

8.06 Spring 2016 Lecture Notes

4. Identical particles

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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 $|\psi(\vec{r}_1, \vec{r}_2)\rangle = |\psi(\vec{r}_2, \vec{r}_1)\rangle$, 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 $\{|+\rangle + |+\rangle, \frac{|+\rangle + |-\rangle + |-\rangle + |+\rangle}{\sqrt{2}}, |-\rangle - |-\rangle\}$ and the basis for $\text{Anti}^2 \mathbb{C}^2$ is $\{\frac{|+\rangle - |-\rangle - |-\rangle + |+\rangle}{\sqrt{2}}\}$. 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

$$|\psi_{\alpha_1, \dots, \alpha_N}^{\text{sym}}\rangle = \mathcal{N} \sum_{\pi \in S_N} |\alpha_{\pi(1)}\rangle \otimes \cdots |\alpha_{\pi(N)}\rangle. \quad (13)$$

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

$$|\psi_{\alpha_1, \dots, \alpha_N}^{\text{anti}}\rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \text{sgn}(\pi) |\alpha_{\pi(1)}\rangle \otimes \cdots |\alpha_{\pi(N)}\rangle. \quad (14)$$

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

$$\det(A) = \sum_{\pi \in S_N} \text{sgn}(\pi) A_{1, \pi(1)} A_{2, \pi(2)} \cdots A_{N, \pi(N)}. \quad (15)$$

Using this and the notation $\psi_{\alpha}(\vec{r}) = \langle \vec{r} | \alpha \rangle$, it is straightforward to show that

$$\langle \vec{r}_1, \dots, \vec{r}_N | \psi_{\alpha_1, \dots, \alpha_N}^{\text{anti}} \rangle = \det \begin{pmatrix} \psi_{\alpha_1}(\vec{r}_1) & \cdots & \psi_{\alpha_1}(\vec{r}_N) \\ \vdots & & \vdots \\ \psi_{\alpha_N}(\vec{r}_1) & \cdots & \psi_{\alpha_N}(\vec{r}_N) \end{pmatrix}. \quad (16)$$

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

$$\psi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{L^{3/2}} \quad \text{where} \quad \vec{k} = \frac{2\pi}{L}\vec{n}, \vec{n} \in \mathbb{Z}^3. \quad (43)$$

$$E_{\vec{k}} = \frac{\hbar^2}{2m}\vec{k}^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \vec{n}^2. \quad (44)$$

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 $63g/mole$, 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

$$\sigma = \frac{ne^2\tau}{m}. \quad (53)$$

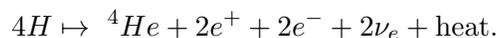
One unsatisfactory feature of this model is the presence of the phenomenological constant τ . On the other hand, a similar calculation (omitted) can express thermal conductivity κ in terms of τ , and predicts that the “Lorentz number” $\frac{\kappa}{\sigma T}$ should be a universal constant. Modeling 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

$$E_{\text{tot}}(R) = \frac{\lambda N^{5/3}}{m_e R^2} - \frac{\kappa N^2}{R}. \tag{54}$$

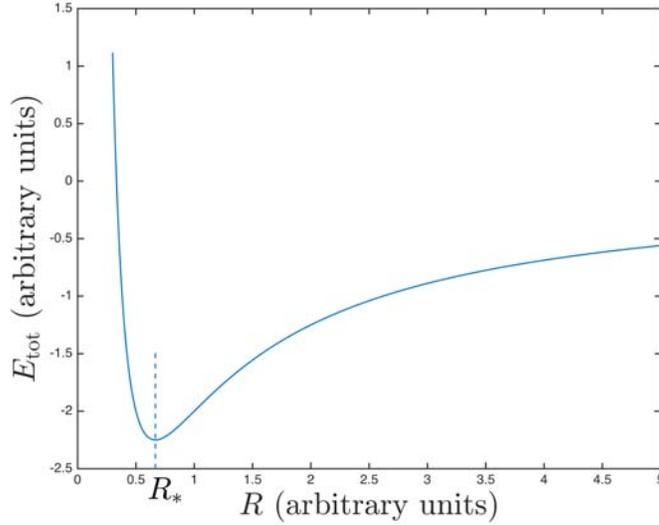


Figure 1: Plot of (54) showing energy from gravity and degeneracy pressure as a function of radius.

