Physics 212C: Advanced Quantum Mechanics
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Lecturer: McGreevy
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0.1 Introductory remarks

By now you know some quantum mechanics (QM), I hope. But it is a vast subject with many applications. There are many directions in which we can generalize from your previous encounters with QM.

One direction is toward situations where things are *faster*. This leads to "relativistic quantum mechanics," which inevitably means quantum field theory. That's the subject of Physics 215 and so I will try to stay away from it to the extent possible.

In this course, we will approach a different frontier: situations where things are *many*. That is: what happens when we put together a whole bunch of quantum degrees of freedom. (As we will see, sometimes this also means quantum field theory!) Sometimes 'a whole bunch' will mean just a big finite number, like the number of electrons in an atom of large atomic number, or a very big finite number, like the number of electrons in a chunk of solid. Sometimes, we'll be interested in *the thermodynamic limit*, where the number of degrees of freedom becomes parametrically large. This is because new (*emergent*) phenomena happen in this limit.

There is some flexibility about what subjects we'll discuss this quarter. Please tell me about topics of interest to you.

0.2 Possible topics (not in order)

Physics phenomena:

Phonons

Radiation (photons, Casimir effect)

Atoms

Molecules

Matter and radiation (photoelectric effect, scattering, lasers)

More interesting states of matter (superfluids and superconductors, magnetic insulators, quantum Hall phases)

Relativistic quantum mechanics

Techniques:

How to describe an indefinite number of particles ('second quantization').

Hartree-Fock, Thomas-Fermi.

Born-Oppenheimer, Berry phases.

Mean field theory of various states of matter

Coherent state path integrals?

Fermi liquid theory?

We'll learn about topics from these list in parallel.

0.3 Sources and acknowledgement

- Commins, *Quantum mechanics, an experimentalist's approach*, Cambridge, 2014.
- Baym, *Lectures on quantum mechanics*, Westview Advanced Book Program, long ago (the front-matter is missing from my copy).
- LeBellac, *Quantum Physics*, Cambridge, 2012.
- Feynman, *Statistical Mechanics: a set of lectures*, Perseus Advanced Book Program, 1972.
- Leggett, *Quantum Liquids*, Oxford, 2006.
- Pines and Nozieres, *The Theory of Quantum Liquids* (two volumes), Perseus Advanced Book Program, 1966.
- Unpublished 212C notes by Tarun Grover.
- Tong, *Topics in Quantum Mechanics*

Some sources I recommend for some of the many topics that we could have studied but did not are:

- Tong, *Lectures on Applications of Quantum Mechanics*
- Littlejohn, Lecture notes for Berkeley Physics 221
- Sakurai, *Advanced Quantum Mechanics*, Addison-Wesley, 1967.

0.4 Conventions

The convention that repeated indices are summed is always in effect unless otherwise indicated.

d is the number of space dimensions, D is the number of spacetime dimensions (it's bigger!).

A consequence of the fact that english and math are written from left to right is that time goes to the left.

A useful generalization of the shorthand $\hbar \equiv \frac{h}{2\pi}$ is $đk \equiv \frac{\mathrm{d}k}{2\pi}$. I will also write $\not{\delta}^d(q) \equiv (2\pi)^d \delta^{(d)}(q)$. I will try to be consistent about writing Fourier transforms as

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} e^{ik\cdot x} \tilde{f}(k) \equiv \int đ^d k \; e^{ik\cdot x} \tilde{f}(k) \equiv f(x).$$

IFF $\equiv$ if and only if.
RHS $\equiv$ right-hand side. LHS $\equiv$ left-hand side. BHS $\equiv$ both-hand side.
IBP $\equiv$ integration by parts. WLOG $\equiv$ without loss of generality.
$+\mathcal{O}(x^n) \equiv$ plus terms which go like x^n (and higher powers) when x is small.
$+h.c. \equiv$ plus hermitian conjugate.
$\mathcal{L} \ni \mathcal{O}$ means the object $\mathcal{L}$ contains the term $\mathcal{O}$.

We work in units where $\hbar$ and the speed of light, c, are equal to one unless you see explicit factors of $\hbar$ or c.

Please tell me if you find typos or errors or violations of the rules above.

1 An indefinite number of identical particles

So far in Physics 212, you've mainly been discussing the quantum theory of particles, where the number of particles is *fixed* (and quite small). There are processes in nature where the number of particles can change – for example photons are created during atomic transitions. How do we describe this kind of thing? The answer is sometimes called quantum field theory or sometimes 'second quantization' (a terrible name), and it is a crucial part of modern physics. We will discover it in a perhaps-unexpected place, momentarily (§1.3).

This discussion also follows logically in that one's study of QM begins (or at least should begin) by discussing a single qubit, and then learning to make composite quantum systems, which basically means two qbits. Here we will take the next step of studying composite quantum systems with *infinitely many* components.

Another side-benefit of being able to describe an indefinite number of particles is that we can also describe superpositions between states with different numbers of particles. This is required to describe a superfluid.

1.1 Harmonic oscillator review, operator solution

[Le Bellac 11.1] The simple harmonic oscillator is ubiquitous in physics, not just because it is exactly solvable both classically and quantum mechanically, but because it arises as the leading approximation to any system near a stable equilibrium. Expanding a potential $V(x)$ in one dimension about its minimum at x_0, Taylor's theorem says

$$V(x) = V(x_0) + 0 + \frac{1}{2}V''(x_0)(x-x_0)^2 + ...$$

and we can often ignore the ... (aka anharmonic terms) for systems that are near their equilibrium configuration. WLOG setting $x_0 \equiv 0$, we are led to study

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{x}^2 = \frac{\hbar\omega}{2}\left(\mathbf{P}^2 + \mathbf{Q}^2\right) = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right)$$

with

$$\mathbf{a} \equiv \frac{1}{\sqrt{2}}\left(\mathbf{Q} + \mathbf{i}\mathbf{P}\right), \quad \mathbf{a}^\dagger \equiv \frac{1}{\sqrt{2}}\left(\mathbf{Q} - \mathbf{i}\mathbf{P}\right).$$

Here I've defined these new operators to hide the annoying constant factors:

$$\mathbf{Q} \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2}\mathbf{x}, \quad \mathbf{P} \equiv \left(\frac{1}{m\hbar\omega}\right)^{1/2}\mathbf{p}.$$

$$[\mathbf{x},\mathbf{p}] = \mathbf{i}\hbar\mathbb{1} \quad \Leftrightarrow \quad [\mathbf{Q},\mathbf{P}] = \mathbf{i}\mathbb{1} \quad \Leftrightarrow \quad [\mathbf{a},\mathbf{a}^\dagger] = \mathbb{1}.$$

The *number operator* $\mathbf{N} \equiv \mathbf{a}^\dagger \mathbf{a}$ is hermitian and satisfies

$$[\mathbf{N}, \mathbf{a}] = -\mathbf{a}, \quad [\mathbf{N}, \mathbf{a}^\dagger] = +\mathbf{a}^\dagger \quad .$$

So $\mathbf{a}$ and $\mathbf{a}^\dagger$ are, respectively, lowering and raising operators for the number operator. The eigenvalues of the number operator have to be positive, since

$$0 \leq \| \, \mathbf{a} \, |n\rangle \, \|^2 = \langle n | \, \mathbf{a}^\dagger \mathbf{a} \, | n \rangle = \langle n | \, \mathbf{N} \, | n \rangle = n \, \langle n | n \rangle$$

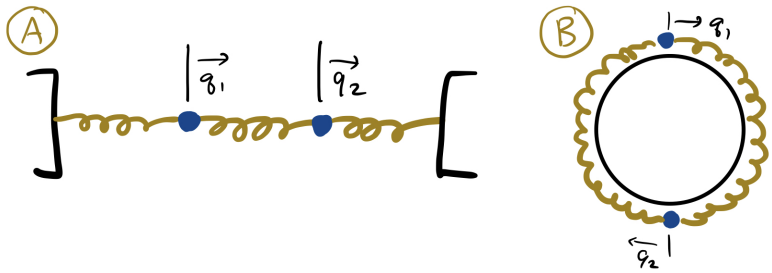
which means that for $n = 0$ we have $\mathbf{a} \, |n = 0\rangle = 0$. If it isn't zero (*i.e.* if $n \geq 1$), $\mathbf{a} \, |n\rangle$ is also an eigenvector of $\mathbf{N}$ with eigenvalue $n - 1$. It has to stop somewhere! So the eigenstates of $\mathbf{N}$ (and hence of $\mathbf{H} = \hbar\omega \left(\mathbf{N} + \frac{1}{2} \right)$) are

$$|0\rangle \, , \quad |1\rangle \equiv \mathbf{a}^\dagger \, |0\rangle \, , \quad ..., |n\rangle = c_n \left(\mathbf{a}^\dagger \right)^n |0\rangle \, ...$$

where we must choose c_n to normalize these states. The answer that gives $\langle n | n \rangle = 1$ is $c_n = \frac{1}{\sqrt{n!}}$.

1.2 Warmup: two modes

As a warmup, consider the following two (quantum) mechanical systems, each consisting of two point masses.



In case A, we have two masses connected by springs and attached to the walls of the box. In case B, the two masses are only connected to each other. In each case, we can write the Hamiltonian as

$$\mathbf{H} = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + V(\mathbf{q}) \tag{1.1}$$

where $V(\mathbf{q})$ is a quadratic function in $\mathbf{q}_1, \mathbf{q}_2$. In case A:

$$V_A(\mathbf{q}) = \frac{1}{2}\kappa(\mathbf{q}_2 - \mathbf{q}_1)^2 + \frac{1}{2}\kappa\mathbf{q}_1^2 + \frac{1}{2}\kappa\mathbf{q}_2^2 = \frac{1}{2}\kappa(\mathbf{q}_1, \mathbf{q}_2) \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} \tag{1.2}$$

and in case B,

$$V_B(\mathbf{q}) = \kappa(\mathbf{q}_2 - \mathbf{q}_1)^2 = \kappa(\mathbf{q}_1, \mathbf{q}_2) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} . \tag{1.3}$$

Recall from mechanics that to solve either of these problems, we can decompose the motion into *normal modes*. In this case, the normal modes are just $\mathbf{q}_\pm = \frac{1}{\sqrt{2}}(\mathbf{q}_1 \pm \mathbf{q}_2)$, which describe the two particles moving together, or the two particles moving oppositely. More mechanically, the eigenvectors of the matrix $\begin{pmatrix} s & 1 \\ 1 & s \end{pmatrix} = s\mathbb{1}_2 - \sigma^x$ are $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$, with respective eigenvalues $s \mp 1$. So

$$\begin{pmatrix} \mathbf{q}_+ \\ \mathbf{q}_- \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} \quad \Leftrightarrow \quad \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \mathbf{q}_+ \\ \mathbf{q}_- \end{pmatrix} . \tag{1.4}$$

There is also a similar relation for the associated canonical momenta:

$$\begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} \mathbf{p}_+ \\ \mathbf{p}_- \end{pmatrix} .$$

Plugging this in:

$$\mathbf{H} = \sum_{\alpha=\pm}\left(\frac{\mathbf{p}_\alpha^2}{2m} + \frac{1}{2}\kappa_\alpha \mathbf{q}_\alpha^2\right) \tag{1.5}$$

the problem breaks apart into two independent oscillators. The normal modes are the eigenvectors of the matrix of spring constants, and κ_α are the associated eigenvalues.

In case A, both spring constants are nonzero, but in case B there is no restoring force for the center of mass mode $\mathbf{q}_+$. This makes sense because if the two particles move together, the springs are not stretched.

To understand the associated quantum system for case A now is easy: just use the above solution of the single SHO for each of the two normal modes. The only tricky part is that we have to introduce a mode operator $\mathbf{a}_\pm, \mathbf{a}_\pm^\dagger$ for each of the oscillators. Here $\pm$ is just a label saying which mode we are talking about.

1.3 Particles and fields

[Le Bellac section 11.3] Let's think about a crystalline solid. The specific heat of solids (how much do you have to heat it up to change its temperature by a given amount) was a mystery before QM. The first decent (QM) model was due to Einstein, where he supposed that the position of each atom is a (independent) quantum harmonic oscillator with frequency ω. This correctly predicts that the specific heat decreases as the temperature is lowered, but is very crude. Obviously the atoms interact: that's why they make a nice crystal pattern, and that's why there are sound waves, as we will see. By treating the elasticity of the solid quantum mechanically, we are going to

discover quantum field theory. One immediate benefit of this will be a framework for quantum mechanics where particles can be created and annihilated.

As a toy model of a one-dimensional crystalline solid, let's consider a chain of point masses m, each connected to its neighbors by springs with spring constant κ. When in equilibrium, the masses form a regular one-dimensional crystal lattice of equally-spaced mass points. Now let q_n denote the displacement of the nth mass from its equilibrium position x_n and let p_n be the corresponding momentum. Assume there are N masses and impose periodic boundary conditions: $q_{n+N} = q_n$. The equilibrium positions themselves are

$$x_n = na, n = 1, 2...N$$

where a is the lattice spacing. The Hamiltonian for the collection of masses is:

$$\mathbf{H} = \sum_{n=1}^{N} \left(\frac{\mathbf{p}_n^2}{2m} + \frac{1}{2}\kappa \left(\mathbf{q}_n - \mathbf{q}_{n-1} \right)^2 \right) + \lambda \mathbf{q}^3. \tag{1.6}$$

I've include a token anharmonic term $\lambda \mathbf{q}^3$ to remind us that we are leaving stuff out; for example we might worry whether we could use this model to describe *melting*. Now set $\lambda = 0$ because we are going to study small deviations from $q = 0$.

This hamiltonian above describes a collection of coupled oscillators, with a matrix of spring constants $V = k_{ab}\mathbf{q}_a\mathbf{q}_b$. If we diagonalize the matrix of spring constants, we will have a description in terms of decoupled oscillators, called *normal modes*.

Notice that the hamiltonian commutes with the *shift* operation

$$\mathcal{T} : (q_n, p_n) \to (q_{n+1}, p_{n+1}) \equiv \left((\mathcal{T}q)_n, (\mathcal{T}p)_n \right)$$

where $\mathcal{T}$ acts on the labels of the masses by

$$\mathcal{T} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

$[\mathbf{H}, \mathcal{T}] = 0$; $\mathcal{T}$ is a symmetry, a discrete translation symmetry.

The eigenvectors of $\mathcal{T}$ are waves:

$$\mathcal{T} e^{\mathbf{i}kx} = e^{\mathbf{i}k(x+a)} = e^{\mathbf{i}ka} e^{\mathbf{i}kx}.$$

Hence these are eigenvectors of k_{ab} as well.

A nice way to summarize this statement is the following slogan: Since our system has (discrete) translation invariance, the normal modes are labelled by a wavenumber k[1]:

$$q_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{\mathbf{i}kx_n} q_n, \quad p_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{\mathbf{i}kx_n} p_n,$$

(Notice that in the previous expressions I didn't use boldface; that's because this step is really just classical physics. Note the awkward (but here, inevitable) fact that we'll have (field) momentum operators $\mathbf{p}_k$ labelled by a wavenumber aka momentum.)

Regulators: Because N is finite, k takes discrete values ($1 = e^{\mathbf{i}kNa}$, so $k = \frac{2\pi j}{Na}, j \in \mathbb{Z}$); this is a long-wavelength "IR" cutoff. Because of the lattice structure, k is periodic (only $e^{\mathbf{i}kan}, n \in \mathbb{Z}$ appears): $k \equiv k + 2\pi/a$; this is a short-distance "UV" cutoff. The range of k can be taken to be

$$0 \leq k \leq \frac{2\pi(N-1)}{Na} \ .$$

Because of the periodicity in k, we can equivalently label the set of wavenumbers by:

$$0 < k \leq \frac{2\pi}{a} \quad \text{or} \quad -\frac{\pi}{a} < k \leq \frac{\pi}{a}.$$

This range of independent values of the wavenumber in a lattice model is called the *Brillouin zone*. There is some convention for choosing a fundamental domain which prefers the last one but I haven't found a reason to care about this.

Summary: Because the system is in a box (periodic), k-space is discrete. Because the system is on a lattice, k-space is periodic. There are N oscillator modes altogether. When I write $\sum_k$ below, it is a sum over these N values.

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[1]The inverse transformation is:

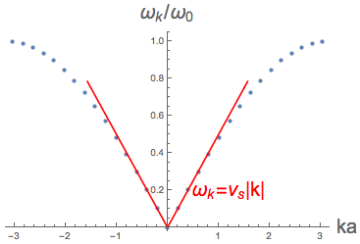
$$q_n = \frac{1}{\sqrt{N}} \sum_{k>0}^{2\pi/a} e^{-\mathbf{i}kx_n} q_k, \quad p_n = \frac{1}{\sqrt{N}} \sum_{k>0}^{2\pi/a} e^{-\mathbf{i}kx_n} p_k.$$

So the whole hamiltonian is a bunch of decoupled oscillators, labelled by these funny wave numbers:

$$\mathbf{H} = \sum_k \left(\frac{\mathbf{p}_k \mathbf{p}_{-k}}{2m} + \frac{1}{2} m\omega_k^2 \mathbf{q}_k \mathbf{q}_{-k} \right) \tag{1.7}$$

where the frequency of the mode labelled k is

$$\omega_k \equiv 2\sqrt{\frac{\kappa}{m}} \sin \frac{|k|a}{2}. \tag{1.8}$$



(The dispersion relation for $N = 40$. ω_k in units of $\omega \equiv \sqrt{\kappa/m}$)

This is called the *dispersion relation* – it says how fast a mode of a given wavenumber propagates; its deviation from linearity in k says how quickly a wave packet will disperse.

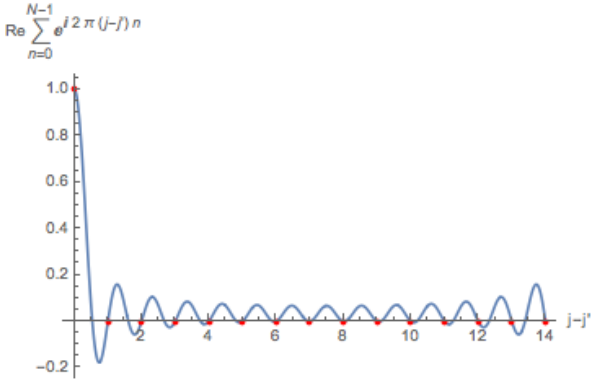
To verify (1.7), let's look more carefully at the expression for the normal modes:

$$q_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{\mathbf{i}kx_n} q_n \equiv \sum_n \mathbf{U}_{kn} q_n \quad , \quad k = j\frac{2\pi}{Na}, \quad j = 1 \ldots N.$$

We can check that $\mathbf{U}$ is indeed a unitary matrix (I am writing $k = \frac{2\pi}{Na} j, k' = \frac{2\pi}{Na} j'$, where $j, j' \in 0 \ldots N-1$ are integers) :

$$\sum_n \mathbf{U}_{kn} \mathbf{U}^\dagger_{nk'} = \sum_n \mathbf{U}_{kn} \mathbf{U}^\star_{k'n} = \frac{1}{N} \sum_n e^{\mathbf{i}kx_n} e^{-\mathbf{i}k'x_n} = \frac{1}{N} \frac{1 - e^{2\pi\mathbf{i}(j-j')}}{1 - e^{2\pi\mathbf{i}(j-j')/N}} = \delta_{jj'} = \delta_{kk'}.$$

At right is what that function looks like for real argument; notice that it vanishes at all the integers other than 0.



