now take $(\xi, \eta, p_\xi, p_\eta)$ to be our canonical variables, so

$$\mathcal{H} = \frac{\hbar\omega_L}{2} [(p_\xi - \eta)^2 + p_\eta^2 + 2\alpha\eta], \quad (73)$$

where $p_\xi = -i\partial/\partial\xi$ and $p_\eta = -i\partial/\partial\eta$.

5.2.2 Eigenstates and eigenenergies

It is quite straightforward to find the eigenenergies and eigenstates of this Hamiltonian. First note that p_ξ is a constant of the motion, $[p_\xi, \mathcal{H}] = 0$. We denote the eigenvalue of p_ξ by k . An eigenstate of p_ξ can be written in coordinate space as,

$$\begin{aligned}\psi(\xi, \eta) &= e^{ik\xi} \varphi(\eta, k) \text{ with} \\ \mathcal{H}(\eta) \varphi(\eta, k) &= \frac{\hbar\omega_L}{2} [p_\eta^2 + 2\alpha\eta + (k - \eta)^2] \varphi(\eta, k) \\ &= \frac{\hbar\omega_L}{2} [p_\eta^2 + (\eta - k + \alpha)^2 + 2\alpha k - \alpha^2] \varphi(\eta, k).\end{aligned}\quad (74)$$

This is simply a one-dimensional harmonic oscillator centered at $\eta = k - \alpha$ with eigenenergies shifted by $\hbar\omega_L(\alpha k - \alpha^2/2)$,

$$\mathcal{E}_n(k) = \hbar\omega_L(n + \frac{1}{2}) + \hbar\omega_L(\alpha k - \frac{\alpha^2}{2}) \quad (75)$$

The associated wavefunction, $\varphi_n(\eta, k)$ is a gaussian (multiplying a Hermite polynomial) strongly localized around $\eta = k - \alpha$,

$$\varphi_n(\eta, k) = \exp -\frac{1}{2}|\eta - k + \alpha|^2 H_n(\eta - k + \alpha). \quad (76)$$

The continuous variable k labels the degeneracy of the Landau levels if $\vec{E} = 0$. When $\vec{E} \neq 0$, the highly degenerate Landau level spreads out into a band with energies that depend on \vec{E} through α as displayed in eq. (75).

5.2.3 Degeneracies

When $\vec{E} = 0$ this problem reduces to motion in a constant magnetic field, B_0 , a problem we have just solved, albeit with a different choice for the vector potential \vec{A} . We can use our earlier solution to help us learn how to count and label the states in the case $\vec{E} \neq 0$.

First consider $\vec{E} = 0$. When we studied Landau levels we learned to expect one state in each energy level in an area containing one quantum of flux, $\Phi_0 = hc/e$. So we expect each Landau level to be N -fold degenerate, where $N = \Phi/\Phi_0$, and Φ is the flux, $\Phi = LWB_0$, passing through the region $0 \leq x \leq W$ and $-L/2 \leq y \leq L/2$. We can relate this degeneracy to the allowed values of k , which labels the degeneracy in eq. (75). From (76) with

$\alpha = 0$ we see that the state with “momentum” k is localized at $\eta = k$ or $y = k\ell_0$. Thus the states in the region $-L/2 \leq y \leq L/2$ correspond to a definite range of k ,

$$-\frac{L}{2\ell_0} \leq k \leq \frac{L}{2\ell_0}. \quad (77)$$

We can associate an interval in k with each state by noting that N states must fit into the k -range given by (77) —

$$\Delta k = \frac{L}{\ell_0 N}. \quad (78)$$

If we substitute $N = \Phi/\Phi_0$, we obtain,

$$\Delta k = \frac{2\pi\ell_0}{W}. \quad (79)$$

The allowed values of k can therefore be labelled by an integer, p ,

$$k_p = \frac{2\pi\ell_0}{W}p + \zeta \quad (80)$$

for $-LW/4\pi\ell_0^2 \leq p \leq LW/4\pi\ell_0^2$. The constant ζ cannot be determined by what we have done so far.