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 $M_{\text{crit}} = N_{\text{crit}} m_p \approx 10^{66} eV/c^2$. By contrast $M_{\text{Sun}} \approx 2 \cdot 10^{30} kg \cdot 6 \cdot 10^{35} \frac{eV/c^2}{kg} \approx 10^{66} eV/c^2$ 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

$$E = \sqrt{m_e^2 c^4 + \hbar^2 \vec{k}^2 c^2} \approx \hbar c |\vec{k}|.$$

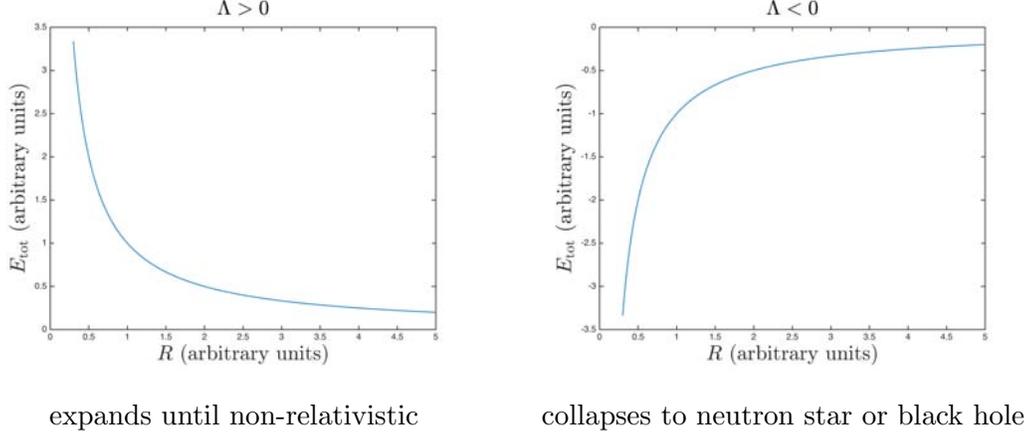


Figure 2: Plot of (56) showing the total energy from gravity and degeneracy pressure of a relativistic free electron gas.

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

$$\begin{aligned}
 E_{\text{gs}} &= \underbrace{\int_0^{k_F} 2 \left(\frac{L}{2\pi} \right)^3 4\pi k^2 dk \hbar c k}_{N_e = \frac{V k_F^3}{3\pi^2}} \\
 &= \frac{V \hbar c}{4\pi^2} k_F^4 \\
 &= \kappa' \frac{N^{4/3}}{V^{1/3}}
 \end{aligned}$$

where $\kappa' \equiv \frac{3}{4} \left(\frac{9\pi}{4} \right)^{1/3} f^{4/3} \hbar c$. Now the total energy is

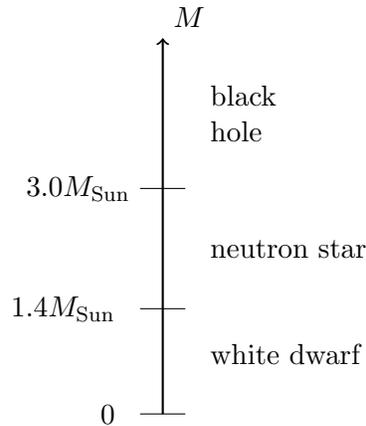
$$E_{\text{tot}} = -\frac{\kappa N^2}{R} + \frac{\kappa' N^{4/3}}{R} \equiv \frac{\Lambda}{R}. \quad (56)$$

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 $[\hat{T}_a, \hat{H}] = 0$ 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

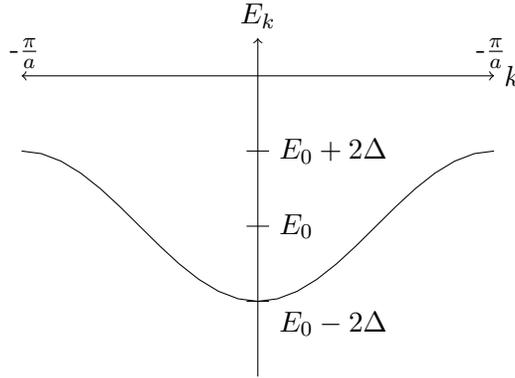
$$T|\psi_k\rangle = e^{ika}|\psi_k\rangle \quad (68)$$

$$H|\psi_k\rangle = E_k|\psi_k\rangle \quad (69)$$

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).