The inverse fourier transform is

$$q_n = \frac{1}{\sqrt{N}} \sum_{k>0}^{2\pi/a} e^{-\mathbf{i}kx_n} q_k = \sum_k \mathbf{U}^\dagger_{nk} q_k = \sum_k \mathbf{U}_{-kn} q_k.$$

Notice that this $\mathcal{T}$ is an operator acting on the *labels* of the quantum states – it's a classical operator. So don't be surprised that we can also Fourier transform the

momenta :

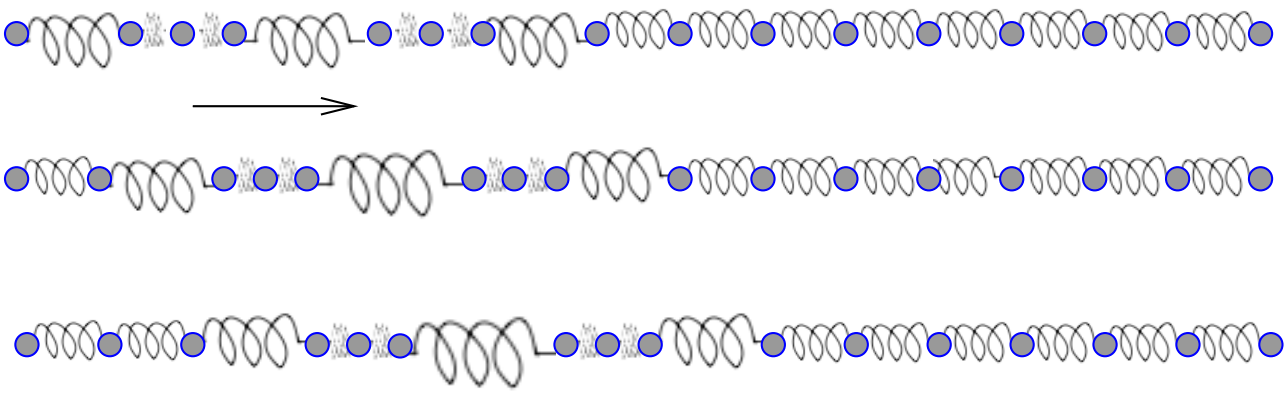
$$p_k = \sum_n \mathbf{U}_{kn} p_n.$$

So far we've actually solved a classical problem of finding normal modes of these coupled oscillators. The world is quantum mechanical so let's remember that our variables are quantum operators now, and figure out what the quantum Hamiltonian is for the normal modes. The kinetic term in the Hamiltonian is

$$\sum_n \mathbf{p}_n^2 = \sum_n \sum_{k,k'} \mathbf{U}_{-kn}\mathbf{U}_{-k'n}\mathbf{p}_k\mathbf{p}_{k'} = \sum_{k,k'} \delta_{k,-k'}\mathbf{p}_k\mathbf{p}_{k'} = \sum_k \mathbf{p}_k\mathbf{p}_{-k}.$$

The potential energy term is

$$\begin{aligned}\sum_n (\mathbf{q}_{n+1} - \mathbf{q}_n)^2 = \sum_n \left((\mathcal{T} - \mathbb{1})\,\mathbf{q}\right)_n^2 &= \sum_n \sum_{k,k'} \left(e^{-\mathbf{i}ka} - 1\right)\left(e^{-\mathbf{i}k'a} - 1\right)\mathbf{U}_{-kn}\mathbf{U}_{-k'n}\mathbf{q}_k\mathbf{q}_{k'} \\ &= \sum_k \left(e^{-\mathbf{i}ka} - 1\right)\left(e^{+\mathbf{i}ka} - 1\right)\mathbf{q}_k\mathbf{q}_{-k} = \sum_k 4\sin^2\left(\frac{ka}{2}\right)\mathbf{q}_k\mathbf{q}_{-k}.\end{aligned}$$



Sound waves. Where does this frequency ω_k matter physically? For one thing, consider the Heisenberg equation of motion for the deviation of one spring:

$$\mathbf{i}\partial_t \mathbf{q}_n = [\mathbf{q}_n, \mathbf{H}] = \frac{\mathbf{p}_n}{m}, \quad \mathbf{i}\partial_t \mathbf{p}_n = [\mathbf{p}_n, \mathbf{H}]$$

Combining these gives:

$$m\ddot{q}_n = -\kappa\left((q_n - q_{n-1}) - (q_n - q_{n+1})\right) = -\kappa\left(2q_n - q_{n-1} - q_{n+1}\right).$$

(You will recognize this as just Newton's equation which would be valid classically.) In terms of the fourier-mode operators, these equations decouple:

$$m\ddot{\mathbf{q}}_k = -\kappa\left(2 - 2\cos ka\right)\mathbf{q}_k \ .$$

Plugging in a fourier ansatz in time as well $q_k(t) = \sum_\omega e^{-\mathbf{i}\omega t} q_{k,\omega}$ turns this into an algebraic equation which says $\omega^2 = \omega_k^2 = \left(\frac{2\kappa}{m}\right) \sin^2 \frac{|k|a}{2}$ for the allowed modes (we used a trigonometric identity here). We see that (the classical version of) this system describes waves:

$$0 = \left(\omega^2 - \omega_k^2\right) q_{k,\omega} \overset{k \ll 1/a}{\simeq} \left(\omega^2 - v_s^2 k^2\right) q_{k,\omega}.$$

The result for small k is the fourier transform of the wave equation:

$$\left(\partial_t^2 - v_s^2 \partial_x^2\right) q(x,t) = 0 \ . \tag{1.9}$$

v_s is the speed of propagation of the waves, in this case the speed of sound. Comparing to the dispersion relation (1.8), we have found

$$v_s = \frac{\partial \omega_k}{\partial k}|_{k \to 0} = a\sqrt{\frac{\kappa}{m}}.$$

The description we are about to give is a description of quantum sound waves. (Below we will also give a description of quantum light waves.) [End of Lecture 1]

Here is a slight generalization, by way of recap. Consider the more general class of Hamiltonians

$$\mathbf{H} = \sum_n \frac{\mathbf{p}_n^2}{2m_n} + \frac{1}{2}\sum_{nm} \kappa_{nm} q_n q_m.$$

We allowed the masses to vary, and we made a whole matrix of spring constants. Notice that only the symmetric part $\frac{1}{2}\left(\kappa_{nm} + \kappa_{mn}\right)$ of this matrix appears in the Hamiltonian. Also κ must be real so that $\mathbf{H}$ is hermitian. To simplify our lives we can redefine variables

$$Q_n \equiv \sqrt{m_n} q_n, \quad P_n = p_n/\sqrt{m_n}, \quad V_{nm} \equiv \frac{\kappa_{nm}}{\sqrt{m_n m_m}}$$

in terms of which

$$\mathbf{H} = \frac{1}{2}\left(\sum_n P_n^2 + \sum_{nm} V_{nm} Q_n Q_m\right).$$

Notice that $[q_n, p_m] = \mathbf{i}\delta_{nm} \Leftrightarrow [Q_n, P_n] = \mathbf{i}\delta_{nm}$.

Now since V_{nm} is a symmetric matrix, and hence hermitian, it can be diagonalized. That is, we can find U so that $UVU^\dagger$ is a diagonal matrix:

$$\sum_{nm} U_{\alpha n} V_{nm} \left(U^\dagger\right)_{m\beta} = \delta_{\alpha\beta}\omega_\alpha^2 \tag{1.10}$$

where I assumed that all the eigenvalues of V are non-negative – otherwise the system is unstable. U is unitary (actually it could be taken to be an orthogonal matrix):

$$\sum_n U_{\alpha n}\left(U^\dagger\right)_{n\beta} = \delta_{\alpha\beta}, \quad \sum_\alpha \left(U^\dagger\right)_{n\beta} U_{\beta m} = \delta_{nm}. \tag{1.11}$$

To take advantage of this, we make the change of variables to the *normal modes*

$$\tilde{Q}_\alpha = \sum_n U_{\alpha n} Q_n.$$

Multiplying the BHS of this equation by $U^\dagger$, we have the inverse relation

$$Q_n = \sum_\alpha \left(U^\dagger\right)_{n\alpha} \tilde{Q}_\alpha.$$

Notice that $Q_n = Q_n^\dagger$ is hermitian. This means

$$Q_n = Q_n^\dagger = \sum_n \left(U^\dagger\right)^\star_{n\alpha} \tilde{Q}^\dagger_\alpha = \sum_n \left(U^T\right)_{n\alpha} \tilde{Q}^\dagger_\alpha = \sum_n \tilde{Q}^\dagger_\alpha U_{\alpha n}.$$

Similarly, we define $\tilde{P}_\alpha = \sum_n U_{\alpha n} P_n$.

Now let's look at what this does to the terms in $\mathbf{H}$:

$$\sum_n P_n^2 = \sum_n P_n^\dagger P_m = \sum_{\alpha\beta} \underbrace{\sum_n U_{\alpha n} \left(U^\dagger\right)_{n\beta}}_{\overset{(1.11)}{=}\delta_{\alpha\beta}} P_\alpha^\dagger P_\beta = \sum_\alpha P_\alpha^\dagger P_\alpha.$$

$$\sum_{nm} V_{nm} Q_n Q_m = \sum_{nm} V_{nm} Q_n^\dagger Q_m = \sum_{\alpha\beta} \underbrace{\sum_{nm} U_{\alpha n} V_{nm} \left(U^\dagger\right)_{m\beta}}_{\overset{(1.10)}{=}\delta_{\alpha\beta}\omega_\alpha^2} Q_\alpha^\dagger Q_\beta = \sum_\alpha \omega_\alpha^2 Q_\alpha^\dagger Q_\alpha.$$

The special case we considered earlier, $\kappa_{nm} = \left(\frac{1}{2}(\mathcal{T} + \mathcal{T}^T) - \mathbb{1}\right)_{nm}$, where each mass is only connected to its two neighbors, is special in three ways:

1. First, it is *local* in the sense that only nearby springs couple to each other, so κ_{nm} is only nonzero when n and m are close together.

2. Second, it is *translation invariant*, meaning κ_{nm} does not depend explicitly on n and m. Because of the latter property, the normal modes are plane waves, $U_{kn} = e^{\mathbf{i}kna}/\sqrt{N}$ which has the consequences that $\left(U^\dagger\right)_{kn} = U_{-k,n}$ and hence that $Q_k^\dagger = Q_{-k}$.

3. Finally, it has a certain additional symmetry that also has a right to be called translation invariance from the microscopic point of view. This is the symmetry under $q_n \to q_n + \epsilon$, which shifts each mass by the same amount. This doesn't stretch the springs at all, and so is a symmetry of H. More precisely, this

symmetry arises because the potential depends on q_n only through differences, $V = V(q_n - q_{n-1})$.

Notice that the transformation on the field q_n is non-linear, in the sense that the field shifts under the symmetry (as opposed to a linear transformation like $q \to Rq$). This is related to the fact that the transformation takes one minimum-energy configuration to another; in this sense, the symmetry is said to be *spontaneously broken*. An important general consequence of a non-linearly realized continuous symmetry is the presence of a massless mode, a Goldstone mode. We've already seen that there is such a massless mode in this system. This is an example of Goldstone's theorem. It's a bit mysterious in this example, but will become clearer later.

Notice that when $k = 0, \omega_k = 0$. We are going to have to treat this mode specially; there is a lot of physics in it.

QM. So far the fact that quantumly $[\mathbf{q}_n, \mathbf{p}_{n'}] = \mathbf{i}\hbar\delta_{nn'}\mathbb{1}$ hasn't mattered in our analysis (go back and check). For the Fourier modes, this implies the commutator

$$[\mathbf{q}_k, \mathbf{p}_{k'}] = \sum_{n,n'} \mathbf{U}_{kn}\mathbf{U}_{k'n'}[\mathbf{q}_n, \mathbf{p}'_n] = \mathbf{i}\hbar\mathbb{1}\sum_n \mathbf{U}_{kn}\mathbf{U}_{k'n} = \mathbf{i}\hbar\delta_{k,-k'}\mathbb{1}. \tag{1.12}$$

where $\mathbf{U}_{kn} = \frac{1}{\sqrt{N}}e^{\mathbf{i}kx_n}$ is again the $N \times N$ unitary matrix realizing the discrete Fourier kernel.

Actually, the Hamiltonian in terms of the normal modes (1.7) is not quite fully diagonalized – it still mixes modes with $+k$ and $-k$. To make the final step to decouple the modes with k and $-k$, introduce the annihilation and creation operators

$$\textbf{For } k \neq 0\textbf{:} \qquad \mathbf{q}_k = \sqrt{\frac{\hbar}{2m\omega_k}}\left(\mathbf{a}_k + \mathbf{a}^\dagger_{-k}\right), \quad \mathbf{p}_k = \frac{1}{\mathbf{i}}\sqrt{\frac{\hbar m\omega_k}{2}}\left(\mathbf{a}_k - \mathbf{a}^\dagger_{-k}\right).$$

To preserve (1.12), they must satisfy

$$[\mathbf{a}_k, \mathbf{a}^\dagger_{k'}] = \delta_{kk'}\mathbb{1}.$$

In terms of these, the hamiltonian is

$$\mathbf{H}_0 = \sum_k \hbar\omega_k\left(\mathbf{a}^\dagger_k\mathbf{a}_k + \frac{1}{2}\right) \quad + \frac{p_0^2}{2m}$$

– it is a sum of decoupled oscillators labelled by k, and a free particle describing the center-of-mass.

Phonons. The groundstate is

$$|0\rangle \equiv |0\rangle_{\rm osc} \otimes |p_0 = 0\rangle\,, \qquad \text{where} \quad \mathbf{a}_k\,|0\rangle_{\rm osc} = 0,\ \forall\ k, \text{and}\ \mathbf{p}_0\,|p_0\rangle = p_0\,|p_0\rangle\ .$$

The lowest excitation above the ground state is of the form

$$\mathbf{a}_k^\dagger\,|0\rangle \equiv |\text{one phonon with momentum } \hbar k\rangle\,.$$

It has energy $\hbar\omega_k$ above the groundstate. (This is an eigenstate because $[N_k, \mathbf{a}_k^\dagger] = \mathbf{a}_k^\dagger$, where $N_k = \mathbf{a}_k^\dagger \mathbf{a}_k$.) The excitation is called a *phonon* with momentum $\hbar k$. This is what in single-particle quantum mechanics we would have called "$|k\rangle$" – a state of a single particle in a momentum eigenstate; we can make a state with one phonon in a position eigenstate by taking superpositions:

$$|\text{one phonon at position } x\rangle = \sum_k e^{\mathbf{i}kx}\,|\text{one phonon with momentum } \hbar k\rangle = \sum_k e^{\mathbf{i}kx}\mathbf{a}_k^\dagger\,|0\rangle\,.$$

This is the state that in single-particle QM we would have called "$|x\rangle$".

The number operator (for the SHO with label k) $\mathbf{N}_k \equiv \mathbf{a}_k^\dagger \mathbf{a}_k$ counts the number of phonons with momentum k. The ground state is the state with no phonons – for this reason, we could also call it the 'vacuum'. We can make a state with two phonons:

$$|k, k'\rangle = \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger\,|0\rangle$$

whose energy above the groundstate is

$$E - E_0 = \omega_k + \omega_{k'}. \tag{1.13}$$

Notice that since $[\mathbf{a}_k, \mathbf{a}_{k'}] = 0$ for $k \neq k'$, we have $|k, k'\rangle = |k', k\rangle$ – only the collection of occupied modes matters, there is no way to specify which particle is in which mode.

So this construction allows us to describe situations where the number of particles $\mathbf{N} = \sum_k \mathbf{N}_k$ can vary! That is, we can now describe dynamical processes in which the number of particles change. This is a huge departure from the description of quantum mechanics where the hilbert space of two particles is a tensor product of the hilbert space of each. How can we act with an operator which enlarges the hilbert space?? We just figured out how to do it.

We can specify basis states for this Hilbert space

$$\frac{\left(\mathbf{a}_{k_1}^\dagger\right)^{n_{k_1}}}{\sqrt{(n_1)!}}\frac{\left(\mathbf{a}_{k_2}^\dagger\right)^{n_{k_2}}}{\sqrt{(n_2)!}}\cdots|0\rangle = |\{n_{k_1}, n_{k_2}, ...\}\rangle$$

by a collection of *occupation numbers* n_k, eigenvalues of the number operator for each normal mode. The energy of this state above the groundstate is $\sum_k \hbar\omega_k$, simply the sum of the phonon energies. There are no interactions between them.

Notice that in this description it is manifest that phonons have no identity. We only keep track of how many of them there are and what is their momentum. They cannot be distinguished. Also notice that we can have as many as we want in the same mode – n_k can be any non-negative integer. Phonons are an example of *bosons*.

It is worth putting together the final relation between the 'position operator' and the phonon annihilation and creation operators:

$$\mathbf{q}_n = \sqrt{\frac{\hbar}{2Nm}} \sum_k \frac{1}{\sqrt{\omega_k}} \left(e^{\mathbf{i}kx} \mathbf{a}_k + e^{-\mathbf{i}kx} \mathbf{a}_k^\dagger \right) + \frac{1}{\sqrt{N}} \mathbf{q}_0 \tag{1.14}$$

and the corresponding relation for its canonical conjugate momentum

$$\mathbf{p}_n = \frac{1}{\mathbf{i}} \sqrt{\frac{\hbar m}{2N}} \sum_k \sqrt{\omega_k} \left(e^{\mathbf{i}kx} \mathbf{a}_k - e^{-\mathbf{i}kx} \mathbf{a}_k^\dagger \right) + \frac{1}{\sqrt{N}} \mathbf{p}_0 .$$

The items in red are the ways in which p and q differ; they can all be understood from the relation $p = m\dot{q}$. To see this, use the Heisenberg equations of motion, $\dot{\mathbf{q}}_n = \mathbf{i}[\mathbf{H}, \mathbf{q}_n]$.

Gaplessness. The state $\mathbf{a}_k^\dagger |0\rangle$ has energy $\hbar\omega_k$ above the groundstate. In a box of size $L = Na$, the smallest energy phonon excitation has $k_1 = \frac{2\pi}{L}$ and energy

$$\Delta E = \hbar\omega_{k_1} \sim \frac{1}{L} \overset{L\to\infty}{\to} 0 \ . \tag{1.15}$$

(Note that here I am taking $L \to \infty$ to implement the thermodynamic limit of infinitely many degrees of freedom; the lattice spacing can remain finite for this purpose – it is not a continuum limit.) So this system is *gapless* in the sense that the gap between the first excited state and the groundstate goes to zero in the thermodynamic limit $L \to \infty$. Gaplessness of a many-body system is something that requires explanation. It isn't even possible for a system with finitely many degrees of freedom.

Why does it happen here? Goldstone[2]: the system has a symmetry under $q_n \to q_n + \epsilon$ for all n. If everyone moves to the left three feet, none of the springs are stretched. This is the dance enacted by the $k = 0$ mode. If *nearly* everyone moves *nearly* three feet to the left, the springs will only be stretched a little; hence the modes with small k have small ω. Hence, in the thermodynamic limit where k can be arbitrarily small, the energy gap ΔE goes to zero.

[2] I should probably give an account of Goldstone's theorem here. The relevant statement for our purposes is: if the groundstate is not invariant under a symmetry of $\mathbf{H}$, then it forms a multiplet of that symmetry. Moreover, if the groundstate is not invariant under a continuous symmetry of $\mathbf{H}$, then the spectrum is gapless.