To summarize: For $\vec{E} = 0$ we have found that the known degeneracy of the Landau levels quantizes the allowed values of the “momentum”, k , according to the rule (80). Referring back to the wavefunction (74), we find that (80) amounts to a periodicity requirement, $\psi(x=0, y) = \psi(x=W, y)$ up to the phase ζW . The phase ζW plays no role in the physics, so we set ζ to zero henceforth.

Now we return to the case of interest, namely $\alpha \neq 0$. We assume that the wavefunction remains periodic in x : $\psi(x=0, y) = \psi(x=W, y)$, and use the y -dependence to find the range of k . For $\alpha \neq 0$, the eigenstates are centered at $\eta = k - \alpha$. This translates into the quantization rule $k = (2\pi\ell_0/W)p$ with

$$-\frac{LW}{4\pi\ell_0^2} + \frac{\alpha W}{2\pi\ell_0} \leq p \leq \frac{LW}{4\pi\ell_0^2} + \frac{\alpha W}{2\pi\ell_0}. \quad (81)$$

The only effect of the electric field is to shift the allowed values of the “momentum” k .

Let us summarize our solution to the problems of electrons propagating in constant crossed electric and magnetic fields —

- The states are labeled by quantum numbers k and n ,

$$\psi(\xi, \eta) = \sqrt{\frac{\ell_0}{W}} e^{ik\xi} \exp -\frac{1}{2} |\eta - k + \alpha|^2 H_n(\eta - k + \alpha) \quad (82)$$

where we have introduced a factor $\sqrt{\ell_0/W}$ so that the wavefunction is normalized to unity over the rectangle of area LW . (We assume $\exp(-\eta^2/2)H_n(\eta)$ is normalized in η .)

- The eigenenergies are

$$\mathcal{E}_n(k) = \hbar\omega_L(n + \frac{1}{2}) + \hbar\omega_L(\alpha k - \frac{\alpha^2}{2}). \quad (83)$$

- The quantum numbers n and k range over the values,

$$\begin{aligned} n &= 0, 1, 2, \dots \\ -\frac{L}{2\ell_0} + \alpha &\leq k \leq \frac{L}{2\ell_0} + \alpha. \end{aligned} \quad (84)$$

- The degeneracy of the Landau levels is broken by the electric field. Each Landau level breaks up into a “band” of very closely spaced levels. The width of the band is $\Delta\mathcal{E} = \hbar\omega_L\alpha L/\ell_0 = eE_0L$, which is just the change in the classical electrostatic energy of the electron over the length of the conductor. As long as the magnetic field is strong we can assume that the now-smeared-out Landau levels remain well separated from one another.
- The other effect of the electric field is to shift the average “momentum” of the electrons in the Landau bands from *zero* to α . We shall now see that this shift has the effect of producing the classical Hall current — with a quantum twist...

5.2.4 The Hall current

Now let us calculate the current that flows in the x -direction in response to the electric field in the $-y$ direction. The electric current carried by a quantum gas of electrons is its probability current multiplied by the electric charge $q = -e$. As you show on a problem set, the expression for the probability current density is

$$\vec{j} = \frac{\hbar}{m} \text{Im} \psi^* \vec{\nabla} \psi - \frac{e}{mc} \vec{A} \psi^* \psi \quad (85)$$

In the gauge we are using, $A_y = 0$. Given this, and given the fact that the harmonic oscillator wavefunctions, H_n , are real, we conclude that there is *no current in the y (\hat{e}_2) direction*. This is remarkable since \hat{e}_2 is the direction of the external electric field! The x -dependence of $\psi(x, y)$ is complex, so a current in the \hat{e}_1 direction may exist. Substituting (82), multiplying by $-e$, we obtain a current density in the \hat{e}_1 direction associated with the state labeled by n and k . This current density depends on the details of the harmonic oscillator wavefunctions. If we integrate over y from $-L/2$ to $L/2$ we obtain a simple expression for the current in the \hat{e}_1 direction from an electron with “momentum” k in the n^{th} Landau level,

$$I_H(n, k) = -\frac{e\hbar k}{m\ell_0 W}. \quad (86)$$

where the subscript H on I reminds us that this is the Hall current. Note that the contribution of the $\vec{A}\psi^*\psi$ term in the current density (85) is odd in y and so vanishes once we integrate over y .