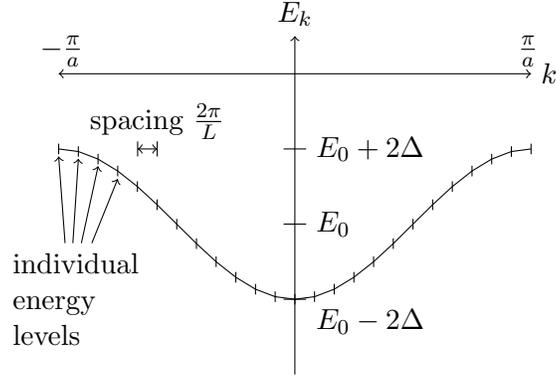
Real solids are not infinite. Suppose there are N sites with periodic boundary conditions, i.e. let $L = Na$ and suppose that $\psi(0) = \psi(L)$. This implies that $T^N|\psi\rangle = \psi$ and therefore for any eigenvalue e^{ika} we must have

$$e^{ikaN} = 1 \quad (71)$$

$$Nka = 2\pi n \quad \text{for some integer } n \quad (72)$$

$$k = \frac{2\pi n}{Na} = \frac{2\pi}{L} n \quad -\frac{N}{2} < n \leq \frac{N}{2} \quad (73)$$

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 $e^{\frac{2\pi inx}{a}}$. Plugging this into (74) we obtain

$$\psi_{n,k}(x) = e^{i\left(\frac{2\pi}{a}n+k\right)x} \quad \text{and} \quad E_{n,k} = \frac{\hbar^2}{2m} \left(\frac{2\pi}{a}n+k\right)^2. \quad (75)$$

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

“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 $m\ddot{\vec{x}} = q(\vec{E} + \frac{\vec{v}}{c} \times \vec{B})$ 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

$$m\ddot{\vec{x}} = \frac{q}{c}\dot{\vec{x}} \times \vec{B}$$

$$\begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix} = \frac{qB}{mc} \begin{pmatrix} \dot{y} \\ -\dot{x} \end{pmatrix}$$

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

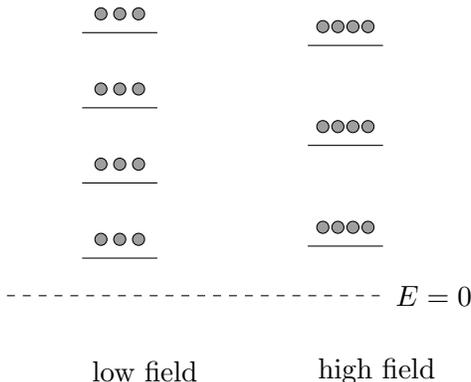
$$\mu_I = -\frac{\partial E}{\partial B} = -(2n + 1)\mu_B.$$

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

$$\nu = \frac{B_0}{B} \quad B_0 \equiv \frac{N\Phi_0}{A}.$$

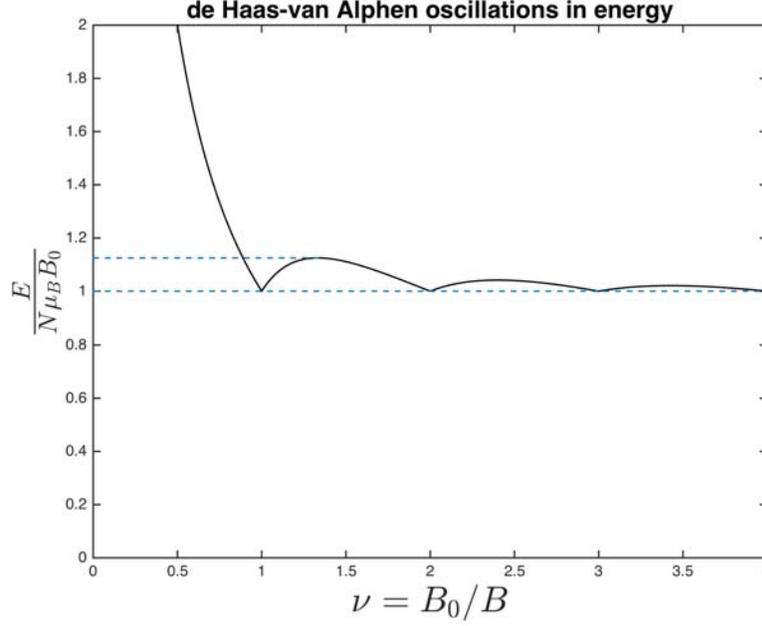


Figure 4: Ground-state energy E as a function of filling fraction, according to (90).