Tower of States: Now I will say a few words about the zeromode, which is horribly mistreated in most textbook discussions of this system that I've seen. There is no potential at all for this mode – it drops out of the $(q_n - q_{n+1})^2$ terms. It just has a kinetic term, which we can think of as the center-of-mass energy of the system. How much energy does it cost to excite this mode? Notice that if everyone moves to the left by a, the system comes back to itself (I am assuming that the masses are themselves indistinguishable particles): $|\{q_n\}\rangle \equiv |\{q_n + a\}\rangle$ are the same state. In terms of the $k = 0$ mode, this is

$$q_0 = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} q_n e^{-\mathbf{i}0x_n} \equiv \frac{1}{\sqrt{N}} \left(\sum_{n=1}^{N} q_n + Na \right), \quad i.e.\ q_0 \equiv q_0 + \sqrt{N}a.$$

This means that the wavefunction for the zeromode must satisfy

$$e^{\mathbf{i}p_0 q_0} = e^{\mathbf{i}p_0(q_0+\sqrt{N}a)} \implies p_0 \in \frac{2\pi\mathbb{Z}}{\sqrt{N}a}$$

and the first excited state has energy

$$\frac{p_0^2}{2m}|_{p_0=\frac{2\pi}{\sqrt{N}a}} = \frac{1}{2}\frac{1}{Nm}\left(\frac{2\pi}{a}\right)^2.$$

This is a victory at least in the sense that we expect the center of mass of the system to have an intertial mass Nm. Notice that the spacing of these states depends differently on the parameters than that of the ones from the nonzero-k phonon states.

But actually this phenomenon is ubiquitous: it happens whenever we take a system that breaks a continous symmetry (here: a solid breaks continuous translation invariance)[3] and put it in finite volume, *i.e.* depart from the thermodynamic limit. In particular, in finite volume the zeromode associated with a conserved quantity (here the momentum) produces a *tower of states* with a different level-spacing (as a function

[3]The fine print:

1. Actually it's important that the order parameter doesn't commute with the Hamiltonian; the exception is ferromagnets, where the order parameter is the total spin itself, which is a conserved quantity and therefore can be nonzero even in finite volume. So the tower is collapsed at zero in that case.

2. Actually, a one-dimensional mattress of oscillators will not spontaneously break continuous translation symmetry even in infinite volume. This is a consequence of the Hohenberg-Coleman-Mermin-Wagner theorem: the positions of the atoms still fluctuate too much, even when there are infinitely many of them in a row; more than one dimension is required to have the crystal really sit still. You'll see the effects of these fluctuations on the problem set when you study the Debye-Waller factors. This does not vitiate our conclusions above at all.

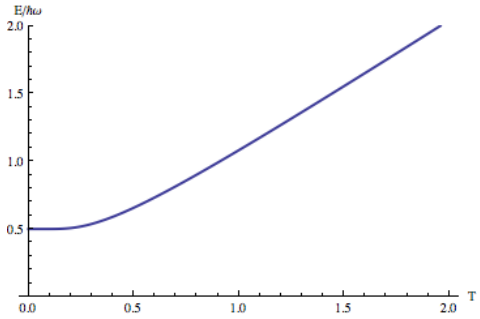
of system size $L = Na$) than the particle excitations (1.15). (It is sometimes called the *Anderson Tower of States* in the study of magnetism or the *Rotator spectrum* in lattice gauge theory). In this case, both towers go like $1/N$, but this is a coincidence. In other cases the tower from the zeromode is more closely spaced (it goes like $\frac{1}{\text{volume}} \sim \frac{1}{L^d} \sim \frac{1}{N}$) than the particle momentum tower (which goes like $\frac{1}{L} \sim \frac{1}{N^{1/d}}$ (or maybe $\frac{1}{L^2}$)), so the tower of states from the zeromode is usually much closer together, and in the thermodynamic limit $L \to \infty$, they combine to form the degenerate vacua associated with spontaneous symmetry breaking. [4]

So you see that we have constructed an approximation to the Fock space of bosonic particles from a system with finitely many degrees of freedom per unit volume (here, length), and in fact finitely many degrees of freedom altogether, since we kept the IR regulator L finite. It is worth pausing to appreciate this: we've been forced to discover a framework for quantum systems in which particles can be created and annihilated, very different from the old-fashioned point of view where we have a fixed Hilbert space for each particle.

Now for some experimental verification of all this hard work:

Heat capacity of (insulating) solids: phonons are real. The simplest demonstration that phonons are real is the dramatic decrease at low temperatures of the heat capacity of insulating solids. At high temperatures, the equipartition theorem of classical thermodynamics correctly predicts that the energy of the solid from the lattice vibrations should be T times the number of atoms, so the pacity, $C_V = \partial_T E$ should be independent of T. At low temperatures $T < \Theta_D$, this is wrong. Θ_D is the temperature scale associated with the frequencies of the lattice vibrations (say the maximum of the curve ω_k above).

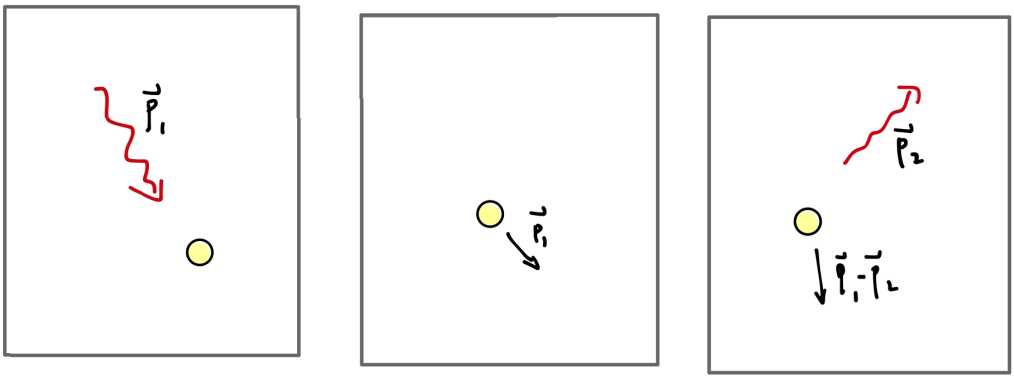
The resolution lies in the thermal energy of a quantum harmonic oscillator which you'll remind yourself of in a homework problem: for $T < \omega$, the energy goes to a constant $\frac{1}{2}\hbar\omega$, so the heat capacity (the slope of this curve) goes to zero as $T \to 0$.



The Mössbauer effect: phonons are real. A nice example where we can see the importance of the tower of states and of the quantization of phonon number is the Mössbauer effect: when scattering high-energy photons off a solid, there is a finite

[4] The definitive discussion of this subject can be found in the last few pages of P. Anderson, *Concepts in Solids*.

amplitude for scattering events which produce *zero* phonons. This means that all the momentum transfer goes to the center of mass mode, which has negligible recoil as $N \to \infty$, since its inertial mass is Nm. This allows for very sharp absorption lines, which if the atom were in free space would be washed out (*i.e.* broadened to a width $E_{\rm recoil} = \frac{(p_\gamma)^2}{2m}$.) by the random recoils of the individual atoms (as depicted in the comic strip below).

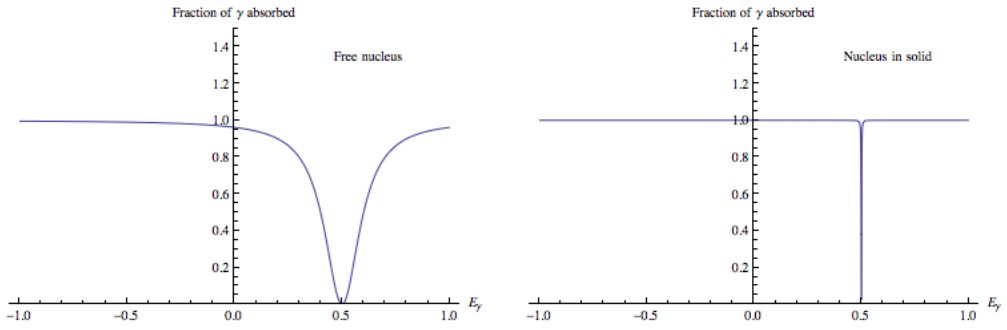


The nuclei of the atoms in a solid have various energy levels; when hit with a γ-ray photon, these nuclei can experience transitions from the groundstate to some excited energy level. If an excited nucleus somewhere in the lattice gets hit by a very energetic photon (a γ-ray) of some very specific energy $E_\gamma = \Delta E \equiv E_{\rm excited} - E_0$, the nucleus can absorb and re-emit that photon. The resulting sharp resonant absorption lines at $E_\gamma = \Delta E$ are indeed observed.

This sounds simple, but here is a mystery about this: Consider a nucleus alone in space in the excited state, after it gets hit by a photon. The photon carried a momentum $p_\gamma = E_\gamma/c$. Momentum is conserved, and it must be made up by some *recoil* of the absorbing nucleus. When it emits a photon again, it needn't do so in the same direction. This means that the nucleus remains in motion with momentum $\Delta\vec{p} = \vec{p}_1 - \vec{p}_2$. But if some of its energy $\Delta E = E_{\rm excited} - E_0$ goes to kinetic energy of recoil, not all of that energy can go to the final photon, and the emitted photon energy will be *less* than E_γ by $E_{\rm recoil} = \frac{\Delta p^2}{2M}$. This can be as big as $E^{\rm max}_{\rm recoil} = \frac{(2\vec{p})^2}{2M} = \frac{(2E\gamma/c)^2}{2M}$ (in the case of scattering by angle π). So instead of a sharp absorption line, it seems that we should see a broad bump of width $\frac{(E\gamma/c)^2}{M}$. But we *do* see a sharp line!

The solution of the puzzle is phonons: for a nucleus in a lattice, its recoil means that the springs are stretched – it must excite a lattice vibration, it must create some phonons. But there is a nonzero probability for it to create *zero* phonons. In this case, the momentum conservation is made up by an acceleration of *the whole solid*, which is very massive, and therefore does not recoil very much at all (it loses only energy $\frac{p_\gamma^2}{2NM}$).

This allows for very sharp resonance lines. In turn, this effect has allowed for some very high-precision measurements.



The different widths in these cartoon absorption spectra don't do justice to the relative factor of N.

[End of Lecture 2]

An essentially similar effect makes it possible to get precise peaks from scattering of X-rays off of a solid (Bragg scattering) – there is a finite amplitude for the scattering to occur without exciting any phonons.

This is actually a remarkable thing: although solids seem ordinary to us because we encounter them frequently, the rigidity of solids is a quantum mechanical emergent phenomenon. You can *elastically* scatter photons off of a solid only because the atoms making up the solid participate in this collective behavior wherein the whole solid acts like a single quantum object!

Here is a sketch of the quantitative calculation of the probability of a nucleus at x_n emitting or absorbing a γ-ray photon without creating any phonons. Recall from your discussion of time-dependent perturbation theory that the transition probability is

$$W(N_i, L_i \to N_f, L_f) \propto |\langle f| \mathbf{H}_{\text{int}} |i\rangle|^2,$$

where $N_{i,f}$ and $L_{i,f}$ are initial and final states of the nucleus and lattice, respectively. $\mathbf{H}_{\text{int}}$ is the perturbing hamiltonian by which the transition can occur. This is Fermi's golden rule. Because the nuclear forces are such high-energy things, we can ignore the density of states of the final states, and we can assume that the transition matrix element factorizes:

$$W(N_i, L_i \to N_f, L_f) \propto |\langle L_f| \mathbf{H}_{\text{L}} |L_i\rangle|^2,$$

where we've factored out some nuclear stuff that we don't care about right now into the $\propto$.

The requirements of translation invariance and Galilean invariance (*i.e.* momentum is conserved, and the transition for a moving observer shouldn't depend on the velocity of the observer) require that

$$\mathbf{H}_{\rm L} = Ae^{\mathbf{i}\vec{K}\cdot\vec{\mathbf{x}}} + \text{h.c.}$$

where $\hbar\vec{K}$ is the momentum of the emitted gamma ray (a c-number), and $\vec{\mathbf{x}}$ is the center-of-mass position of the nucleus in question. [5] But, in the 1d case at least, we have an expression for $\mathbf{x}$ in terms of the phonon creation operators:

$$\mathbf{x}_n = na + \mathbf{q}_n = na + \sum_k \mathcal{N}_k \left(e^{\mathbf{i}kna}\mathbf{a}_k + e^{-\mathbf{i}kna}\mathbf{a}_k^\dagger \right), \tag{1.16}$$

where a is the lattice spacing and $\mathcal{N}_k = \sqrt{\frac{\hbar}{2mN\omega_k}}$.

Now the amplitude for emitting no phonons is the 'vacuum-persistence amplitude', i.e. the amplitude for $|L_i\rangle = |0\rangle$ to stay that way:

$$P_{\text{Mössbauer}} \propto |\langle 0| e^{\mathbf{i}K(na+\mathbf{q}_n)} |0\rangle|^2 .$$

Now it is an exercise in harmonic oscillator physics to get a function out of this. A useful general fact is that for harmonic oscillators (and any gaussian theory)

$$\left\langle e^{\mathbf{i}K\mathbf{q}} \right\rangle = e^{-\frac{1}{2}K^2\langle \mathbf{q}^2\rangle} .$$

Applying this here, and using (1.16),

$$P_{\text{Mössbauer}} \propto e^{-\frac{1}{2}K^2\sum_k \frac{\hbar}{4mN\omega_k}} \overset{d=1}{\sim} e^{-K^2\frac{\hbar}{2m}\frac{a}{v_s}\ln(N)} .$$

Here Na is the system size, so this actually vanishes in the thermodynamic limit; this (IR) divergence is a 1d artifact related to the absence of continuous symmetry-breaking in $d = 1$. In $d > 1$, we would get a finite function of K[6].

[5] It is possible to show that the interactions with the EM field, to be discussed next, I promise, meet these requirements and reproduce this form of the answer. The relevant term is from $\mathbf{H}_{\rm int} = \frac{1}{2m}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) \in \frac{1}{2m}(\mathbf{p}+\mathbf{A})^2$. Then we use the fact that the Maxwell field representing a photon is a wave $\mathbf{A} \propto e^{\mathbf{i}\vec{K}\cdot\vec{\mathbf{x}}}$, evaluated at the position of the nucleus.

[6] To see this, let's think directly about the infinite-volume limit, but keep the lattice spacing finite. Then any divergence we find is an IR divergence. Let's think about a cubic lattice. In this case, the answer for the thing in the exponent of the Debye-Waller factor is proportional to

$$\oint_{\rm BZ} \frac{d^dk}{\omega_k} = \int_{-\pi/a}^{\pi/a} \cdots \int_{-\pi/a}^{\pi/a} \frac{d^dk}{\sqrt{\sum_{\mu=1}^d \sin^2(k_\mu a/2)}} .$$

Near $k = 0$, the integrand behaves like $1/k = \sqrt{\sum_\mu k_\mu^2}$, and $\int_0 \frac{d^dk}{k}$ is finite near the lower limit of integration. At larger $|k|$, of order $1/a$, the integrand looks nothing like this, but is manifestly finite. So the integral away from $k = 0$ is clearly finite, and the integral at $k = 0$ is finite, so the integral is finite. It seems Mathematica cannot do the integral analytically, but NIntegrate gives 50.76 and 225.90 for $d = 2$ and $d = 3$ respectively. So: in infinite volume with finite lattice spacing the answer is finite, and therefore there is no IR divergence.

For future reference, these effects of fluctuations of the lattice on photon scattering are called *Debye-Waller factors*.

Two final comments, to make connections with future excitement in this course:

I've made a big deal about the regulators here. One reason we care about them is if we remove them ($N \to \infty, a \to 0$) and ask bad questions, we'll get infinity. For example, we could think about the vacuum energy $E_0 = \frac{1}{2}\sum_k \hbar\omega_k$. There is physics in there (*e.g.* Casimir forces), to which we'll return.

Notice that since $\omega_k \propto \sin|k|a/2$, there are some energies where there aren't any phonon states. In particular, the function (1.8) has a maximum. More generally, in a system with discrete translation invariance, there are *bands* of allowed energies.

Interactions. Many aspects of the above discussion are special to the fact that our hamiltonian was quadratic in the operators. Certainly our ability to completely solve the system is. Notice that the number of phonons *of each momentum* $\mathbf{N}_k \equiv \mathbf{a}_k^\dagger \mathbf{a}_k$ is conserved for each k. But if we add generic cubic and quartic terms in $\mathbf{q}$ (or if we couple our atoms to the photon field) even the total number of phonons $\sum_k \mathbf{N}_k$ will no longer be a conserved quantity[7]. So a description of such particles which forced us to fix their number wouldn't be so great.

For example, think about expanding a general cubic term $\sum_{nml} \lambda_{nml} q_n q_m q_l$ in oscillators. It has terms like

$$a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}^\dagger, \quad a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}, \quad a_{k_1}^\dagger a_{k_2} a_{k_3}, \quad a_{k_1} a_{k_2} a_{k_3}$$

all of which change the number of phonons. A quartic terms will also contain terms like $a^\dagger a^\dagger a a$ which preserve the number of phonons, but describe an interaction between them, where they exchange momentum.

1.4 Scalar field theory

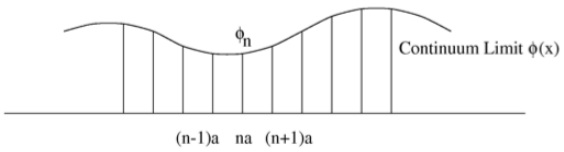
Above, we have stumbled upon an example of a *quantum field theory* (so far, a scalar field in one spatial dimension). Let me explain in terms of the action.

The action for our collection of oscillators is

$$S[q] = \int dt \left(\sum_n \frac{1}{2} m_n \dot{q}_n^2 - V(\{q\}) \right)$$

with $V(\{q\}) = \sum_n \frac{1}{2}\kappa \left(q_{n+1} - q_n\right)^2$. Now let's try to take the continuum limit $a \to 0, N \to \infty$ (here N is the number of points in space).

Basically the only thing we need is to think of $q_n = q(x = na)$ as defining a smooth function, as in the figure at right. [Note that the continuum field is often called $\phi(x)$ instead of $q(x)$ for some reason. At least the letters $q(x)$ and $\phi(x)$ look similar.]



[7] Note that it *is* possible to make a non-quadratic action for conserved particles, but this requires adding more degrees of freedom – the required $\mathsf{U}(1)$ symmetry must act something like

$$(q^1, q^2) \to (\cos\theta q^1, \sin\theta q^2).$$

We can reorganize this as a complex field $\Phi = q^1 + \mathbf{i} q^2$ on which the symmetry acts by $\Phi \to e^{\mathbf{i}\theta}\Phi$.

We now have

$$(q_n - q_{n-1})^2 \simeq a^2 (\partial_x q)^2 |_{x=na}$$

Now the action becomes:

$$S[q] = \int dt \int dx \frac{1}{2} \left(\mu (\partial_t q)^2 - \mu v_s^2 (\partial_x q)^2 - r q^2 - u q^4 - ... \right) \equiv \int dt \int dx \mathcal{L} \quad (1.17)$$

where I've introduced some parameters μ, v_s, r, u determined from $m, \kappa ...$ in some ways that we needn't worry about. $\mathcal{L}$ is the Lagrangian *density* whose integral over space is the Lagrangian $L = \int dx \mathcal{L}$.

The equation of motion is

$$0 = \frac{\delta S}{\delta q(x,t)} = -\mu \ddot{q} - \mu v_s^2 \partial_x^2 q - r q - 2 u q^3 - ...$$

From the phonon problem, we automatically found $r = u = 0$, and the equation of motion is just the wave equation (1.9). This happened because of the symmetry $q_n \to q_n + \epsilon$. This is the operation that *translates* the whole crystal, It guarantees low-energy phonons near $k = 0$ because it means $q(x)$ can only appear in S via its derivatives.