Now let us suppose that *all states in a given Landau band are filled* and calculate the associated current. This means that we sum (86) over the allowed range of k . For $\alpha = 0$ the negative and positive values of k cancel and we get $\vec{j} = 0$ for $\alpha = 0$. For $\alpha \neq 0$ we replace the sum over p by an integral,

$$I_H(n) = -\frac{e\hbar}{m\ell_0 W} \int_{p_-}^{p_+} k(p) dp \quad (87)$$

where p_{\pm} are the limits on p given in eq. (81). This yields,

$$I_H(n) = -\frac{e^2}{h} E_0 L \quad (88)$$

corresponding to a Hall conductance of $\sigma = e^2/h$ *independent of the size of the sample (L and W) and n — the label of the Landau band*. If N Landau bands are filled then the conductance is $-Ne^2/h$. In the matrix notation of the previous section, we have found that the idealized quantum problem leads to a purely *off-diagonal* conductance matrix

$$\sigma = \begin{pmatrix} 0 & -\frac{Ne^2}{h} \\ +\frac{Ne^2}{h} & 0 \end{pmatrix}, \quad (89)$$

The resistance matrix is the inverse of σ .

To summarize: *If* the idealized quantum treatment is justified, the conductance is purely off-diagonal: an external field in the \hat{e}_2 direction leads to a current in the \hat{e}_1 direction; and *if* N Landau bands *are filled* then the off diagonal (Hall) conductance is quantized in multiples of e^2/h .

5.2.5 A description of the integer quantum Hall effect

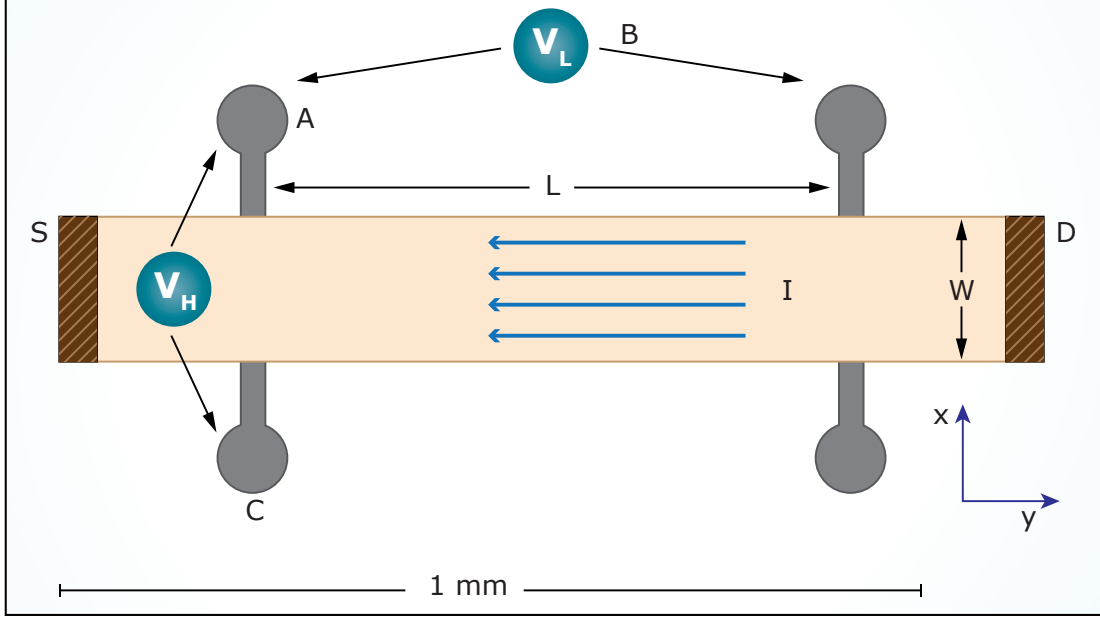


Image by MIT OpenCourseWare,

adapted from R. E. Prange and S. M. Girvin, *The Quantum Hall Effect*, Springer-Verlag, Berlin, 1987.