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.

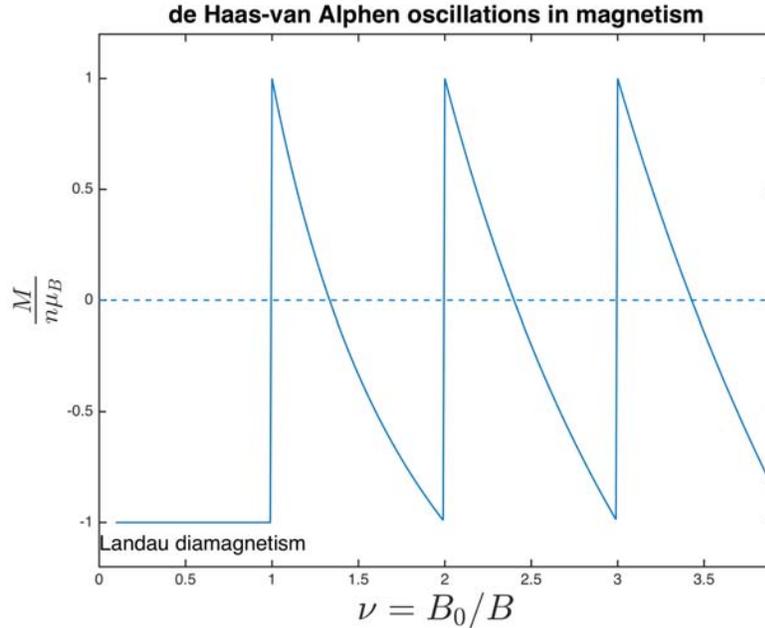


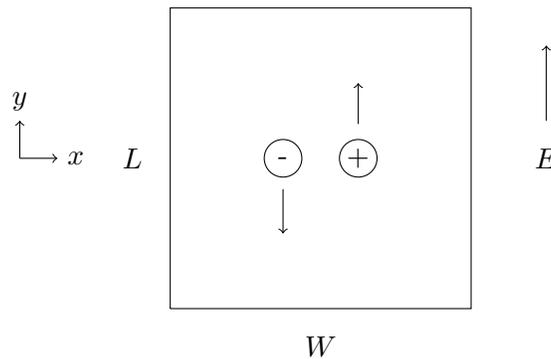
Figure 5: Magnetism M as a function of filling fraction, according to (91).

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.



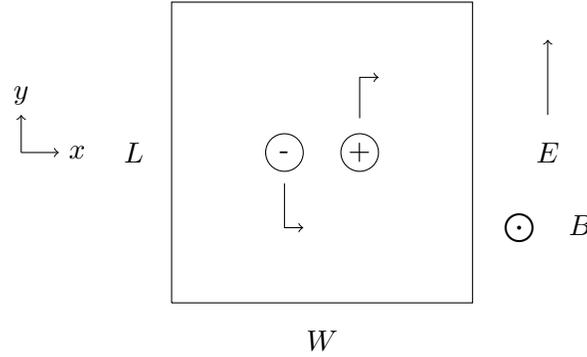
As discussed above, if the mean time between scattering events is τ_0 then there is a drift velocity $\vec{v}_d = \frac{q}{m} \tau_0 \vec{E}$ giving rise to a current density $\vec{j} = nq\vec{v}_d = \frac{nq^2\tau_0}{m} \vec{E}$. Thus the conductivity is $\sigma_0 = \frac{nq^2\tau_0}{m}$. We can also 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

$$\vec{v}(t) + A^{-1}\vec{b} = e^{At}(\vec{v}(0) + A^{-1}\vec{b}),$$

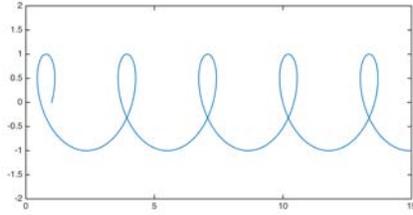


Figure 6: Motion of a charged particle subject to crossed electric and magnetic fields.