The following will be quite useful for our subsequent discussion of quantum light. Notice that we can construct a hamiltonian from this action by defining a canonical field-momentum $\pi(x) = \frac{\partial \mathcal{L}}{\partial_t q} = \mu \partial_t q$ and doing the Legendre transformation:

$$H = \sum_n (p_n \dot{q}_n - L_n) = \int dx (\pi(x) \dot{q}(x) - \mathcal{L}) = \int dx \left(\frac{\pi(x)^2}{2\mu} + \mu v_s^2 (\partial_x q(x))^2 + r q^2 + u q^4 + ... \right) . \quad (1.18)$$

(Note that I suppress the dependence of all the fields on t just so it doesn't get ugly, not because it isn't there.)

If we were feeling fancy, we could now talk more about the *field operator*

$$\mathbf{q}(x) = \sqrt{\frac{\hbar}{2\mu L}} \sum_k \frac{1}{\sqrt{\omega_k}} \left(e^{\mathbf{i} k x} \mathbf{a}_k + e^{-\mathbf{i} k x} \mathbf{a}_k^\dagger \right)$$

and its canonical conjugate momentum

$$\boldsymbol{\pi}(x) = \frac{1}{\mathbf{i}} \sqrt{\frac{\hbar \mu}{2L}} \sum_k \sqrt{\omega_k} \left(e^{\mathbf{i} k x} \mathbf{a}_k - e^{-\mathbf{i} k x} \mathbf{a}_k^\dagger \right) .$$

($\boldsymbol{\pi}(x)$ is the quantum operator associated with the field-momentum π above.) Notice that the position along the chain x here is just a *label* on the fields, not a quantum

operator. The point of the mode operators $\mathbf{a}$ is that in terms of them, the Hamiltonian is a sum of independent terms

$$\mathbf{H} = \sum_k \hbar\omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \frac{1}{2} \right).$$

The field q is called a *scalar field* because it doesn't have any indices decorating it. This is to be distinguished from the Maxwell field, which is a vector field, and which is our next subject. (Note that vibrations of a crystal in three dimensions actually do involve vector indices. We will omit this complication from our discussion.)

The lattice spacing a and the size of the box Na in the discussion above are playing very specific roles in *regularizing* our 1-dimensional scalar field theory. The lattice spacing a implies a maximum wavenumber or shortest wavelength and so is called an "ultraviolet (UV) cutoff", because the UV is the short-wavelength end of the visible light spectrum. The size of the box Na implies a maximum wavelength mode which fits in the box and so is called an "infrared (IR) cutoff".

There is one annoying thing I should mention about the infinite-volume limit. In that limit, the wavenumbers become continuous, and the $\sum_k$ wants to become an integral. The correct replacement is $\frac{1}{L}\sum_k \overset{L\to\infty}{\rightsquigarrow} \int đk \equiv \int \frac{dk}{2\pi}$. Note that the units work out. We will also want to replace the Kronecker delta in $[\mathbf{a}_k, \mathbf{a}_{k'}^\dagger] = \delta_{k,k'} \overset{L\to\infty}{\rightsquigarrow} 2\pi\delta(k-k')$ with a Dirac delta function. Here the units don't work. This last step requires a change in normalization of the $\mathbf{a}_k$s by a factor of $\sqrt{L}$.

Continuum (free) scalar field theory in $d+1$ dimensions

Notice that these continuum expressions are easy to generalize to scalar field theory in any number of dimensions: The action is

$$S[\phi] = \int dt d^d x \left(\frac{1}{2}\mu\dot{\phi}^2 - \frac{1}{2}\mu v_s^2 \vec{\nabla}\phi \cdot \vec{\nabla}\phi - V(\phi) \right)$$

and the Hamiltonian is

$$\mathbf{H} = \int d^d x \left(\frac{\boldsymbol{\pi}(x)^2}{2\mu} + \frac{1}{2}\mu v_s^2 \left(\vec{\nabla}\boldsymbol{\phi} \cdot \vec{\nabla}\boldsymbol{\phi} \right) + V(\phi) \right)$$

with $\pi = \mu\dot{q}$. Again, think of $q_n(t) \equiv \boldsymbol{\phi}(x_n, t), p_n(t) \equiv \boldsymbol{\pi}(x_n, t)$ as defining the fields via their values at the grid points. The equations of motion are

$$0 = \frac{\delta S}{\delta\phi(t,\vec{x})} = -\mu\ddot{\phi} + \mu v_s^2 \nabla^2\phi + \frac{\partial V}{\partial\phi}.$$

Let's think about the special case where $V(\phi) = \frac{1}{2}m^2\phi^2$, so the model is gaussian, and the equation of motion is linear in ϕ. A translation invariant linear problem is

solved by Fourier transforms: $\boldsymbol{\phi}(x) = \frac{1}{\sqrt{L^d}} \sum_k e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \boldsymbol{\phi}_k, \boldsymbol{\pi}(x) = \frac{1}{\sqrt{L^d}} \sum_k e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \boldsymbol{\pi}_k$, this is

$$\mathbf{H} = \sum_k \left(\frac{1}{2\mu} \boldsymbol{\pi}_k \boldsymbol{\pi}_{-k} + \frac{1}{2} \left(\mu v_s^2 k^2 + m^2 \right) \boldsymbol{\phi}_k \boldsymbol{\phi}_{-k} \right)$$

where $k^2 = (-\mathbf{i}\vec{k}) \cdot (\mathbf{i}\vec{k}) = \vec{k} \cdot \vec{k}$. Using

$$\boldsymbol{\phi}_k \equiv \sqrt{\frac{\hbar}{2\mu V \omega_k}} \left(\mathbf{a}_k + \mathbf{a}_{-k}^\dagger \right), \boldsymbol{\pi}_k \equiv \frac{1}{\mathbf{i}} \sqrt{\frac{\hbar \mu \omega_k}{2V}} \left(\mathbf{a}_k - \mathbf{a}_{-k}^\dagger \right),$$

this is

$$\mathbf{H} = \sum_k \hbar \omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \frac{1}{2} \right)$$

where

$$\omega_k^2 = v_s^2 k^2 + m^2.$$

The field operators

$$\boldsymbol{\phi}(x) = \sum_k \sqrt{\frac{\hbar}{2\mu N \omega_k}} \left(e^{\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k + e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k^\dagger \right),$$
$$\boldsymbol{\pi}(x) = \frac{1}{\mathbf{i}} \sum_k \sqrt{\frac{\hbar \mu \omega_k}{2N}} \left(e^{\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k - e^{-\mathbf{i}\vec{k}\cdot\vec{x}} \mathbf{a}_k^\dagger \right),$$

satisfy the canonical commutation relation

$$[\boldsymbol{\phi}(\vec{x}), \boldsymbol{\pi}(\vec{x}')] = \mathbf{i}\hbar \mathbb{1} \delta^d(\vec{x} - \vec{x}').$$

This is morally the same equation as our starting point for each ball on springs:

$$[\mathbf{q}_n, \mathbf{p}_{n'}] = \mathbf{i}\hbar \mathbb{1} \delta_{nn'}.$$

[End of Lecture 3]

1.5 Quantum light: Photons

The quantization of the Maxwell field is logically very similar to the preceding discussion. There are just a few complications from its several polarizations, and from the fact that quantum mechanics means that the vector potential is real and necessary (whereas classically it is just a convenience).

Maxwell's equations are :

$$\vec{\nabla} \cdot \vec{B} = 0, \quad \vec{\nabla} \times \vec{E} = -\partial_t \vec{B}, \tag{1.19}$$

$$\vec{\nabla} \cdot \vec{E} = \rho/\varepsilon_0, \quad c^2 \vec{\nabla} \times \vec{B} = \partial_t \vec{E} + \vec{j}/\varepsilon_0. \tag{1.20}$$

The first two equations (1.19) are constraints on $\vec{E}$ and $\vec{B}$ which mean that their components are not independent. This is annoying for trying to treat them quantumly. To get around this we introduce *potentials* which determine the fields by taking derivatives and which automatically solve the constraints (1.19):

$$\vec{E} = -\vec{\nabla}\Phi - \partial_t \vec{A}, \quad \vec{B} = \vec{\nabla} \times \vec{A}.$$

Potentials related by a *gauge transformation*

$$\vec{A} \to \vec{A}^\lambda = \vec{A} - \vec{\nabla}\lambda, \quad \Phi \to \Phi^\lambda = \Phi + \partial_t \lambda$$

for any function $\lambda(\vec{r}, t)$, give the same $\vec{E}, \vec{B}$. The Bohm-Aharonov effect (below?) is proof that (some of the information in) the potential is real and useful, despite this redundancy. We can partially remove this redundancy be choosing our potentials to satisfy *Coulomb gauge*

$$\vec{\nabla} \cdot \vec{A} = 0 \ .$$

In the absence of sources $\rho = 0 = \vec{j}$, we can also set $\Phi = 0$. In this gauge, Ampere's law becomes

$$c^2 \vec{\nabla} \times \left(\vec{\nabla} \times \vec{A} \right) = c^2 \vec{\nabla} \cdot \left(\vec{\nabla} \cdot \vec{A} \right) - c^2 \nabla^2 \vec{A} = -\partial_t^2 \vec{A} \quad i.e. \ \boxed{\partial_t^2 \vec{A} - c^2 \nabla^2 \vec{A} = 0}.$$

This wave equation is different from our scalar wave equation (1.9) in three ways:

- we're in three spatial dimensions,
- the speed of sound v_s has been replaced by the speed of light c,
- the field $\vec{A}$ is a vector field obeying the constraint $\vec{\nabla} \cdot \vec{A} = 0$. In fourier space $\vec{A}(x) = \sum_k e^{i\vec{k}\cdot\vec{x}} \vec{A}(k)$ this condition is

$$0 = \vec{k} \cdot \vec{A}(k)$$

  – the vector field is *transverse*.

Recall that the energy density of a configuration of Maxwell fields is $u = \frac{\epsilon_0}{2}\left(\vec{E}^2 + c^2\vec{B}^2\right)$. So the quantum Hamlitonian is

$$\mathbf{H} = \frac{\varepsilon_0}{2}\int d^3r\left(\vec{E}^2 + c^2\vec{B}^2\right) = \frac{\varepsilon_0}{2}\int d^3r\left(\left(\partial_t\vec{A}\right)^2 + \left(\vec{\nabla}\times\vec{A}\right)^2\right) \quad . \tag{1.21}$$

Here $\vec{E} = -\partial_t\vec{A}$ plays the role of field momentum $\pi(x)$ in (1.18), and $\vec{B} = \vec{\nabla}\times\vec{A}$ plays the role of the spatial derivative $\partial_x q$. We immediately see that we can quantize this system just like for the scalar case (by analogy, replacing $L \to L^3, \mu \to \epsilon_0$) by expanding the quantum Maxwell field in terms of independent creation and annihilation operators:

$$\vec{\mathbf{A}}(\vec{r}) = \sum_{\vec{k}}\sum_{s=1,2}\sqrt{\frac{\hbar}{2\epsilon_0\omega_k L^3}}\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}} + \mathbf{a}^\dagger_{\vec{k},s}\vec{e}^\star_s(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}}\right) \quad .$$

We're going to need to know how this evolves in time (for example, because we'll need to construct $\vec{\mathbf{E}} = -\partial_t\vec{\mathbf{A}}$). One way to do this is to solve the Heisenberg evolution equation $\partial_t\vec{\mathbf{A}} = \frac{\mathbf{i}}{\hbar}[\mathbf{H}, \vec{\mathbf{A}}]$ (using the fact that $\mathbf{H}$ is time-independent) to write $\vec{\mathbf{A}}(\vec{r},t) = e^{-\mathbf{i}\mathbf{H}t/\hbar}\vec{\mathbf{A}}(\vec{r})e^{\mathbf{i}\mathbf{H}t/\hbar}$. Alternatively, we can just write the general positive-energy, transverse solution of the Maxwell equation (two polarizations for each $\vec{k}$), as a superposition of each such solution $e^{\mathbf{i}\vec{k}\cdot\vec{r}-\mathbf{i}\omega_k t}\vec{e}_s(\hat{k})$ (where $\hat{k}\cdot\vec{e}_s = 0$ guarantees transverseness and $\omega_k^2 = c^2k^2$ solves the Maxwell equations for $\vec{A}$); then replace the constant coefficient in front of each solution with its own annihilation operator, $\mathbf{a}_{\vec{k},s}$ satisfying

$$[\mathbf{a}_{ks}, \mathbf{a}^\dagger_{k's}] = \delta_{kk'}\delta_{ss'}. \tag{1.22}$$

The result is

$$\vec{\mathbf{A}}(\vec{r},t) = \sum_{\vec{k}}\sum_{s=1,2}\sqrt{\frac{\hbar}{2\epsilon_0\omega_k L^3}}\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}-\mathbf{i}\omega_k t} + \mathbf{a}^\dagger_{\vec{k},s}\vec{e}^\star_s(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}+\mathbf{i}\omega_k t}\right) \quad .$$

The field momentum is (up to a factor of ε_0) $\vec{\mathbf{E}} = -\partial_t\vec{A}$:

$$\vec{\mathbf{E}}(\vec{r},t) = \mathbf{i}\sum_{\vec{k}}\sum_{s=1,2}\sqrt{\frac{\hbar\omega_k}{2\epsilon_0 L^3}}\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}-\mathbf{i}\omega_k t} - \mathbf{a}^\dagger_{\vec{k},s}\vec{e}^\star_s(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}+\mathbf{i}\omega_k t}\right)$$

[8] Also, the magnetic field operator is

$$\vec{\mathbf{B}} = \vec{\nabla}\times\vec{\mathbf{A}} = \sum_{\vec{k}}\sum_{s}\sqrt{\frac{\hbar}{2\epsilon_0\omega_k L^3}}\mathbf{i}\vec{k}\times\left(\mathbf{a}_{\vec{k},s}\vec{e}_s(\hat{k})e^{\mathbf{i}\vec{k}\cdot\vec{r}-\mathbf{i}\omega_k t} - \mathbf{a}^\dagger_{\vec{k},s}\vec{e}^\star_s(\hat{k})e^{-\mathbf{i}\vec{k}\cdot\vec{r}+\mathbf{i}\omega_k t}\right)$$

[8] I should say a bit more about the *polarization vectors*, $\vec{e}_s$. They conspire to make it so that there are only two independent states for each $\vec{k}$ and they are transverse $\vec{k}\cdot\vec{e}_s(\hat{k}) = 0$, so $s = 1, 2$. The polarization vectors for a given k can be chosen to satisfy a completeness relation:

$$\sum_s e_{si}(\hat{k})e^\star_{sj}(\hat{k}) = \delta_{ij} - \hat{k}_i\hat{k}_j \ . \tag{1.23}$$

This says that they span the plane perpendicular to $\hat{k}$.

where I've highlighted in red the places where these expressions differ from that for $\vec{\mathbf{A}}$.

It seems like the canonical commutator should generalize according to

$$[\phi(x), \pi(x')] = \mathbf{i}\hbar\delta(x-x') \qquad \overset{?}{\rightsquigarrow} \qquad [\mathbf{A}_i(\vec{r}), \mathbf{E}_j(\vec{r}')] \overset{?}{=} -\mathbf{i}\hbar\delta^3(\vec{r}-\vec{r}')\delta_{ij}/\varepsilon_0$$

where $i, j = 1..3$ are spatial indices. This is not quite true. If we plug in the expressions above and use (1.22) and (1.23) we find instead

$$[\mathbf{A}_i(\vec{r}), \mathbf{E}_j(\vec{r}')] = -\mathbf{i}\hbar \int \text{đ}^3k \; e^{\mathbf{i}\vec{k}\cdot(\vec{r}-\vec{r}')} \left(\delta_{ij} - \hat{k}_i\hat{k}_j\right)/\varepsilon_0$$

As a check, note that using this Hamiltonian and the canonical commutator, we can reproduce Maxwell's equations:

$$\partial_t^2 \vec{A} = -\partial_t \vec{E} = -\frac{\mathbf{i}}{\hbar}[\mathbf{H}, \vec{E}] = c^2\vec{\nabla}^2\vec{A}.$$

The last step is a bit nontrivial (see the homework).

Plugging these expressions into the Hamiltonian (1.21), we can write it in terms of these oscillator modes (which create and annihilate *photons*). As for the scalar field, the definitions of these modes were designed to make this simple: It is:

$$\mathbf{H} = \sum_{\vec{k},s} \hbar\omega_k \left(\mathbf{a}^\dagger_{\vec{k},s}\mathbf{a}_{\vec{k},s} + \frac{1}{2}\right).$$

The groundstate is the vacuum $|0\rangle$ annihilated by all the annihilation operators $\mathbf{a}_{ks}|0\rangle = 0$. Notice that the vacuum energy is

$$E_0 \equiv \langle 0|\,\mathbf{H}\,|0\rangle = \frac{1}{2}\sum_{\vec{k},s}\hbar\omega_k = \frac{1}{2}L^3\int \text{đ}^3k\hbar ck. \tag{1.24}$$

The fact that in the continuum $\sum_k$ is no longer a finite sum might be something to worry about. We will see below in §1.6 that this vacuum energy has physical consequences.

The first excited states have the form

$$\mathbf{a}^\dagger_{k,s}|0\rangle$$

and represent a single *photon* of momentum k in the polarization state s. Note that the polarization represents a double-degeneracy of each k-state. We can make states of two photons $\mathbf{a}^\dagger_{k,s}\mathbf{a}^\dagger_{k',s'}|0\rangle = \mathbf{a}^\dagger_{k',s'}\mathbf{a}^\dagger_{k,s}|0\rangle$. Photons are identical bosons. Again we can make a basis for the full Hilbert space by specifying the occupation numbers of each mode

$$\frac{\left(\mathbf{a}^\dagger_{k_1,s_1}\right)^{n_{k_1}}}{\sqrt{(n_1)!}}\frac{\left(\mathbf{a}^\dagger_{k_2,s_2}\right)^{n_{k_2}}}{\sqrt{(n_2)!}}\cdots|0\rangle = |\{n_{k_1,s_1}, n_{k_2,s_2}, ...\}\rangle \ .$$

Consolidation of understanding

So far in this chapter, we have studied systems of increasing complexity: the simple harmonic oscillator, a scalar field, and the EM field. They all have the same structure, in the following sense.