Figure 3: (From R. E. Prange and S. M. Girvin, *The Quantum Hall Effect*, Springer-Verlag, Berlin, 1987.

Now it is necessary to translate the rather abstract calculation we have just completed into a description of the effect observed by von Klitzing and others. I don't have the time or expertise to do justice to the richness of the phenomena in realistic conductors, but I will try to sketch the physics in a somewhat idealized situation.

Figure 4 shows the results of a measurement of the Hall resistance (on the left vertical axis) and the longitudinal resistance (on the right vertical axis) as a function of $n\hbar c/eB_0$, measured on an idealized sample at low temperature. Two effects stand out: (1) the Hall conductance ($1/R_H$) is quantized in integer multiples of e^2/h over *ranges* of magnetic field strength. The plateaus in $1/R_H$ are very flat and separated by steep increases as $1/R_H$ grows from one integer value to another. (2) The longitudinal resistance, on the other hand, vanishes when R_H is constant, and is finite when R_H is varying. The longitudinal resistance depends on the geometry of the sample as it does for normal metals under normal conditions. The possible values of the Hall resistance, on the other hand, are independent of the geometry of the

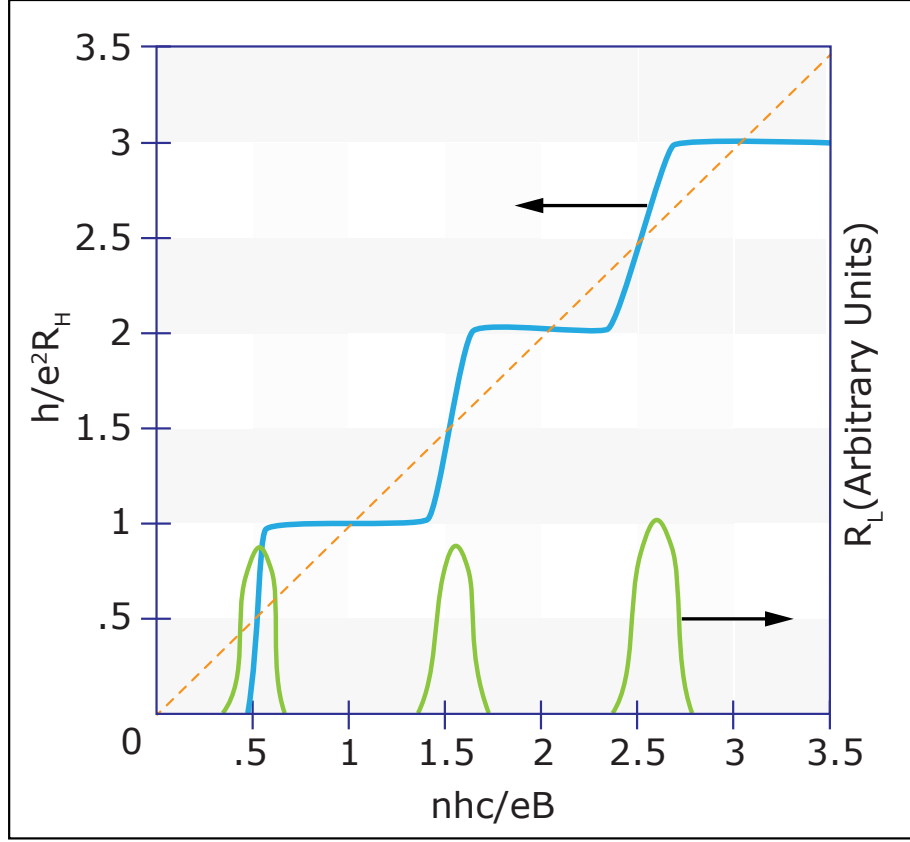


Figure by MIT OpenCourseWare, adapted from R. E. Prange and S. M. Girvin, *The Quantum Hall Effect*, Springer-Verlag, Berlin, 1987.