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

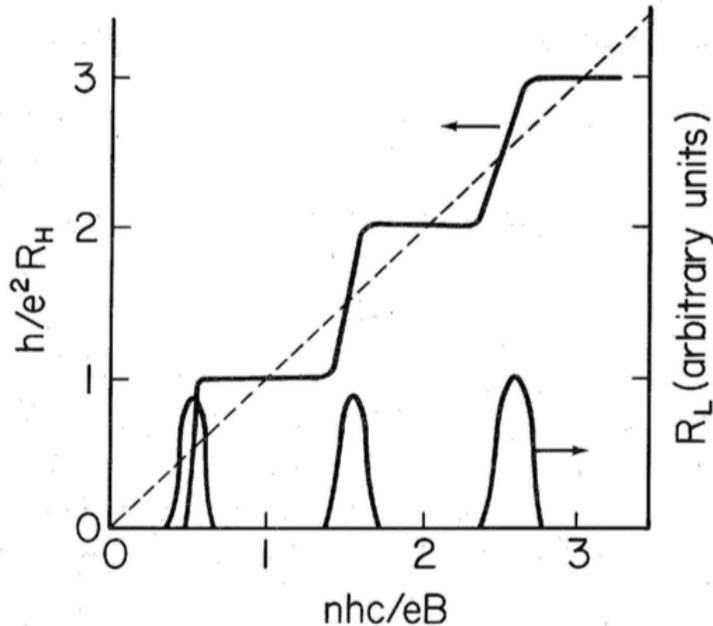


Figure 7: The dashed line is the classical prediction for the transverse resistance. We see instead that it rises quickly around integer values of ν but is nearly flat (in fact, flat to within a factor of 10^{-9}) in between. The longitudinal resistance (and also conductivity) is mostly zero but jumps 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 $\nu = \frac{B_0}{B} = \frac{nhc}{eB} = \frac{nehc}{B} \frac{h}{e^2} = \frac{\sigma_H}{\sigma_0}$. 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

$$H|_{k_x} = \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2(y - y_0)^2 - qEy \quad y_0 \equiv -\ell_0^2 k_x \quad (100)$$

$$= \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2 \left(y^2 - 2yy_0 + y_0^2 - \frac{2qE}{m\omega_L^2} y \right) \quad (101)$$

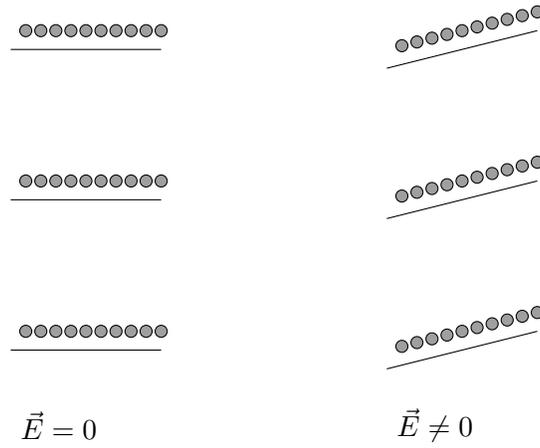
$$= \frac{p_y^2}{2m} + \frac{1}{2}m\omega_L^2 (y - y_0 - y_1)^2 - \frac{1}{2}m\omega_L^2 (2y_0 y_1 + y_1^2) \quad y_1 \equiv \frac{qE}{m\omega_L^2} = \frac{qE}{m\omega_L} \frac{qB}{mc} = \frac{E}{B} \frac{c}{\omega_L} = \frac{v_H}{\omega_L} \quad (102)$$