In the following, Here $\mathrm{Re}\mathbf{A} \equiv \frac{1}{2}\left(\mathbf{A} + \mathbf{A}^\dagger\right)$ as usual. The normalization constant in finite volume V is $\mathcal{N}_k = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega_k V}}$.

$$\mathbf{H}_{SHO} = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}m\omega^2\mathbf{q}^2 = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right)$$

$$[\mathbf{q}, \mathbf{p}] = \mathbf{i}\hbar \implies [\mathbf{a}, \mathbf{a}^\dagger] = \mathbb{1}.$$

$$\mathbf{q} = \mathrm{Re}\mathcal{N}\mathbf{a}, \quad \mathbf{p} = m\mathrm{Im}\omega\mathcal{N}\mathbf{a}.$$

$$\mathbf{H}_{1d\ scalar} = \int dx \left(\frac{1}{2\mu}\boldsymbol{\pi}^2 + \frac{1}{2}\mu c^2\left(\partial_x\boldsymbol{\phi}\right)^2\right) = \sum_k \hbar\omega_k\left(\mathbf{a}_k^\dagger\mathbf{a}_k + \frac{1}{2}\right)$$

$$[\mathbf{a}_k, \mathbf{a}_{k'}^\dagger] = \mathbf{i}\hbar\delta_{kk'} \Leftrightarrow [\boldsymbol{\phi}(x), \boldsymbol{\pi}(x')] = \mathbf{i}\hbar\delta(x - x').$$

$$\boldsymbol{\phi}(x) = \mathrm{Re}\left(\sum_k \mathcal{N}_k e^{\mathbf{i}kx}\mathbf{a}_k\right), \quad \boldsymbol{\pi}(x) = \mu\mathrm{Im}\left(\sum_k \omega_k\mathcal{N}_k e^{\mathbf{i}kx}\mathbf{a}_k\right).$$

$$\mathbf{H}_{EM} = \int d^3x \left(\frac{\epsilon_0}{2}\vec{\mathbf{E}}^2 + \frac{\epsilon_0 c^2}{2}\vec{\mathbf{B}}^2\right) = \sum_{k,s=1,2} \hbar\omega_k\left(\mathbf{a}_{ks}^\dagger\mathbf{a}_{ks} + \frac{1}{2}\right)$$

$$[\mathbf{a}_{ks}, \mathbf{a}_{k's'}^\dagger] = \hbar\delta_{k,k'}\delta_{ss'} \Leftrightarrow [\mathbf{A}_i(x), \mathbf{E}_j(x')] \stackrel{?}{=} \mathbf{i}\hbar\delta^3(x - x')\delta_{ij}.$$

$$\vec{\mathbf{A}}(x) = \mathrm{Re}\left(\sum_k \mathcal{N}_k e^{\mathbf{i}\vec{k}\cdot\vec{x}}\mathbf{a}_{ks}\vec{e}_s(\hat{k})\right), \quad \vec{\mathbf{E}}(x) = \mu\mathrm{Im}\left(\sum_k \omega_k\mathcal{N}_k e^{\mathbf{i}\vec{k}\cdot\vec{x}}\mathbf{a}_{ks}\vec{e}_s(\hat{k})\right).$$

Note that $\vec{\mathbf{E}}$ is the canonical momentum of $\vec{\mathbf{A}}$ since (in Coulomb gauge) $\vec{E} = -\partial_t\vec{A}$. I wrote the not-quite-true form of the commutator of A and E; this agrees with the more correct expression when acting on transverse vectors, like A itself.

Mössbauer more microscopically

As an example where you can see the photon machinery in action, we return to our discussion of the Mössbauer effect. Now we can answer in more detail the question: where did that $\mathbf{H}_{\rm int}$ that we used in the Mössbauer effect come from? This requires information from all of the previous subsections: it involves both phonons and photons. A more microscopic description of the transition rate would include the radiation field, too:

$$W(N_i, L_i, R_i \to N_f, L_f, R_f) \propto |\langle f| \mathbf{H}_{\rm int} |i\rangle|^2,$$

where now $N_{i,f}, L_{i,f}, R_{i,f}$ denote initial and final states of the nucleus (and electrons), lattice and radiation field, respectively. We are working in a big hilbert space $\mathcal{H} = \mathcal{H}_N \otimes \mathcal{H}_L \otimes \mathcal{H}_R$.

Again we ignore the nuclear stuff:

$$W(N_i, L_i, R_i \to N_f, L_f, R_f) \propto |\langle L_f| \otimes \langle R_f| \mathbf{H}_{LR} |L_i\rangle \otimes |R_i\rangle|^2.$$

If the photon gets absorbed, the final state of the radiation field is the vacuum, no photons:

$$\langle R_f| = {}_R\langle 0|$$

which is annihilated by the photon annihilation operators: $\mathbf{a}_{K,s} |0\rangle_R = 0$ and hence ${}_R\langle 0| \mathbf{a}^\dagger_{K,s} = 0$. The initial state is one photon of momentum K and some polarization s:

$$|R_i\rangle = |K, s\rangle_R = \mathbf{a}^\dagger_{K,s} |0\rangle_R \ .$$

What is the interaction hamiltonian $\mathbf{H}_{\rm int}$? As you'll remind yourself on the homework, the hamiltonian for a charged particle (such as an ion in the solid) in an EM field is

$$\mathbf{H}_1 = \frac{1}{2m}\left(\vec{\mathbf{p}} + e\vec{\mathbf{A}}(\mathbf{x})\right)^2 = \frac{1}{2m}\left(\mathbf{p}^2 + e\mathbf{p}\mathbf{A} + e\mathbf{A}\mathbf{p} + e^2\mathbf{A}^2\right) = \frac{\mathbf{p}^2}{2m} + \mathbf{H}_{\rm int}.$$

Think of e as small, so that we may treat $\mathbf{H}_{\rm int}$ as a perturbation. Here we should use our expression above for the quantized photon field:

$$\mathbf{A}(x) \sim \sum_K \left(\mathbf{a}_K e^{\mathbf{i}Kx} + \mathbf{a}^\dagger_K e^{-\mathbf{i}Kx}\right).$$

The catch here is that we have to evaluate this *at the location of the ion*, which means that the x appearing in the argument is an operator, $\mathbf{x}$!

The final term in $\mathbf{H}_1$ proportional to $\mathbf{A}^2$ changes the number of photons by an even number, and so doesn't participate in the process we are talking about where one

photon is absorbed. So we just need to think about the middle terms with one $\mathbf{A}$. The $\mathbf{p}$ is pretty innocuous:

$$\mathbf{p}e^{i\mathbf{K}\mathbf{x}} + e^{i\mathbf{K}\mathbf{x}}\mathbf{p} = (\mathbf{p} + K)\, e^{i\mathbf{K}\mathbf{x}}$$

and we'll just focus on the second term. So the matrix element is:

$$W \propto |\, \langle L_f| \otimes {}_R\langle 0|\, e^{i\mathbf{K}\mathbf{x}}\mathbf{a}_K\, |L_i\rangle \otimes \mathbf{a}_K^\dagger\, |0\rangle_R\, |^2$$

$$= |\, \langle L_f|\, e^{i\mathbf{K}\mathbf{x}}\, |L_i\rangle\, |^2 |{}_R\langle 0|\, \mathbf{a}_K\mathbf{a}_K^\dagger\, |0\rangle_R\, |^2 = |\, \langle L_f|\, e^{i\mathbf{K}\mathbf{x}}\, |L_i\rangle\, |^2$$

which is our previous expression.

[End of Lecture 4]

1.6 Casimir effect: vacuum energy is real

[Le Bellac, 11.5.12 page 399; A. Zee, *Quantum Field Theory in a Nutshell*] This subsection has two purposes. One is to show that the $\frac{1}{2}\hbar\omega$ energy of the vacuum of the quantum harmonic oscillator is real. Sometimes we can get rid of it by choosing the zero of energy (which doesn't matter unless we are studying dynamical gravity). But it is meaningful if we can *vary* ω (or the collection of ωs if we have many oscillators as for the radiation field) and compare the difference.

The other purpose is to give an object lesson in asking the right questions. In physics, the right question is often a question which can be answered by an experiment, at least in principle. The answers to such questions are less sensitive to our silly theoretical prejudices, *e.g.* about what happens to physics at very short distances.

In the context of the bunch of oscillators making up the radiation field, we can change the spectrum of frequencies of these oscillators $\{\omega_k\}$ by putting it in a box and varying the size of the box. In particular, two parallel conducting plates separated by some distance d experience an attractive force from the change in the vacuum energy of the EM field resulting from their presence. The plates put boundary conditions on the field, and therefore on which normal modes are present.

To avoid some complications of E&M which are not essential for our point here, we're going to make two simplifications:

- we're going to solve the problem in 1+1 dimensions
- and we're going to solve it for a scalar field.

To avoid the problem of changing the boundary conditions *outside* the plates we use the following device with *three* plates:

$$| \leftarrow d \rightarrow | \longleftarrow \qquad L - d \qquad \longrightarrow |$$

(We will consider $L \gg d$, so we don't really care about the far right plate.) The 'perfectly conducting' plates impose the boundary condition that our scalar field $q(x)$ vanishes there. The normal modes of the scalar field $q(x)$ in the left cavity are then

$$q_j = \sin\left(j\pi x/d\right), \quad j = 1, 2, ...$$

with frequencies $\omega_j = ck_j = \frac{\pi|j|}{d}c$. There is a similar expression for the modes in the right cavity which we won't need. We're going to add up all the $\frac{1}{2}\hbar\omega$s for all the modes in both cavities to get the vacuum energy $E_0(d)$; the force on the middle plate is then $-\partial_d E_0$.

The vacuum energy between the outer plates is the sum of the vacuum energies of the two cavities

$$E_0(d) = f(d) + f(L-d)$$

where

$$f(d) = \frac{1}{2}\hbar\sum_{j=1}^{\infty}\omega_j = \hbar c\frac{\pi}{2d}\sum_{j=1}^{\infty} j \stackrel{?!?!!}{=} \infty.$$

We have done something wrong. Our crime is hubris: we assumed that we knew what the modes of arbitrarily large mode number k (arbitrarily short wavelength, arbitrarily high frequency) are doing, and in particular we assumed that they cared about our silly plates. In fact, no metal in existence can put boundary conditions on the modes of large enough frequency – those modes don't care about d. The reason a conductor puts boundary conditions on the EM field is that the electrons move around to compensate for an applied field, but there is a limit on how fast the electrons can move (*e.g.* the speed of light). The resulting cutoff frequency is called the *plasma frequency* but we don't actually need to know about all these details. To parametrize our ignorance of what the high-frequency modes do, we must *cut off* (or *regularize*) the contribution of the high-frequency modes. Let's call modes with $\omega_j \gg \pi/a$ high frequency, where here a is some short time[9].

Then one possible model of the microphysics, which makes the sum both finite and doable, is realized by making the replacement:

$$\begin{aligned} f(d) \rightsquigarrow f(a,d) &= \hbar c\frac{\pi}{2d}\sum_{j=1}^{\infty} e^{-a\omega_j/\pi} j \\ &= -\frac{\pi\hbar c}{2}\partial_a \underbrace{\left(\sum_{j=1}^{\infty} e^{-aj/d}\right)}_{=\frac{1}{1-e^{-a/d}}-1} \\ &= +\frac{\pi\hbar c}{2d}\frac{e^{a/d}}{\left(e^{a/d}-1\right)^2} \\ &\stackrel{a\ll d}{\simeq} \hbar\left(\underbrace{\frac{\pi d}{2a^2}}_{\to\infty \text{ as } a\to 0} - \frac{\pi}{24d} + \frac{\pi a^2}{480 d^3} + \ldots\right) \end{aligned} \tag{1.25}$$

Answers that don't depend on a have a chance of being meaningful. The thing we can measure is the force:

$$F = -\partial_d E_0 = -\left(f'(d) - f'(L-d)\right)$$

[9] You can think of a as the time it takes the waves to move by one lattice spacing. If we work in units where the velocity is $c = 1$, this is just the lattice spacing.

$$
\begin{aligned}
&= -\hbar c \left(\left(\frac{\pi}{2a^2} + \frac{\pi}{24d^2} + \mathcal{O}(a^2) \right) - \left(\frac{\pi}{2a^2} + \frac{\pi}{24\,(L-d)^2} + \mathcal{O}(a^2) \right) \right) \\
&\overset{a\to 0}{=} -\frac{\pi\hbar c}{24} \left(\frac{1}{d^2} - \frac{1}{(L-d)^2} \right) \\
&\overset{L\gg d}{=} -\frac{\pi\hbar c}{24d^2} \left(1 + \mathcal{O}(d/L)\right) \ . \qquad (1.26)
\end{aligned}
$$

This is an attractive force between the plates.

The analogous force between real conducting plates, caused by the change of boundary conditions on the electromagnetic field, has been measured.

The string theorists will tell you that $\sum_{j=1}^{\infty} j = -\frac{1}{12}$, and our calculation above agrees with them in some sense. But what this foolishness means is that if we compute something which is not dependent on the cutoff we have to get the same answer no matter what cutoff we use. Notice that it is crucial to ask the right questions.

An important question is to what extent could we have picked a different cutoff function (instead of $e^{-\pi\omega/a}$) and gotten the same answer for the physics. This interesting question is answered affirmatively in Zee's wonderful book, 2d edition, section I.9 (available electronically here!).

A comment about possible physical applications of the calculation we actually did: you could ask me whether there is such a thing as a Casimir force due to the vacuum fluctuations of *phonons*. Certainly it's true that the boundary of a chunk of solid puts boundary conditions on the phonon modes, which change when we change the size of the solid. The problem with the idea that this might produce a measurable force (which would lead the solid to want to shrink) is that it is hard to distinguish the 'phonon vacuum energy' from the rest of the *energy of formation* of the solid, that is, the energy difference between the crystalline configuration of the atoms and the configuration when they are all infinitely separated. Certainly the latter is not well-described in the harmonic approximation ($\lambda = 0$ in (1.6)).

A few comments about the 3+1 dimensional case of E&M.

Assume the size of the plates is much larger than their separation L. Dimensional analysis shows that the force per unit area from vacuum fluctuations must be of the form

$$P = \alpha \frac{\hbar c}{L^4}$$

where α is a numerical number. α is not zero!

Use periodic boundary conditions in the xy planes (along the plates). The allowed

wave vectors are then

$$\vec{k} = \left(\frac{2\pi n_x}{L_x}, \frac{2\pi n_y}{L_y}, \frac{\pi n}{L} \right)$$

with n_x, n_y, n integers.

We have to do a bit of E&M here. Assume the plates are perfect conductors (this is where the hubris about the high-frequency modes enters). This means that the transverse component of the electric field must vanish at the surface. Instead of plane waves in z, we get standing waves: $E_{x,y}(z) \propto \sin(n\pi z/L)$.

The frequencies of the associated standing waves are then

$$\omega_n(\vec{k}) = c\sqrt{\frac{\pi^2 n^2}{L^2} + \vec{k}^2}, n = 0, 1, 2...$$

Also, there is only one polarization state ($\vec{E} \propto \hat{z}$) for $n = 0$.

So the zero-point energy is

$$E_0(L) = \frac{\hbar}{2} \left(2 \sum_{n,\vec{k}}{}' \omega_n(\vec{k}) \right)$$

where it's useful to define

$$\sum_{n,\vec{k}}{}' \equiv \frac{1}{2} \sum_{n=0,\vec{k}} + \sum_{n\geq 1,\vec{k}}$$

Now you can imagine introducing a regulator like the one we used above, and replacing

$$\sum_{n,\vec{k}}{}' \cdot \rightsquigarrow \sum_{n,\vec{k}}{}' e^{-a\omega_n(\vec{k})/\pi}.$$

and doing the sums and integrals and extracting the small-a behavior. The result is $\alpha = -\frac{\pi^2}{2 \cdot 5!}$, an attractive force. It was measured in 1998.

1.7 Identical particles

[Griffiths chapter 5, Le Bellac chapter 13, Weinberg §4.5, Baym §18]

Every photon is the same as every other photon, except for their position (or momentum) and polarization state. This is an immediate consequence of how we discovered photons by quantizing the Maxwell field: the state with n photons of the same momentum and polarization is

$$\left| n \text{ photons with } \vec{k}, \alpha \right\rangle = \frac{\left(\mathbf{a}^\dagger_{\vec{k},\alpha}\right)^n}{\sqrt{n!}} |0\rangle \,.$$

In fact, the same is true of all the other kinds of particles we know about, including electrons (for which we haven't seen a similar classical field description).

This means that we can write the state of N such *indistinguishable particles* merely by specifying a collection of positions and of polarization (or spin) states – we don't need to say which is which (and in fact, we cannot).

Indistinguishable means that the probability of finding N such particles in a state labelled $k_1\alpha_1 \cdots k_N\alpha_N$ must be invariant under permutations of the particles:

$$P(k_1\alpha_1 \cdots k_N\alpha_N) = P(k_{\pi_1}\alpha_{\pi_1} \cdots k_{\pi_N}\alpha_{\pi_N})$$

where here π denotes a permutation on N objects $(12...N) \to (\pi_1\pi_2...\pi_N)$. This means that the wavefunction ($P = |\Psi|^2$) must be preserved up to a phase:

$$\Psi(k_1\alpha_1 \cdots k_N\alpha_N) = e^{\mathbf{i}\theta}\Psi(k_{\pi_1}\alpha_{\pi_1} \cdots k_{\pi_N}\alpha_{\pi_N}).$$

What can we say about this phase?

A wavefunction for N such particles is of the form

$$\Psi(k_1, \alpha_1; ...; k_N, \alpha_N) \equiv \langle k_1\alpha_1; \cdots; k_N, \alpha_N|\Psi\rangle = \langle 0| \, \mathbf{a}_{k_1\alpha_1}\mathbf{a}_{k_2\alpha_2} \cdots \mathbf{a}_{k_N\alpha_N} \, |\Psi\rangle \,.$$

(Here I am anticipating the second-quantized description.) But the same state is described if we switch the labels of any two of the particles:

$$\Psi(k_2, \alpha_2; k_1, \alpha_1; ....) = a\Psi(k_1, \alpha_1; k_2, \alpha_2; ....)$$

where a is some phase (recall: multiplying the whole wavefunction by a phase does not change the state). Switching them back gives back the first state[10]:

$$\Psi(k_1, \alpha_1; k_2, \alpha_2; ....) = a^2\Psi(k_1, \alpha_1; k_2, \alpha_2; ....)$$

[10] In two spatial dimensions, something interesting can happen. The phase a can depend on the topological class of the path by which we exchange the particles. Going around one way can be

so $a^2 = 1$. There are two solutions: $a = +1$ and $a = -1$ and the two classes of particles associated with these two choices are called respectively *bosons* and *fermions*. For bosons, the wavefunction is simply permutation invariant:

$$\Psi_B(1 \cdots N) = \Psi_B(\pi_1 \cdots \pi_N).$$

For fermions, the sign of the wavefunction changes under an *odd* permutation:

$$\Psi_F(1 \cdots N) = (-1)^\pi \Psi_F(\pi_1 \cdots \pi_N).$$

An odd permutation is one that can be made from an odd number of transpositions. (For example $(123) \to (213)$ is odd, but $(123) \to (231)$ is even.)

Note that the Hilbert space of N indistinguishable particles is therefore not quite a tensor product of the Hilbert spaces of the individual particles. In fact, both the bosonic states and the fermionic states fit easily into $\mathcal{H}_1^{\otimes N}$. If $D \equiv \dim \mathcal{H}_1$, then

$$\dim \mathcal{H}_F = \frac{D!}{N!(D-N)!} = \binom{D}{N}$$

$$\dim \mathcal{H}_B = \frac{(N+D-1)!}{N!(D-1)!} = \binom{N+D-1}{N}$$

and in fact $\dim \mathcal{H}_F + \dim \mathcal{H}_B \leq \dim \mathcal{H}_1^{\otimes N} = D^N$ (for $N > 1$).

---

different from going around the other way. This leads to the possibility of *anyons*.

One way to see that something is different in $D = 2+1$ is to think about the path integral for, say two particles. In the special case of $2+1$ dimensions, the worldlines of the particles can *braid* around each other; undoing a braid requires a collision between the particles. In more dimensions, the paths can be unlinked without any collision. This means that in $D = 2+1$, the sum over paths can be divided up into topological sectors, labelled by the number of times n the particles wind around each other. Nothing can stop us from weighting the contributions of paths in different sectors differently:

$$Z = \sum_n e^{\mathbf{i}n\theta} Z_n$$

where Z_n is the sum over all paths in the sector labelled n. The phase θ determines the statistics of the particles.

There is an even more dramatic thing that can happen, again only in $D = 2+1$. There can be a degenerate subspace of the Hilbert space associated with the presence of two anyons. Exchanging the two particles, or moving them around each other, can then result in not just a phase, but a whole unitary operator acting within this degenerate subspace. Since two such unitaries generally do not commute, such particles are called *non-abelian anyons*.