Figure 4: Longitudinal and transverse resistance for the quantum Hall effect. (From Prange and Girvin.)

sample. It depends on the sample only through the magnetic field strength, B_0 and the charge density, n . Note that a smooth line interpolating through the steps in R_H gives the *classical* relationship $1/R_H = nec/B_0$ as expected from the classical analysis at the beginning of this section (see eq. (69)).

To understand Fig. 4 it is necessary to figure out what is happening to the electron spectrum as nhc/eB_0 is increased. Since electrons obey the Pauli exclusion principle, only two electrons (one of each spin projection) can be placed in each spatial state. For $B_0 = 0$ the states available to the electrons form (essentially) a continuum. For $B_0 \neq 0$ the continuum breaks up into Landau levels separated by gaps. Each Landau level can hold one electron in an area corresponding to a single flux quantum. That area is given by hc/eB_0 . The number of electrons that can be accommodated in a

given Landau level grows as B_0 increases. When B_0 is extremely large, all the electrons can be placed in the lowest Landau level. For large B_0 , the splitting between spin up and spin down electron levels also becomes large, so we can ignore the higher spin state. The ratio of the number of electrons per unit area, n , and the number per unit area per Landau level, eB_0/hc , gives us the number of Landau levels that must be occupied as a function of B_0 (at fixed n),

$$N(B_0) = nhc/eB_0, \quad (90)$$

which is exactly the independent variable in Fig. 4.

We know from the analysis of the previous section that the Hall conductance is quantized when a Landau level is *exactly* full. Fig. 4 together with our interpretation of the variable nhc/eB_0 seems to be saying that $1/R_H$ behaves as though the Landau level were exactly full for a range of B_0 .

The key to understanding the integer quantum Hall effect is the role of *impurities*. We have treated the electrons as an ideal gas, free to orbit in Landau levels. Real experiments are done using almost-two-dimensional electron systems called “inversion layers”, in which the electrons are essentially free to move in the xy -plane but are localized in z at a planar interface between one type of semi-conductor and another. In any real system, there are impurities. This means that while many electron energy levels are *delocalized* as in the ideal case — allowing them to move through the two-dimensional system and respond to external \vec{E} and \vec{B} fields, other energy levels remain pinned, *ie. localized*, around impurities. Electrons that fill these localized levels do not conduct current. A picture of the energy levels in a realistic two-dimensional electron gas is shown in Fig. 5: localized states in between bands (in this case Landau levels) of delocalized states. The striking appearance of the integer quantum Hall effect can be understood by considering the sequential filling of localized and delocalized states as a function of $1/B_0$.

We begin with very large B_0 , at the far left of Fig. 4. The lowest Landau level is only partially filled. Electrons in a partially filled Landau level give rise to a Hall conductance that is a fraction (the “filling fraction”) of the quantum e^2/h . As B_0 decreases, the Landau level fills. The conductance is exactly e^2/h . As B_0 decreases further electrons are forced into higher *localized* levels between the first and second Landau levels. These electrons do not conduct, so the Hall conductance stays fixed at e^2/h . When B_0 decreases still further, the second Landau level quickly fills and the conductance rises to $2e^2/h$. Succeeding intervals of filling localized and delocalized levels gives

rise to the step-like pattern shown in Fig. 4. Eventually, at low magnetic field strength, the steps smooth out to follow the interpolating dashed line that marks the classical Hall resistance.