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 eigenstate 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

$$\int_0^L S_x dy = \frac{\omega_L}{W} \int_0^L |\phi_n(y - y_0 - y_1)|^2 (y - y_0) \quad (108a)$$

$$\approx \frac{\omega_L}{W} \int_0^\infty |\phi_n(y - y_0 - y_1)|^2 (y - y_0) \quad (108b)$$

$$= \frac{\omega_L}{W} \int_0^\infty \underbrace{|\phi_n(y - y_0 - y_1)|^2}_{\text{even}} \underbrace{(y - y_0 - y_1 + y_1)}_{\text{odd}} \quad (108c)$$

$$= \frac{\omega_L}{W} y_1 \quad (108d)$$

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

$$\sigma_H = \frac{j_x}{E_y} = \frac{qc}{AB} = \frac{qc}{\Phi} = \frac{hc e^2}{e h \Phi} = \sigma_0 \frac{\Phi_0}{\Phi} = \nu \sigma_0. \quad (109)$$

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

$$P' = P + \int_{\text{path}} \vec{\nabla} f \cdot d\vec{l} = P + f(\vec{x}_2) - f(\vec{x}_1). \quad (112)$$

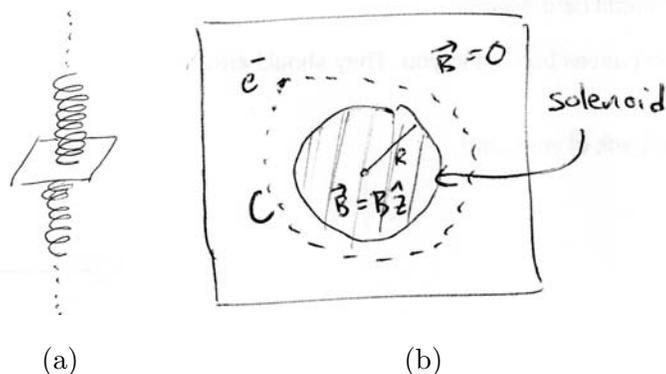


Figure 8: (a) An infinite solenoid of radius R intersects a plane. (b) A cross-section of that plane. The magnetic field inside the solenoid is $B\hat{z}$. An electron and the curve C are entirely outside the solenoid.

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 $\vec{B} = 0$.

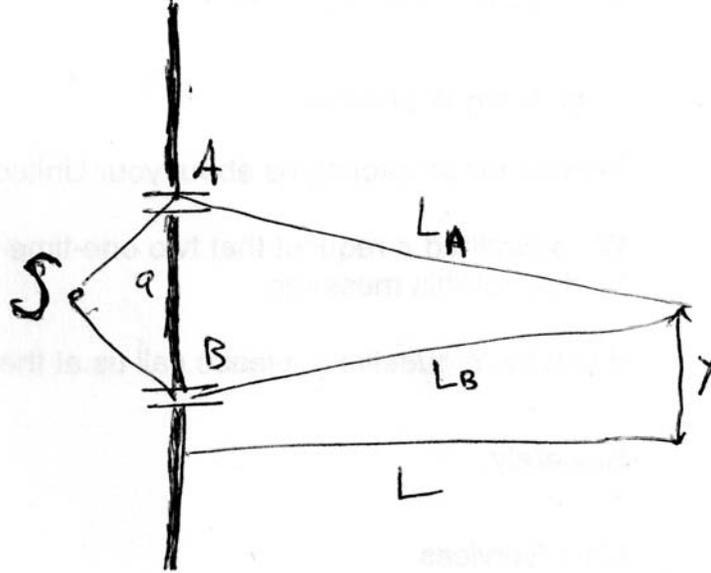
However, the vector potential cannot be zero outside the solenoid. Indeed consider a curve C enclosing the solenoid such as the dashed line in Fig. 8(b). The loop integral of \vec{A} around C is

$$\oint_C \vec{A} \cdot d\vec{\ell} = \pi R^2 B = \Phi \neq 0. \quad (114)$$

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

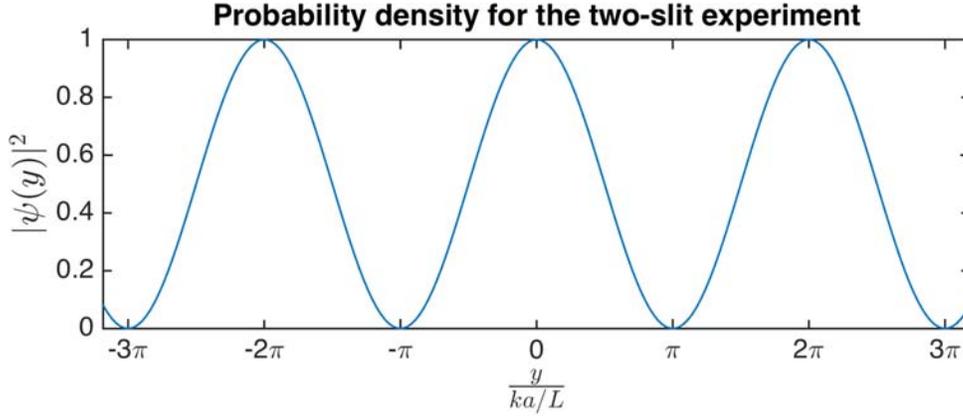
$$\psi(y) = \psi(S \rightarrow A \rightarrow y) + \psi(S \rightarrow B \rightarrow y). \quad (116)$$