How then can we ever discuss the wavefunction of a single electron?? Don't we have to antisymmetrize it with the state of all the other electrons in the world? Suppose there were only two electrons in the world, and the two single-particle states involved were $\psi_H(x)$ and $\psi_T(x)$ ('H' for 'here' and 'T' for 'there'). The full state is

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\psi_H(x_1)\psi_T(x_2) - \psi_T(x_1)\psi_H(x_2)\right). \tag{1.27}$$

What is the probability of finding an electron somewhere around here at location x?

$$P(\text{an electron at } x) = \int dx_2 |\Psi(x, x_2)|^2 + \int dx_1 |\Psi(x_1, x)|^2 \tag{1.28}$$

$$= |\psi_H(x)|^2 \int dy |\Psi_T(y)|^2 + |\psi_T(x)|^2 \int dy |\Psi_H(y)|^2$$
$$- 2\mathrm{Re}\,\psi_H(x)\psi_T^\star(x) \int dy \psi_H^\star(y)\psi_T(y)\ . \tag{1.29}$$

But suppose we know that the two states don't overlap: $\psi_T(x)\psi_H(x) = 0$ for all x. Then the last interference term vanishes, and one or the other of the first two terms vanishes wherever we look, and by normalization of ψ_T and ψ_H, the other reduces to the formula we would have used if we didn't know about this antisymmetrization stuff.
Conclusion: you only need to worry about antisymmetrizing states that overlap.

Compare the mind-set of first-quantized and second-quantized descriptions. In the first-quantized formalism, we must answer the question: which particles are in which single-particle states? For example, we can write states like $|\alpha\rangle_1 \otimes |\beta\rangle_2$ or $|\beta\rangle_1 \otimes |\alpha\rangle_2$, where α, β are two different singie-particle states. Only the combinations

$$|\alpha\rangle_1 \otimes |\beta\rangle_2 \pm |\beta\rangle_1 \otimes |\alpha\rangle_2 \tag{1.30}$$

are allowed states of bosons and fermions, respectively. In the second-quantized formalism, we only need to answer: how many particles are in each single-particle state? Then the states (1.30) would be denoted

$$|n_\alpha = 1, n_\beta = 1\rangle$$

with no further fuss. The second-quantized language is like *Newspeak*, the language in Orwell's *1984* in which it is not possible to formulate heretical statements. But in a good way.

A second advantage of the second-quantized language is that the single-particle language quickly becomes unwieldy as the the number of particles grows. Above in (1.30) I wrote a state of two identical bosons or fermions. Its wavefunction, in position space, say, is

$$\Psi_{B/F}(x_1, x_2) = u_\alpha(x_1)u_\beta(x_2) \pm u_\beta(x_1)u_\alpha(x_2).$$

Here each $u_\alpha(x) \equiv \langle x|\alpha\rangle$ is a single-particle wavefunction. Suppose I had three particles. What does the wavefunction look like if I fill three levels α, β, γ? Here's a trick for the Fermi case:

$$\Psi_F(x_1, x_2, x_3) = \det M \tag{1.31}$$

where

$$M \equiv \begin{pmatrix} u_\alpha(x_1) & u_\alpha(x_2) & u_\alpha(x_3) \\ u_\beta(x_1) & u_\beta(x_2) & u_\beta(x_3) \\ u_\gamma(x_1) & u_\gamma(x_2) & u_\gamma(x_3) \end{pmatrix}.$$

The structure of the determinant

$$\det M = \sum_{\pi \in S_N} (-1)^\pi M_{1\pi_1} \cdots M_{N\pi_N}$$

makes it automatic that this is antisymmetric under interchange of the position labels, $\Psi_F(x_1, x_2, x_3) = -\Psi_F(x_2, x_1, x_3)$. The wavefunction (1.31) is called a *Slater determinant*. For N fermions the state associated to a collection of single-particle levels $\{\alpha_1 \cdots \alpha_N\}$ is $\Psi_F^{(\alpha_1 \cdots \alpha_N)}(x_1 \cdots x_N) = \det_{ij} u_{\alpha_i}(x_j)$.

To make the wavefunction for bosons made from these same single-particle states, just remove all the minus signs involved in constructing the determinant:

$$\Psi_B(x_1 \cdots x_N) = \sum_{\pi \in S_N} M_{1\pi_1} \cdots M_{N\pi_N} \equiv \mathrm{Per}(M),$$

which is called the *permanent* of M. Now the α_i don't all have to be different.

An immediate consequence of the minus sign under exchange of fermion labels is the *Pauli exclusion principle*:

$$\Psi_{\text{Fermions}}(k_1, \alpha_1; k_1, \alpha_1; ...) = 0.$$

No two fermions can occupy the same single-particle state. The ground state of a collection of (non-interacting) fermions is therefore quite interesting, since we must find a different single-particle state in which to put each of our fermions. This has many dramatic consequences, including the periodic table of elements, and the distinction between metals and insulators that we discuss next. [End of Lecture 5]

1.7.1 Band structure: metals and insulators

Now we will say some words about fermions in periodic potentials. This will allow us to quickly understand a way to distinguish metals and insulators. Then we'll translate to the second-quantized language.

Consider a collection of fermions that care about each other only because of the Pauli principle – the hamiltonian is a sum of terms involving the fermions one at a time. Suppose that each fermion (call them electrons) can live at one of N sites in a one dimensional crystal, and can hop from one site to the next by some tunneling process. Further suppose that each site involves several (we'll say two for simplicity) atomic orbitals (or spin states), so the one-particle hilbert space is $\mathcal{H}_1 = \text{span}\{|n\rangle \otimes |\alpha\rangle, n = 1...N, \alpha = 0, 1\}$. We'll suppose that each electron is governed by the hamiltonian

$$\mathbf{H}_1 = -t \sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right) \otimes \mathbb{1} + \sum_n |n\rangle\langle n| \otimes \epsilon |1\rangle\langle 1| \equiv \mathbf{H}_t + \mathbf{H}_\epsilon.$$

The first term allows the electrons to hop. The second term says that one of the orbitals has lower energy than the other ($|0\rangle$ is the ground state and $|1\rangle$ has energy $\epsilon > 0$). For example, if α is a spin label, this could be the result of a Zeeman field of strength ϵ.

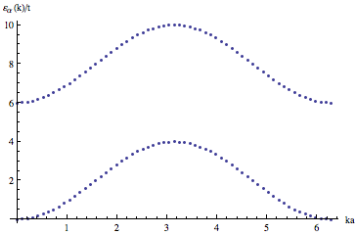
What is the spectrum of $\mathbf{H}_1$, the hamiltonian of *one* electron hopping in this solid? The two terms commute $[\mathbf{H}_t, \mathbf{H}_\epsilon] = 0$, so we can simultaneously diagonalize them. Let's assume periodic boundary conditions for simplicity. Notice that the problem has a discrete translation invariance, which should be familiar by now. Moreover, it's just two copies of the problem on the problem set; the eigenstates are eigenstates of the momentum

$$|k\rangle \otimes |\alpha\rangle = \frac{1}{\sqrt{N}} \sum_n e^{ikna} |n\rangle \otimes |\alpha\rangle \qquad \alpha = 0, 1$$

with eigenvalues[11]

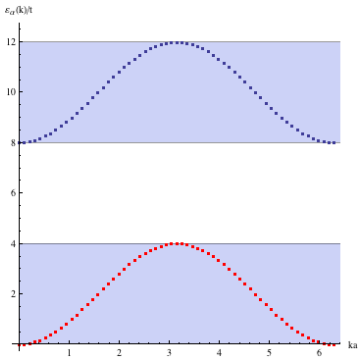
$$\varepsilon_\alpha(k) = -2t \cos ka + \epsilon \delta_{\alpha,1}. \tag{1.32}$$

For finite N, the allowed independent wave numbers are $\{k_j = \frac{2\pi}{Na} j, j = 1..N\}$. Here is the spectrum for $\epsilon/t = 6$, with $N = 60$ sites. There are $120 = 2N$ dots because this is the size of our single-particle Hilbert space. The two curves are sometimes called 'bands'. This is because they describe *bands* of allowed energies. The *bandwidth* here is $4t$. In this plot there is a gap between the bands, which depends on ϵ.

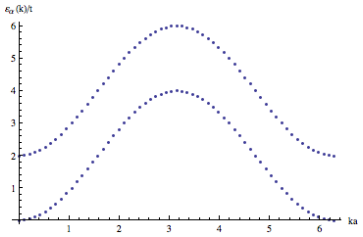


[11] I picked this example for simplicity so we don't waste time diagonalizing lots of matrices. More generally, it's interesting to consider a more generic action of $\mathbf{H}_1$ on the orbital degree of freedom. This would give us more interesting bands. On the next homework, you'll get to study such an example.

Here the allowed bands of energies are highlighted:

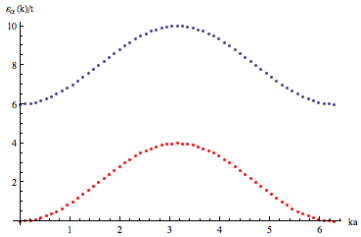


Here is the spectrum for $\epsilon/t = 2$:
Now the bands overlap.



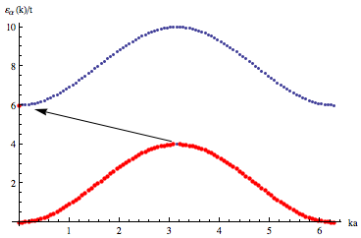
To understand the important consequence of this distinction, now consider what happens if we have many fermions. If we have one fermion, the ground state is found by putting it in the lowest energy state, here $k = 0, \alpha = 0$. If we have two, the Pauli principle forces us to put them in different states; we should put the second (note that they don't really have an order) in the second lowest energy state; here it is $\alpha = 0, k = \frac{2\pi}{Na}$. Each fermion we add fills the next-lowest-energy state. So each dot in these figures is a possible cubbyhole in which to stash our electrons. Only one electron fits in each hole. In the ground state, the electrons pile up in the lowest holes.

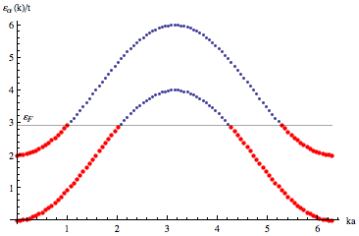
Suppose we have N fermions – one per ion site. This is natural if we think of the ions as carrying positive charge; with N electrons the whole thing will be neutral and happy. The ground state is constructed by filling the lowest *half* of the one-electron states – recall that we have $2N$ single-particle states altogether. If the bands don't overlap (if $\epsilon > 4t$), this means we just fill the bottom band:



Filled states are indicated in red.

The lowest energy excitation of this system is achieved by taking one of the electrons out of a filled state in the bottom ('valence')band and raising it all the way to the empty

('conduction') band:  This costs energy $\Delta E = \epsilon - 4t$ which is finite even as $N \to \infty$. A system of fermions with completely filled bands describes an insulator (aka semiconductor). It has an energy gap: the energy of the first excited state is above the ground state energy (even as $N \to \infty$). It is hard to excite. If we apply an infinitesimal electric field, nothing will happen, no Ohm's law.

As we decrease the orbital energy difference ϵ, the excited atomic states start to matter and eventually (for $\epsilon < 4t$) they are filled in the ground state. 

The name for the energy of the last filled level is the *Fermi energy* ε_F. (and the name of its momentum is the *Fermi momentum*, k_F). [12] Now the first excited state of the N-electron system is achieved by a very small change – we can stay in the same band. The energy cost to excite the system from the ground state is of order $\Delta k \partial_k \varepsilon|_{\varepsilon_F} \sim \frac{1}{N}$ (where $\Delta k = \frac{2\pi}{Na}$) which goes to zero as $N \to \infty$. There is no energy gap. When the Fermi energy is in the middle of a band, the system is a *metal*.

Groundstates of such macroscopic ($N \to \infty$) systems can be called *states of matter*. This sort of sharp distinction between possible behaviors of states of matter – like whether there is an energy gap – is the central preoccupation of condensed matter physics.

By the way, what we have really shown here is that when the Fermi energy is in the middle of the band, the system has very low-energy excitations. The fact that it actually conducts electricity is also a consequence of quantum mechanics. It happens because the wavefunctions of these low-energy excitations are *extended* across the material – they are (quasi-)momentum (k) eigenstates. This means that they can carry a current across the sample, $\mathrm{Im}\,\psi_k^\star \partial_x \psi_k \neq 0$. Notice that this picture departs dramatically from the classical (Drude) picture of charge transport by a charged particle bouncing around in the lattice. Notice that the form of the lattice is already built into the wavefunctions ψ_k! (At this point we actually have the opposite problem that the answer we would compute for the resistance of such a metal is zero. To get the right

[12] Partly because we chose such a simple example for our Hamiltonian, we find several (4) places where the bands cross the Fermi energy – several Fermi momenta.

finite answer we would need to include some form of *disorder* in the lattice, or phonons, and/or interactions between the electrons.)

Fermionic operators. What is the analog of the description of the many-body system in terms of mode operators $\mathbf{a}_k$ that we had for phonons and photons? We can introduce operators that *create* and *annihilate* electrons just like we did before:

$$\mathbf{c}_{n\alpha}\left|0\right\rangle = 0, \qquad \mathbf{c}^\dagger_{n\alpha}\left|0\right\rangle = \left|n\right\rangle \otimes \left|\alpha\right\rangle .$$

Notice that they are labelled by a position n and an orbital label $\alpha = 0, 1$. Our boson creation operators satisfied the algebra $1 = [\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a}$ (for each mode) and this led to boson statistics. We need somehow to prevent two electrons from being in the same state. We can accomplish the Pauli principle simply by demanding that

$$\boxed{\mathbf{c}^2 = 0}$$

for each mode, *i.e.* $\left(\mathbf{c}_{n\alpha}\right)^2 = 0 = \left(\mathbf{c}^\dagger_{n\alpha}\right)^2$. It's just zero. More generally, in order to make sure that the wavefunction is antisymmetric under interchange,

$$\left|\alpha, \beta\right\rangle = c^\dagger_\alpha c^\dagger_\beta \left|0\right\rangle = -c^\dagger_\beta c^\dagger_\alpha \left|0\right\rangle = -\left|\beta, \alpha\right\rangle ,$$

we also need to change a key sign:

$$1 = \{\mathbf{c}, \mathbf{c}^\dagger\} \equiv \mathbf{c}\mathbf{c}^\dagger + \mathbf{c}^\dagger\mathbf{c}.$$

This is called an *anticommutator*. With the labels the algebra should be:

$$\{\mathbf{c}_{n\alpha}, \mathbf{c}^\dagger_{n'\alpha'}\} = \delta_{\alpha\alpha'}\delta_{nn'}, \qquad \{\mathbf{c}_{n\alpha}, \mathbf{c}_{n'\alpha'}\} = 0. \tag{1.33}$$

This last statement is weird: fermion operators, even if they create particles that are far apart, do not commute. Rather they anticommute. Fermions are weird in this sense. (We saw above however that this does not mean that you have to worry about all the electrons in the world when thinking about the physics of the electrons you're interested in.)

Note that each fermionic operator $\mathbf{c}$ satisfying

$$\mathbf{c}^2 = 0, \qquad \{\mathbf{c}, \mathbf{c}^\dagger\} = 1$$

constructs the Hilbert space of a qubit (*i.e.* a two-state system) as follows:

$$\mathbf{c}\left|\downarrow\right\rangle = 0, \quad \mathbf{c}^\dagger\left|\downarrow\right\rangle = \left|\uparrow\right\rangle .$$

The two states of the qubit just describe the presence or absence of the fermion in this state. Exercise: we can rewrite the Pauli operators as

$$\boldsymbol{\sigma}^x = \mathbf{c} + \mathbf{c}^\dagger, \quad \boldsymbol{\sigma}^y = \frac{1}{\mathbf{i}}\left(\mathbf{c} - \mathbf{c}^\dagger\right), \quad \boldsymbol{\sigma}^z = 2\mathbf{c}^\dagger\mathbf{c} - \mathbb{1}.$$

These operators satisfy the Pauli algebra, $\boldsymbol{\sigma}^i\boldsymbol{\sigma}^j = \mathbf{i}\epsilon^{ijk}\boldsymbol{\sigma}^k$. Also note that $\boldsymbol{\sigma}^+ = c^\dagger, \boldsymbol{\sigma}^- = c$ and the number operator $\mathbf{c}^\dagger\mathbf{c}$ (whose eigenvalues are 0 and 1) is $\mathbf{c}^\dagger\mathbf{c} = \frac{1}{2}\boldsymbol{\sigma}^z + \mathbb{1}$.

Now we can write the many-fermion Hamiltonian as

$$\mathbf{H}_{\text{many}} = -t\sum_n \left(\mathbf{c}^\dagger_{n\alpha}\mathbf{c}_{n+1,\alpha} + \mathbf{c}^\dagger_{n+1,\alpha}\mathbf{c}_{n\alpha}\right) + \sum_n \epsilon_{\alpha\beta}\mathbf{c}^\dagger_{n\alpha}\mathbf{c}_{n\beta}.$$

Such a Hamiltonian is sometimes called a tight-binding model, since we've restricted the allowed positions of the electrons to certain well-defined orbitals, labelled by n. Above we have chosen the very simple case where $\epsilon_{\alpha\beta} = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}$.

This hamiltonian is of the form

$$\mathbf{H}_{\text{many}} = \sum_A \mathbf{c}^\dagger_A h_{AB}\mathbf{c}_B$$

(here $A = n\alpha$ is a multi-index labelling an arbitrary state in the single-particle Hilbert space) and can be diagonalized by choosing a more favorable linear combination of the creation operators, which diagonalize the (ordinary c-number) matrix h which acts within the single-particle Hilbert space. Because of translation invariance, these more-favorable modes are (no surprise) momentum eigenstates (we solved this problem above):

$$\mathbf{c}_{\alpha k} \equiv \frac{1}{\sqrt{N}}\sum_n e^{\mathbf{i}kx_n}\mathbf{c}_{n\alpha}$$

in terms of which

$$\mathbf{H}_{\text{many}} = \sum_{k,\alpha} \mathbf{c}^\dagger_{\alpha k}\mathbf{c}_{\alpha k}\varepsilon_\alpha(k)$$

with $\varepsilon_\alpha(k)$ given above in (1.32). The ground state of n such electrons is

$$|\text{ground state}\rangle = \prod_{n\ (k,\alpha) \text{ with the smallest } \epsilon_\alpha(k)} \mathbf{c}^\dagger_{\alpha k}\,|0\rangle\,.$$

The groundstate wavefunction is

$$\Psi(r_1\alpha_1, \cdots r_n\alpha_n) = \langle r_1\alpha_1 \cdots r_n\alpha_n|\text{ground state}\rangle = \langle 0|\,\mathbf{c}_{r_1\alpha_1}\cdots\mathbf{c}_{r_n\alpha_n}\,|\text{ground state}\rangle$$

is the Slater determinant of the n lowest single-particle wavefunctions:

$$\Psi(r_1\alpha_1, \cdots r_n\alpha_n) = \det_{ij}{}^{n}\, u_{k_i\beta_i}(r_j\alpha_j)$$

where the single-particle wavefunctions are $u_{k\beta}(r\alpha) = \frac{1}{\sqrt{N}}e^{\mathbf{i}kr}\delta_{\alpha\beta}$. (The dependence on α, β is so simple because of our simple choice of Hamiltonian.) [End of Lecture 6]

1.8 Second quantization, from scratch

Above, we discovered the second quantized description in an organic way. Let's back up and consider the formalism more generally on its own terms.