The explanation of the behavior of the longitudinal resistance also depends crucially on the existence of impurities. In the last section we found that electrons in Landau levels do not contribute to the longitudinal conductivity of a sample. This idealization breaks down in the presence of electron scattering from impurities. Such scattering generates a normal, longitudinal resistance when Landau levels are partially full. However, when a given Landau level is exactly full, the electrons have no unoccupied levels into which to scatter and the longitudinal resistance vanishes. In the domains of B_0 where the localized states are filling the situation remains unchanged — the localized electrons do not participate. When a Landau level again begins to fill, scattering again generates a longitudinal resistance.

We have only scratched the surface of the myriad of phenomena associated with the behavior of materials in the presence of magnetic fields. Many aspects of these systems are studied by condensed matter theorists and experimenters in the MIT Physics Department. For further readings we recommend the book by Prange and Girvin.

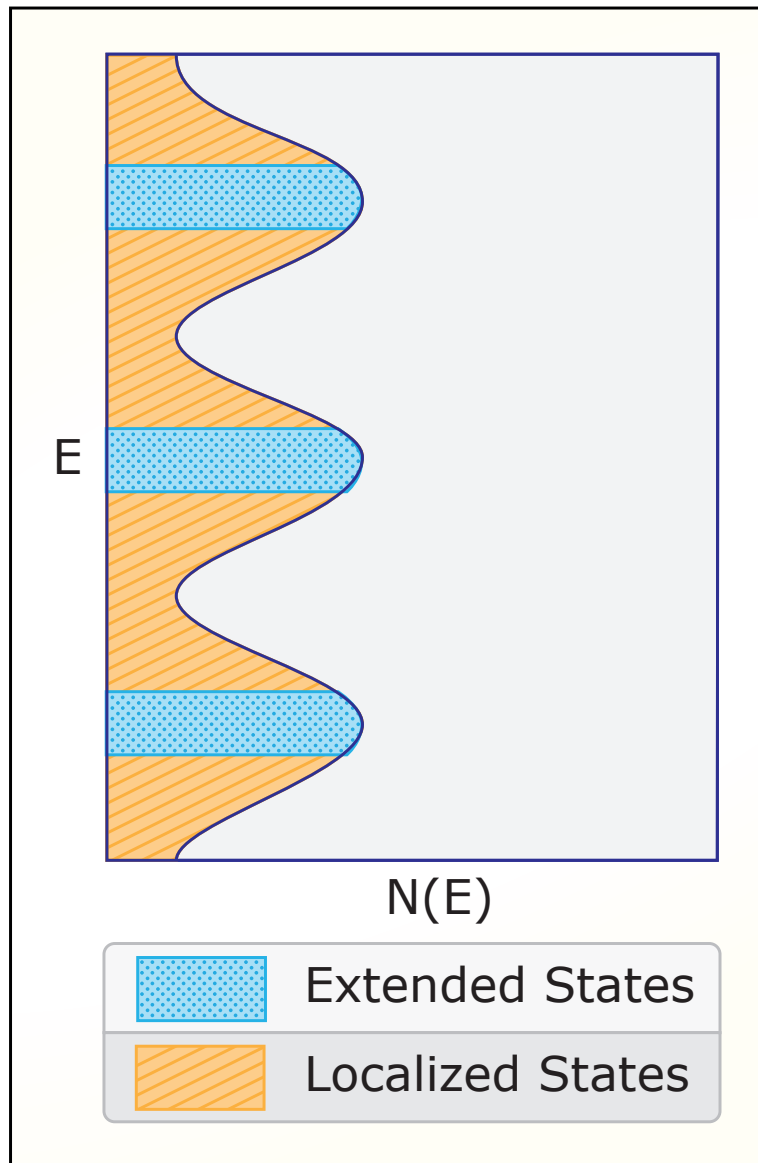


Image by MIT OpenCourseWare, adapted from R. E. Prange and S. M. Girvin, *The Quantum Hall Effect*, Springer-Verlag, Berlin, 1987.

Figure 5: Localized and extended states in a “realistic” two-dimensional electron gas. (From Prange and Girvin.)

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Spring 2016

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