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.

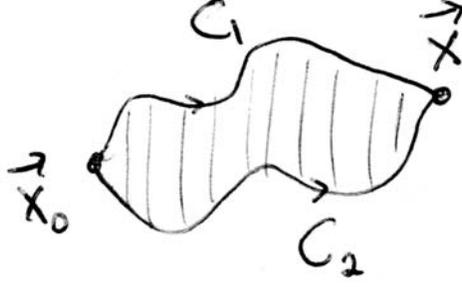


Figure 9: Two curves from \vec{x}_0 to \vec{x} and the region enclosed by them.

To prove (120), consider two curves C_1, C_2 with the same endpoint. Then

$$g(\vec{x}, C_1) - g(\vec{x}, C_2) = \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x}}^{\text{along } C_1} \vec{A} \cdot d\vec{\ell} - \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x}}^{\text{along } C_2} \vec{A} \cdot d\vec{\ell} \quad (121a)$$

$$= \frac{q}{\hbar c} \int_{\vec{x}_0 \rightarrow \vec{x}}^{\text{along } C_1} \vec{A} \cdot d\vec{\ell} + \frac{q}{\hbar c} \int_{\vec{x} \rightarrow \vec{x}_0}^{\text{along } C_2} \vec{A} \cdot d\vec{\ell} \quad (121b)$$

$$= \frac{q}{\hbar c} \oint_{\text{along } C_1 \text{ then } C_2}^{\vec{x}_0 \rightarrow \vec{x} \rightarrow \vec{x}_0} \vec{A} \cdot d\vec{\ell} \quad (121c)$$

$$= \frac{q}{\hbar c} \Phi \quad (121d)$$

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

$$He^{ig} = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)e^{ig} = e^{ig}\frac{\vec{p}^2}{2m} = e^{ig}H^{(0)}. \quad (125)$$

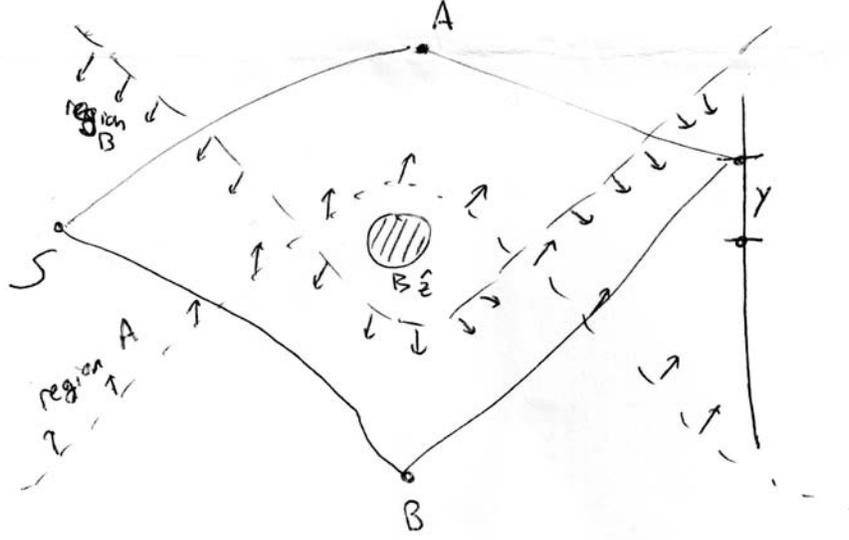


Figure 10: A two-slit experiment is conducted with a solenoid between the two paths. We define two simply connected regions A and B , both of which include the source and the screen where we observe interference. Region A contains paths $S \rightarrow A \rightarrow y$ and region B contains paths $S \rightarrow B \rightarrow y$.