Creation operators for general one-particle states. Given a one-particle state with momentum-space wavefunction $\varphi(k) \equiv \langle k|\varphi\rangle$, let

$$\mathbf{a}^\dagger(\varphi) \equiv \sum_k \mathbf{a}_k^\dagger \varphi(k). \tag{1.34}$$

Then if $|k\rangle = \mathbf{a}_k^\dagger |0\rangle$, we have

$$\mathbf{a}^\dagger(\varphi)|0\rangle = \sum_k \underbrace{\mathbf{a}_k^\dagger |0\rangle}_{=|k\rangle} \varphi(k) = |\varphi\rangle .$$

So this operator creates a single particle in the state φ.

The commutation relations of such operators are as follows. If

$$\mathbf{a}_k \mathbf{a}_{k'}^\dagger - \zeta \mathbf{a}_{k'}^\dagger \mathbf{a}_k = \delta_{kk'}$$

where $\zeta = \pm 1$ for bosons and fermions respectively, then I claim that

$$\mathbf{a}(\varphi_1)\mathbf{a}^\dagger(\varphi_2) - \zeta \mathbf{a}^\dagger(\varphi_2)\mathbf{a}(\varphi_1) = \langle \varphi_2|\varphi_1\rangle .$$

One-body operators. An arbitrary operator acting on the one-particle Hilbert space $\mathcal{H}_1 = \mathrm{span}\{|\alpha\rangle\}$ (assume this is an orthonormal basis) can be written as

$$\mathbf{A}_1 = \sum_{\alpha\beta} |\alpha\rangle\langle\beta| A_{\alpha\beta}.$$

How do we write the corresponding operator on the many-body Hilbert space? In the first-quantized language, a basis for the states with n particles is of the form

$$|u_1 \cdots u_N\rangle = \sum_\pi \zeta^\pi |u_{\pi_1}\rangle \otimes |u_{\pi_2}\rangle \otimes \cdots \otimes |u_{\pi_n}\rangle$$

where u_i are some single-particle states (they could be the same basis as α, β), $\pi \in S_n$ is a permutation, and again $\zeta = \pm$ for B/F. Here by $(-1)^\pi$ I mean -1 if π is an odd permutation and $+1$ otherwise. On such a state, we want $\mathbf{A}$ to act as

$$\mathbf{A}|u_1 \cdots u_N\rangle = \sum_\pi \zeta^\pi \left[\underbrace{(\mathbf{A}_1 |u_{\pi_1}\rangle)}_{=\sum_{\alpha\beta} A_{\alpha\beta}|\alpha\rangle\langle\beta|u_{\pi_1}\rangle} |u_{\pi_2} \cdots u_{\pi_n}\rangle + |u_{\pi_1}\rangle (\mathbf{A}_1 |u_{\pi_2}\rangle) |u_{\pi_3} \cdots u_{\pi_n}\rangle + \cdots \right] \tag{1.35}$$

The effect of the operation $|\alpha\rangle\langle\beta|$ is to replace the state β with the state α. On the many-body Hilbert space, this happens wherever the $\mathbf{A}_1$ acts. But this is precisely what is accomplished by the many-body operator

$$\mathbf{a}^\dagger(\alpha)\mathbf{a}(\beta)$$

– it destroys a particle in state β and creates a particle in state α. Notice that this is a bosonic object, no matter what are the statistics of the **a**s. If there is no such particle to destroy, it just gives zero. Therefore,

$$\mathbf{A} = \sum_{\alpha\beta} \mathbf{a}^\dagger(\alpha)\mathbf{a}(\beta)A_{\alpha\beta}.$$

For example, we can write the kinetic energy of a collection of free particles in this language. The single-particle operator is just $\mathbf{H}_1 = \frac{\mathbf{p}^2}{2m}$. On n particles, we would write

$$\mathbf{H}_n = \sum_{i=1}^{n} \frac{\mathbf{p}_i^2}{2m}.$$

On an *indefinite* number of particles, we can write instead

$$\mathbf{H} = \sum_k \mathbf{a}_k^\dagger \mathbf{a}_k \frac{(\hbar k)^2}{2m}.$$

In this last expression, $p = \hbar k$ is just a number – $\frac{k^2}{2m}$ are the matrix elements of $A_{\alpha\beta}$ in this example, which happens to be diagonal in the k basis of the one-particle Hilbert space. Notice that the fixed-particle-number operators above can be written as

$$\mathbf{H}_n = \Pi_n \mathbf{H} \Pi_n$$

where Π_n is the projector onto states with exactly n particles.

Above, I claimed without much proof that the state we get by filling single-particle levels and (anti)symmetrizing is a Slater determinant or permanent. Let me clarify that statement. Consider an n-particle state

$$|\alpha_1 \cdots \alpha_n\rangle = \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} \zeta^\sigma |\alpha_{\sigma_1}\rangle \otimes \cdots \otimes |\alpha_{\sigma_n}\rangle$$

where the α_i are arbitrary 1-particle states. Then the overlap between any two such

states is

$$\langle\alpha_1\cdots\alpha_n|\beta_1\cdots\beta_n\rangle = \frac{1}{n!}\sum_{\sigma,\pi}\zeta^\pi\zeta^\sigma\left(\langle\alpha_{\sigma_1}|\cdots\langle\alpha_{\sigma_n}|\right)\left(|\beta_{\pi_1}\rangle\otimes\cdots\otimes|\beta_{\pi_n}\rangle\right) \tag{1.36}$$

$$= \frac{1}{n!}\sum_{\sigma,\pi}\zeta^\pi\zeta^\sigma\,\langle\alpha_{\sigma_1}|\beta_{\pi_1}\rangle\cdots\langle\alpha_{\sigma_n}|\beta_{\pi_n}\rangle \tag{1.37}$$

$$= \frac{1}{n!}\sum_{\sigma,\pi}\zeta^{\pi\sigma^{-1}}\left\langle\alpha_1|\beta_{\pi\sigma^{-1}(1)}\right\rangle\cdots\left\langle\alpha_n|\beta_{\pi\sigma^{-1}(n)}\right\rangle \tag{1.38}$$

$$= \sum_{\rho=\pi\sigma^{-1}}\zeta^\rho\,\langle\alpha_1|\beta_{\rho_1}\rangle\cdots\langle\alpha_n|\beta_{\rho_n}\rangle \tag{1.39}$$

$$= \left|\begin{pmatrix}\langle\alpha_1|\beta_1\rangle & \cdots & \langle\alpha_1|\beta_n\rangle\\ \vdots & \ddots & \vdots\\ \langle\alpha_n|\beta_1\rangle & \cdots & \langle\alpha_n|\beta_n\rangle\end{pmatrix}\right|_\zeta \tag{1.40}$$

where $|A|_\zeta \equiv \sum_\pi \zeta^\pi A_{1\pi_1}\cdots A_{n\pi_n}$ is the determinant or permanent for $\zeta=-1$ or $+1$ respectively. In the tricky step after (1.37) we permuted the factors in the product by the permutation σ (they are just numbers after all), and used $\zeta^\pi\zeta^\sigma = \zeta^\pi\zeta^{\sigma^{-1}} = \zeta^{\pi\sigma^{-1}}$.

Particles in free space. [Baym, chapter 19] Let's focus for a bit on the special but important example of particles (bosons or fermions) living in a rectangular periodic box of volume $V = L_xL_yL_z$ in the continuum. Then a useful basis of single-particle states is the plane waves

$$u_p(r) = \langle r|p\rangle = \frac{e^{\mathbf{i}\vec{p}\cdot\vec{r}}}{\sqrt{V}},\quad p_i = \frac{2\pi n_i}{L_i},\quad n_i\in\mathbb{Z},\quad i=x,y,z.$$

We can include a spin label $s=\uparrow,\downarrow$, too. So $\mathbf{a}^\dagger_{ps}$ adds a particle with momentum p and spin s; the amplitude for the particle to be at r is $u_p(r)$. And $\mathbf{a}_{ps}$ removes such a particle. These particles are bosons or fermions according to the algebra of the $\mathbf{a}$s

$$\mathbf{a}_{ps}\mathbf{a}^\dagger_{p's'} - \zeta\mathbf{a}^\dagger_{p's'}\mathbf{a}_{ps} = \mathbb{1}\delta_{pp'}\delta_{ss'}.$$

Now consider

$$\psi^\dagger_s(r) \equiv \sum_p u^\star_p(r)\mathbf{a}^\dagger_{ps}.$$

This adds a particle in a particular superposition of plane waves. In the state $\psi^\dagger_s(r)\,|0\rangle$, the amplitude for finding the particle at position r' is[13] (using the completeness relation

[13] More precisely, including the spin label, the amplitude to find a particle at position at r' with

for our single-particle basis $\mathbb{1}_1 = \sum_p |p\rangle\langle p|$)

$$\langle r'| \psi^\dagger(r) |0\rangle = \sum_p u_p^\star(r) u_p(r') = \delta(r - r').$$

(The δ function on the RHS here is a d-dimensional δ-function, $\delta^d(r - r')$ but I'll omit the superscript d to avoid clutter.) So we can say that $\psi^\dagger(r)$ adds a particle at position r. (Notice that this is a special case of the general formula (1.34); if we wanted to be uniform, we would call it $a^\dagger(r)$.) The $\psi(r)$ are called "field operators," just like ϕ in our discussion of scalar field theory or $A_\mu(x)$ in our discussion of electrodynamics in vacuum. A big difference is that now ψ may be a fermionic object (if $\zeta = -1$). What I mean by this is that they satisfy

$$\psi_s(r)\psi^\dagger_{s'}(r') - \zeta\psi^\dagger_{s'}(r')\psi_s(r) = \sum_{pp'} u_p(r)u^\star_{p'}(r')\delta_{ss'} \underbrace{\left(\mathbf{a}_{ps}\mathbf{a}^\dagger_{p's'} - \zeta\mathbf{a}^\dagger_{p's'}\mathbf{a}_{ps}\right)}_{=\delta_{pp'}\delta_{ss'}} = \delta_{ss'}\delta(r - r'). \tag{1.41}$$

$$\psi(r)\psi(r') - \zeta\psi(r')\psi(r) = 0, \quad \psi^\dagger(r)\psi^\dagger(r') - \zeta\psi^\dagger(r')\psi^\dagger(r) = 0. \tag{1.42}$$

When adding or creating particles at different points, the order doesn't matter (up to a sign for fermions). But at the same point, it matters if there is a particle there already. For example, if there is no particle there then $\psi^\dagger\psi = 0$, but $\psi\psi^\dagger \neq 0$.

Now we can make a position eigenstate of n particles (let's forget about spin for a moment):

$$\begin{aligned} |r_1 r_2 \cdots r_n\rangle &= \frac{1}{\sqrt{n!}}\psi^\dagger(r_n)\cdots\psi^\dagger(r_2)\psi^\dagger(r_1)|0\rangle \\ &= \zeta |r_2 r_1 \cdots r_n\rangle . \end{aligned} \tag{1.43}$$

The statistics are automatic.

To add one more particle, we can try to do

$$\psi^\dagger(r)|r_1\cdots r_n\rangle = \sqrt{n+1}\,|r_1\cdots r_n, r\rangle$$

and again the state is automatically (anti)symmetrized. To *remove* a particle, we just

---

spin s' is

$$\langle r's'|\psi^\dagger(r)|0\rangle = \sum_p u_p^\star(r)\langle r's'|\mathbf{a}^\dagger_{ps}|0\rangle = \sum_p u_p^\star(r)u_p(r')\delta_{ss'} = \delta(r-r')\delta_{ss'} .$$

So we can conclude that $|rs\rangle = \psi^\dagger_s(r)|0\rangle$.

do

$$\psi(r)\,|r_1\cdots r_n\rangle = \frac{1}{\sqrt{n!}}\psi(r)\psi^\dagger(r_n)\cdots\psi^\dagger(r_2)\psi^\dagger(r_1)\,|0\rangle \tag{1.44}$$

$$= \frac{1}{\sqrt{n!}}\left(\delta(r-r_n)+\zeta\psi^\dagger(r_n)\psi(r)\right)\psi^\dagger(r_{n-1})\cdots\psi^\dagger(r_1)\,|0\rangle \tag{1.45}$$

$$= \cdots \tag{1.46}$$

$$= \frac{1}{\sqrt{n}}\left(\delta(r-r_n)\,|r_1\cdots r_{n-1}\rangle + \zeta\delta(r-r_{n-1})\,|r_1\cdots r_{n-2}r_n\rangle + \cdots\zeta^{n-1}\delta(r-r_1)\,|r_2\cdots r_n\rangle\right). \tag{1.47}$$

So this is only nonzero if the position r at which we try to remove the particle is one of the positions r_i of the particles that are present. If it is, then we get a perfectly (anti)symmetrized $n-1$-particle state.

A similar calculation tells us the inner product between these states:

$$\langle r'_1\cdots r'_n|r_1\cdots r_n\rangle = \frac{\delta_{nn'}}{n!}\sum_{\pi\in S_n}\zeta^\pi\left(\delta(r_1-r'_{\pi_1})\delta(r_2-r'_{\pi_2})\cdots\delta(r_n-r'_{\pi_n})\right).$$

Warning: Actually the state (1.43) is not normalized. Consider for example $n=2$ with $r_1\neq r_2$, where

$$\langle r_1r_2|r_1r_2\rangle = \frac{1}{2}\langle 0|\,\psi(r_2)\,\underbrace{\psi(r_1)\psi^\dagger(r_1)}_{=\zeta\psi^\dagger(r_1)\psi(r_1)+\mathbb{1}}\,\psi^\dagger(r_2)\,|0\rangle \overset{(1.41)(1.42)}{=} \frac{1}{2}. \tag{1.48}$$

The reason is basically that $|r_1r_2\rangle$ and $|r_2r_1\rangle$ are not different and each count as half a state in the resolution of the identity we'll find below – they aren't different states! If we wanted to, we could normalize this state to one and try to sum only over $r_1\leq r_2$. This requires putting an order on the points and is annoying. Feynman (in his wonderful *Lectures on Statistical Mechanics*, §6.7), for example, chooses to normalize his states without the $\sqrt{n!}$ and put a $1/n!$ in his resolution of the identity. However, his states are then not normalized when *e.g.* $r_1=r_2$.

How to write the n-particle state $|\Psi\rangle$ whose wavefunction of the n particles is $\Psi(r_1\cdots r_n)$? This is easy:

$$|\Psi\rangle = \sum_{r_1\cdots r_n}\Psi(r_1\cdots r_n)\,|r_1\cdots r_n\rangle.$$

Notice that this state is correctly (anti)symmetrized, even if the function $\Psi(r_1\cdots r_n)$ is not; the un-(anti)symmetric part simply disappears. The amplitude in this state for

observing the particles at $r'_1 \cdots r'_n$ is

$$\langle r'_1 \cdots r'_n | \Psi \rangle = \sum_{r_1 \cdots r_n} \Psi(r_1 \cdots r_n) \langle r'_1 \cdots r'_n | r_1 \cdots r_n \rangle \tag{1.49}$$

$$= \frac{1}{n!} \sum_{\pi} \zeta^{\pi} \Psi(r'_{\pi_1}, r'_{\pi_2} \cdots r'_{\pi_n}) \tag{1.50}$$

$$\text{if } \Psi \text{ is (anti)symmetric:} \quad = \Psi(r'_1 \cdots r'_n). \tag{1.51}$$

We can also check that the norm is

$$\langle \Psi | \Psi \rangle = \sum_{r_1 \cdots r_n} |\Psi(r_1 \cdots r_n)|^2.$$

And more generally, for any two n-particle states,

$$\langle \Phi | \Psi \rangle = \sum_{r_1 \cdots r_n} \Phi^{\star}(r_1 \cdots r_n) \Psi(r_1 \cdots r_n) = \sum_{r_1 \cdots r_n} \langle \Phi | r_1 \cdots r_n \rangle \langle r_1 \cdots r_n | \Psi \rangle .$$

(The overlap with an n'-particle state for $n \neq n'$ is zero because an extra annihilation operator will hit $|0\rangle$ or an extra creation operator will hit $\langle 0|$.) Since this is true for all $\langle \Phi|$, we can just erase the Φ and get

$$|\Psi\rangle = \sum_{r_1 \cdots r_n} |r_1 \cdots r_n\rangle\langle r_1 \cdots r_n | \Psi \rangle.$$

But this is also true for any Ψ, so we have

$$\mathbb{1}_n = \sum_{r_1 \cdots r_n} |r_1 \cdots r_n\rangle\langle r_1 \cdots r_n|$$

is the identity operator on n-particle states,

$$\mathbb{1}_{n'} |\Phi_n\rangle = \delta_{nn'} |\Phi_n\rangle .$$

The identity on the whole Fock space is

$$\mathbb{1} = \sum_n \mathbb{1}_n = |0\rangle\langle 0| + \sum_{n=1}^{\infty} \mathbb{1}_n.$$

Operators on the Fock space. Ignore spin for a moment. I claim that $\rho(r) \equiv \psi^{\dagger}(r)\psi(r)$ is the *density* of particles at r. The idea is simply: try to remove one, and if you find one there, put it back (otherwise you get zero). Here is a more formal

demonstration of this claim. If Ψ, Ψ' are n-particle states,

$$\begin{aligned}
\langle\Psi'|\,\rho(r)\,|\Psi\rangle &= \langle\Psi'|\,\psi^\dagger(r)\psi(r)\,|\Psi\rangle && (1.52)\\
&= \langle\Psi'|\,\psi^\dagger(r)\mathbb{1}\psi(r)\,|\Psi\rangle && (1.53)\\
&= \langle\Psi'|\,\psi^\dagger(r)\mathbb{1}_{n-1}\psi(r)\,|\Psi\rangle && (1.54)\\
&= \sum_{r_1\cdots r_{n-1}} \langle\Psi'|\,\psi^\dagger(r)|r_1\cdots r_{n-1}\rangle\langle r_1\cdots r_{n-1}|\psi(r)\,|\Psi\rangle && (1.55)\\
&= n\sum_{r_1\cdots r_{n-1}} \langle\Psi'|\,(|r_1\cdots r_{n-1}r\rangle\langle r_1\cdots r_{n-1}r|)\,|\Psi\rangle && (1.56)\\
&= \sum_{r_1\cdots r_n} \langle\Psi'|r_1\cdots r_n\rangle\,\langle r_1\cdots r_n|\Psi\rangle \sum_{i=1}^n \delta(r-r_i) && (1.57)
\end{aligned}$$

where here $\sum_i \delta(r-r_i)$ counts the number of particles at r. Similarly, with spin, $\rho_s(r) \equiv \psi_s^\dagger(r)\psi_s(r)$ counts the number of particles of spin s at r, and $\sum_s \rho_s(r)$ counts the total number of particles at r.

$$\mathbf{N} = \sum_r \rho(r) = \sum_{p,s} \mathbf{a}_{ps}^\dagger \mathbf{a}_{ps}$$

counts the total number of particles. [End of Lecture 7]

Let's write some other one-body operators in terms of ψ. We saw above that the kinetic energy was

$$K = \sum_{ps} \mathbf{a}_{ps}^\dagger \mathbf{a}_{ps} \frac{p^2}{2m}.$$

Inverting the relation between $\mathbf{a}_p$ and ψ_r

$$\mathbf{a}_{ps} = \sum_r \frac{e^{\mathbf{i}pr}}{\sqrt{V}}\psi_s(r)^\dagger, \quad \mathbf{a}_{ps}^\dagger = \sum_r \frac{e^{-\mathbf{i}pr}}{\sqrt{V}}\psi_s(r)$$

we have (using $\vec{p}e^{\mathbf{i}pr} = -\mathbf{i}\vec{\nabla}e^{\mathbf{i}pr}$),

$$K = \frac{1}{2mV}\sum_p \sum_{rr'} \left(\vec{\nabla}e^{\mathbf{i}pr}\right)\left(\vec{\nabla}'e^{-\mathbf{i}pr'}\right)\psi_s(r)^\dagger\psi_s(r') \overset{\text{IBP}\times 2}{=} \sum_{rr'} \underbrace{\frac{1}{V}\sum_p e^{\mathbf{i}p(r-r')}}_{=\delta_{rr'}} \frac{\vec{\nabla}\psi^\dagger\cdot\vec{\nabla}\psi}{2m} = \sum_r \frac{\vec{\nabla}\psi^\dagger\cdot\vec{\nabla}\psi}{2m}.$$

The particle current is

$$\vec{j}(r) = \frac{1}{2m\mathbf{i}}\left(\psi^\dagger(r)\vec{\nabla}\psi(r) - \left(\vec{\nabla}\psi^\dagger(r)\right)\psi(r)\right)$$

and the spin density is

$$\vec{S}(r) = \sum_{ss'} \psi_s^\dagger(r)\frac{\vec{\sigma}_{ss'}}{2}\psi_{s'}(r),$$

where $\vec{\sigma}$ are the Pauli matrices.