Thus we have (using also the fact that $\partial_t g = 0$) that

$$H\psi = He^{ig}\psi^{(0)} = e^{ig}H^{(0)}\psi^{(0)} = e^{ig}i\hbar\partial_t\psi^{(0)} = i\hbar\partial_t e^{ig}\psi^{(0)} = i\hbar\partial_t\psi. \quad (126)$$

□

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 $\frac{q}{\hbar c} = -2\pi \frac{\Phi}{\Phi_0}$ and the phase shift is $-2\pi \frac{\Phi}{\Phi_0}$. The resulting interference pattern is then

$$|\psi(y)|^2 \propto \cos^2 \left(\frac{1}{2} \left(\frac{kay}{L} - 2\pi \frac{\Phi}{\Phi_0} \right) \right). \quad (131)$$

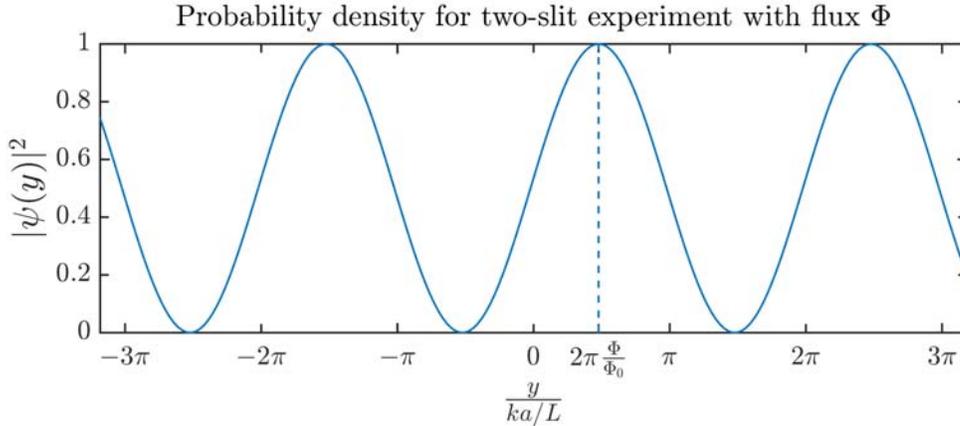


Figure 11: Observed interference pattern when performing the two-slit experiment with a magnetic flux Φ enclosed between the two paths.

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.

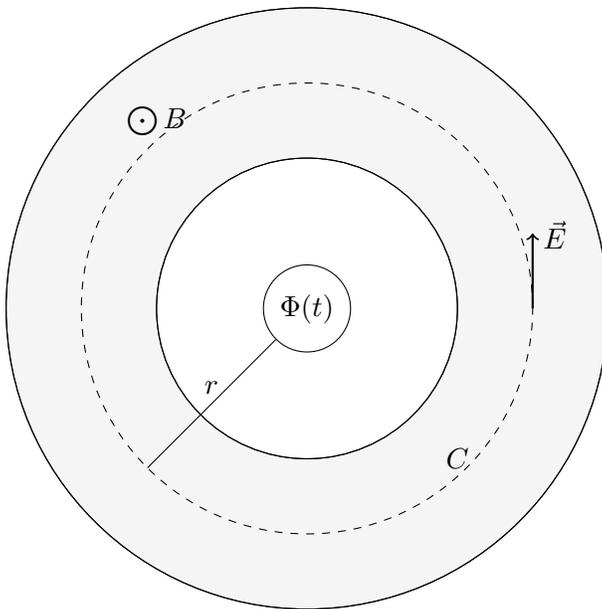


Figure 12: Hall effect on an annulus. There is still a B field in the \hat{z} direction, but now the electric field points in the $\hat{\phi}$ direction. We can think of it as being induced by a time-dependent flux in the center of the annulus. The Hall current now flows radially outward and can be measured 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

$$\Delta Q = \int_0^T \frac{dQ}{dt} dt = \int_0^T 2\pi r j_H dt = 2\pi r \frac{\sigma_H}{2\pi r c} \Phi_0 = \frac{x \frac{e^2}{h}}{c} \frac{hc}{e} = xe. \quad (135)$$

We conclude that x is an integer, as desired.

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