Now I can explain the origin of the weird and misleading name 'second quantization'. The above expressions bear some visual similarity with the corresponding single-particle expressions, were I to mistake the field operator $\psi(r)$ for a single-particle wavefunction. So it looks as if we've taken the single-particle QM expressions for various observables and in each of them replaced the wavefunction with an operator. That's not actually what we did!

The many body hamiltonian for a collection of non-interacting particles in a potential (for which the one-body hamiltonian is $\mathbf{H} = \frac{\mathbf{p}^2}{2m} + V(r)$) is then

$$\mathbf{H} = \sum_r \left(\frac{\vec{\nabla}\psi^\dagger \cdot \vec{\nabla}\psi}{2m} + \psi^\dagger(r)\psi(r)V(r) \right). \tag{1.58}$$

Why do I call this non-interacting? Well, notice that each of these operators we've written is of the form $\psi^\dagger\psi$ – whenever it removes a particle, it puts it right back. An interaction is something involving more powers of ψ, so that the doings of one particle have an influence on those of another.

Interactions. [Feynman §6.8] For example, we might wish to consider a 2-body interaction $V^{(2)}(x_i, y_i)$, which acts within the 2-particle Hilbert space as

$$V^{(2)} = \frac{1}{2}\sum_x \sum_y |x,y\rangle\langle x,y|V^{(2)}(x,y).$$

An example to think about is the Coulomb potential, $V^{(2)}(x,y) = \frac{e^2}{|x-y|}$. We want to find an operator that acts on an n-particle state as

$$\hat{V}\,|r_1 \cdots r_n\rangle = \frac{1}{2}\sum_{ij} V^{(2)}(r_i, r_j)\,|r_1 \cdots r_n\rangle\,. \tag{1.59}$$

A first guess might be

$$\hat{V}_{\text{guess}} = \frac{1}{2}\sum_{x,y} V^{(2)}(x,y)\rho(x)\rho(y)$$

where $\rho(x) \equiv \psi^\dagger(x)\psi(x)$ is the particle density operator. This is almost correct. However

$$\rho(x)\rho(y) = \psi_x^\dagger\psi_x\psi_y^\dagger\psi_y = \zeta\psi_x^\dagger\psi_y^\dagger\psi_x\psi_y + \delta_{xy}\psi_x^\dagger\psi_y = \psi_x^\dagger\psi_y^\dagger\psi_y\psi_x + \delta_{xy}\rho(x)$$

it is not *normal-ordered*. Normal-ordered means all annihilation operators are to the right of all creation operators. This is a good feature because it will mean that there is no part of the operator that is secretly a single-particle operator. The correct $\hat{V}$

$$\hat{V} = \hat{V}_{\text{guess}} - \frac{1}{2}\sum_x V^{(2)}(x,x)\rho(x)$$

subtracts off this 'self-energy' term.

Let's check that this definition

$$\hat{V} = \frac{1}{2}\sum_{xy} \psi_x^\dagger \psi_y^\dagger \psi_y \psi_x V^{(2)}(x,y)$$

achieves the goal (1.59). First[14]

$$\psi_y \psi_x \left|r_1 \cdots r_n\right\rangle = \psi_y \sum_{i=1}^{n} \zeta^{n-i-1} \delta_{x,r_i} \left|r_1 \cdots \widehat{r_i} \cdots r_n\right\rangle \frac{1}{\sqrt{n}} \tag{1.60}$$

$$= \sum_{i=1}^{n} \zeta^{n-i-1} \delta_{x,r_i} \sum_{j=1, j\neq i}^{n} \eta_{ji} \delta_{y,r_j} \left|r_1 \cdots \widehat{r_i} \cdots \widehat{r_j} \cdots r_n\right\rangle \frac{1}{\sqrt{n(n-1)}} \tag{1.61}$$

where a hat means that that particle is missing, and $\eta_{ji} = \begin{cases} \zeta^{n-j-1}, & j < i \\ \zeta^{n-j}, & j > i \end{cases}$. So we get some horrible signs to keep track of. Now

$$\psi_x^\dagger \psi_y^\dagger \psi_y \psi_x \left|r_1 \cdots r_n\right\rangle = \sum_{i=1}^{n} \zeta^{n-i-1} \delta_{x,r_i} \sum_{j=1, j\neq i}^{n} \eta_{ji} \delta_{y,r_j} \left|x, y, r_1 \cdots \widehat{r_i} \cdots \widehat{r_j} \cdots r_n\right\rangle \tag{1.62}$$

$$= \sum_{i=1}^{n} \zeta^{n-i-1} \delta_{x,r_i} \sum_{j=1, j\neq i}^{n} \eta_{ji} \delta_{y,r_j} \left|r_i, r_j, r_1 \cdots \widehat{r_i} \cdots \widehat{r_j} \cdots r_n\right\rangle \tag{1.63}$$

$$= \sum_{i\neq j}^{n} \delta_{x,r_i} \delta_{y,r_j} \left|r_1 \cdots r_n\right\rangle \tag{1.64}$$

All of the signs cancel out when putting the particles back in this order. Therefore

$$\frac{1}{2}\sum_{xy} V^{(2)}(x,y) \psi_x^\dagger \psi_y^\dagger \psi_y \psi_x \left|r_1 \cdots r_n\right\rangle = \frac{1}{2}\sum_{i\neq j} V^{(2)}(r_i, r_j) \left|r_1 \cdots r_n\right\rangle$$

as we asked for. Notice that this is a true interaction, in the sense that it vanishes if the number of particles is less than two.

We will learn more about interacting many-body systems. There's actually quite a bit more to say about non-interacting systems first.

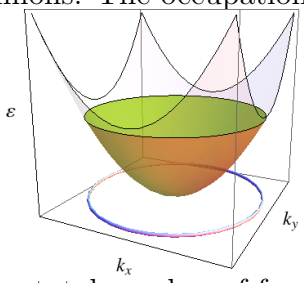
1.9 Many bosons versus many fermions

[still Baym, chapter 19] Let's return to the groundstate of a Fermi gas. Letting the fermions move wherever they want, and not just on particular orbitals can be achieved

[14] Beware the conventions for the order of the operators in $\left|r_1 \cdots r_n\right\rangle \propto \psi(r_n)^\dagger \cdots \psi(r_1)^\dagger \left|0\right\rangle$. With this convention, the operator ψ_x has to move through $n-i-1$ of its friends to get to $\psi(r_i)^\dagger$.

by taking the continuum limit of the model we studied in §1.7.1. This involves two steps: take $N \to \infty$, so the momentum space becomes continuous, and focus on low energies – Taylor expand about the minimum of the band, where $\epsilon(p) = \frac{p^2}{2m} + \mathcal{O}(p^4)$, and ignore the p^4 terms.

Alternatively, we could just start from scratch, using the non-interacting many-body Hamiltonian (1.58), and set $V = 0$. Either way, the single-particle levels are $\epsilon(p) = \frac{p^2}{2m}$, and in the groundstate $|\Psi_0\rangle$ we fill them from the bottom until we run out of fermions. The occupation numbers are



$$n_{ps} \equiv \langle \Phi_0 | \, \mathbf{a}^\dagger_{ps} \mathbf{a}_{ps} \, | \Phi_0 \rangle = \begin{cases} 1, & |p| < p_F \\ 0, & |p| > p_F \end{cases} . \tag{1.65}$$

The total number of fermions is

$$N = \sum_{sp} n_{ps} = 2 \sum_{|p|<p_F} 1 \overset{V\to\infty}{=} 2V \int_0^{p_F} \text{đ}^d p \overset{d=3}{=} \frac{p_F^3}{3\pi^2} V \tag{1.66}$$

which determines the Fermi momentum $p_F^d = 3\pi^2 \frac{N}{V} \equiv 3\pi^2 n$ in terms of the average particle number density $n = N/V$:

$$p_F \propto \left(\frac{N}{V}\right)^{1/d} .$$

Fermi pressure. This groundstate of free fermions is actually quite an interesting state. One reason is that it can contain particles with quite large momentum. These particles exert a pressure on the walls of a container holding such a gas, even at zero temperature. To see this *Fermi pressure*, consider the groundstate energy:

$$E_0 = \langle \Phi_0 | \mathbf{H} | \Phi_0 \rangle = \langle \Phi_0 | \sum_{ps} \mathbf{a}^\dagger_{ps} \mathbf{a}_{ps} \frac{p^2}{2m} \, | \Phi_0 \rangle \tag{1.67}$$

$$= \sum_s \sum_{|p|<p_F} \frac{p^2}{2m} \overset{V\to\infty}{=} 2V \int_{|p|<p_F} \text{đ}^d p \frac{p^2}{2m} \tag{1.68}$$

$$\overset{d=3}{=} 2V \frac{4\pi}{(2\pi)^3} \int_0^{p_F} \frac{p^2}{2m} p^2 dp = \frac{p_F^2}{2m} \frac{p_F^3 V}{5\pi^2} \overset{(1.66)}{=} \frac{3}{5} \frac{p_F^2}{2m} N = \frac{3}{5} \varepsilon_F N \tag{1.69}$$

where $\varepsilon_F = \frac{p_F^2}{2m}$ is the *Fermi energy*, the energy of the last-filled single-particle state. That is, the groundstate energy per particle is

$$\frac{E_0}{N} = \frac{3}{5} \varepsilon_F .$$

Now recall the definition of pressure[15]: at zero temperature,

$$P = -\frac{dE_0}{dV}|_N. \tag{1.70}$$

This gives

$$P = -\partial_V|_N \left(\frac{3}{5}\frac{N}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}\right) = +\frac{3}{5}\frac{2}{3}\frac{1}{2m}N^{5/3}(3\pi^2)^{2/3}V^{-5/3} = \frac{2}{3}\frac{E_0}{V}.$$

Contrast this with the pressure for a classical ideal gas as $T \to 0$!

This degeneracy pressure is what holds up white dwarfs (from electrons) and neutron stars (from neutrons). In fact, the contribution from the electron degeneracy pressure plays an important role in determining the lattice spacing of solids. Moreover, its contribution to holding up the volume of a solid is *necessary* for the stability of matter, as demonstrated here in this wonderful paper by Freeman Dyson, where he shows that the Coulomb repulsion is insufficient. [End of Lecture 8]

1.9.1 Correlations in the groundstate of the Fermi gas

As a warmup, let's look at the density in the groundstate

$$\langle \rho(r)\rangle_{\Phi_0} = \sum_s \left\langle \Phi_0|\psi_s^\dagger(r)\psi_s(r)|\Phi_0\right\rangle = \sum_{spp'} u_p^\star(r)u_{p'}(r)\underbrace{\langle \Phi_0|\, \mathbf{a}_{ps}^\dagger \mathbf{a}_{p's}\,|\Phi_0\rangle}_{=\delta_{pp'}n_{ps}} = \frac{1}{V}\sum_{ps} n_{ps} = n,$$

where n_{ps} is the groundstate occupation number (1.65). Indeed the density is uniform, and therefore equal to the average density.

Now consider the similar but more interesting quantity, sometimes called the one-particle density matrix, which depends on two positions:

[15] If you like, you can think about it thermodynamically,

$$dE = TdS - PdV + \mu dN.$$

We are at $T = 0$ and fixed N, so we get (1.70).

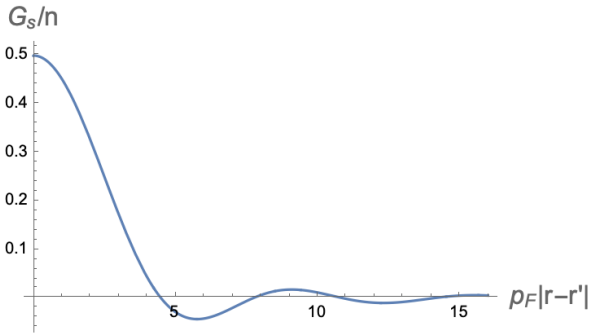
$$G_s(r-r') \equiv \left\langle \Phi_0 | \psi_s^\dagger(r) \psi_s(r') | \Phi_0 \right\rangle \tag{1.71}$$

$$= \frac{1}{V} \sum_p e^{-\mathbf{i}p\cdot(r-r')} n_{ps} \tag{1.72}$$

$$= \int_0^{p_F} \mathrm{đ}^d p e^{-\mathbf{i}p\cdot(r-r')} \tag{1.73}$$

$$\overset{d=3}{=} \frac{1}{4\pi^2} \int_0^{p_F} dp p^2 \underbrace{\int_{-1}^{1} d\mu e^{-\mathbf{i}p|r-r'|\mu}}_{=2\frac{\sin p|r-r'|}{p|r-r'|}} \tag{1.74}$$

$$= \frac{3n}{2} \left(\frac{\sin x - x\cos x}{x^3} \right) \tag{1.75}$$



where $x \equiv p_F|r-r'|$. This function is depicted at left. Notice that we used translation invariance to anticipate that $G(r,r')$ would only depend on the difference of positions. It oscillates with a period $2\pi/p_F$ with a power-law decaying envelope.[16]

Pair correlation functions. Fermions avoid each other. Bosons not only don't avoid each other, but they clump. Here we will justify these vague words by figuring out what is

$$\mathrm{Prob}_{\Phi_0}(\text{particle at } r' | \text{particle at } r)$$

– the probability of finding a particle at r' given that there is a particle at r (in the groundstate)? To do this, we first *remove* a particle from the groundstate of N particles:

$$|\Phi(rs)\rangle_{N-1} \equiv \psi_s(r) |\Phi_0\rangle .$$

Of course this is zero if there is no such particle at r. Then in *this* state, we ask about

[16] A number of people have asked me about the physical significance of $G_s(r)$. One answer is that in some systems it can be measured by angle-resolved photoemission. This is an experiment where we kick a particle out of the system (for example by hitting it with a high-energy photon with known momentum and energy k, E), then we measure the momentum and energy p, ω of the particle we kicked out. The intensity as a function of $(k-p, E-\omega)$ is the imaginary part of the Fourier transform of G. You can see this by using Fermi's golden rule.

the expected density at r' (which is the probability to find a particle at r'[17]):

$$\text{Prob}_{\Phi_0}(\text{particle at } r' | \text{particle at } r) = \tag{1.80}$$

$$\text{Prob}_{\Phi(rs)}(\text{particle at } r') = \langle \Phi(rs)| \psi^\dagger_{s'}(r')\psi_{s'}(r') |\Phi(rs)\rangle \tag{1.81}$$

$$= \langle \Phi_0| \psi^\dagger_s(r)\psi^\dagger_{s'}(r')\psi_{s'}(r')\psi_s(r) |\Phi_0\rangle \equiv \left(\frac{n}{2}\right)^2 g_{ss'}(r-r')$$

$$= \frac{1}{V^2}\sum_{pp'qq'} e^{-\mathbf{i}(p-p')r-\mathbf{i}(q-q')r'} \langle \Phi_0| \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{qs'}\mathbf{a}_{q's'}\mathbf{a}_{p's} |\Phi_0\rangle \ . \tag{1.82}$$

The matrix element is zero unless the particles we remove with the $\mathbf{a}$s have the same labels as the particles we put back with the $\mathbf{a}^\dagger$s.

First consider $s \neq s'$. Then the only possibility is $p' = p, q' = q$, so

$$\langle \Phi_0| \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{qs'}\mathbf{a}_{q's'}\mathbf{a}_{p's} |\Phi_0\rangle = \delta_{pp'}\delta_{qq'}s^2 \langle \Phi_0| \mathbf{a}^\dagger_{ps}\mathbf{a}_{ps}\mathbf{a}^\dagger_{qs'}\mathbf{a}_{qs'} |\Phi_0\rangle = \delta_{pp'}\delta_{qq'}n_{ps}n_{qs'}$$

Therefore, for $s \neq s'$,

$$g_{ss'}(r-r') = \left(\frac{2}{n}\right)^2 \frac{1}{V^2}\sum_{pq} n_{ps}n_{qs'} = \left(\frac{2}{n}\right)^2 \frac{1}{V^2} N_s N_{s'} = 1,$$

since $N_s = \frac{N}{2}$ for each spin. This is the classical behavior of non-interacting particles – the locations of particles of different spins are uncorrelated.

Now consider $s = s'$. Then there are two ways to put back what we took out: $p = p', q = q'$ or $p = q', q = p'$. So in this case

$$\langle \Phi_0| \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{qs}\mathbf{a}_{q's}\mathbf{a}_{p's} |\Phi_0\rangle = \delta_{pp'}\delta_{qq'} \left\langle \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{qs}\mathbf{a}_{qs}\mathbf{a}_{ps}\right\rangle + \delta_{pq'}\delta_{qp'} \left\langle \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{qs}\mathbf{a}_{ps}\mathbf{a}_{qs}\right\rangle \tag{1.83}$$

$$= (\delta_{pp'}\delta_{qq'} - \delta_{pq'}\delta_{qp'}) \underbrace{\left\langle \mathbf{a}^\dagger_{ps}\mathbf{a}^\dagger_{ps}\mathbf{a}_{qs}\mathbf{a}_{qs}\right\rangle}_{=n_{ps}n_{qs}} \ . \tag{1.84}$$

[17] Actually this step is maybe not obvious. Here's the idea: if Φ is an N-particle state, then

$$\text{Prob}_\Phi(\text{particle at } r') = N \sum_{r_2\cdots r_N} |\langle r' r_2 \cdots r_N|\Phi\rangle|^2 \tag{1.76}$$

$$= N \langle \Phi| \left(\sum_{r_2\cdots r_N} |r' r_2 \cdots r_n\rangle\langle r' r_2 \cdots r_N| \right) |\Phi\rangle \tag{1.77}$$

$$= \frac{N}{N} \langle \Phi| \psi^\dagger(r') \underbrace{\sum_{r_2\cdots r_N} |r_2 \cdots r_N\rangle\langle r_2 \cdots r_N|}_{=\mathbb{1}_{N-1}} \psi(r') |\Phi\rangle \tag{1.78}$$

$$= \langle \Phi| \psi^\dagger(r')\psi(r') |\Phi\rangle \, . \tag{1.79}$$

The factor of N in the first line is because the particle we find could be any of the N particles (as in (1.28)). Note that $\int dr \text{Prob}_\Phi(r) = N$, but this is OK, since finding particles at different places are not exclusive events! (Note that if r is continuous then by 'Prob' I mean probability density.)

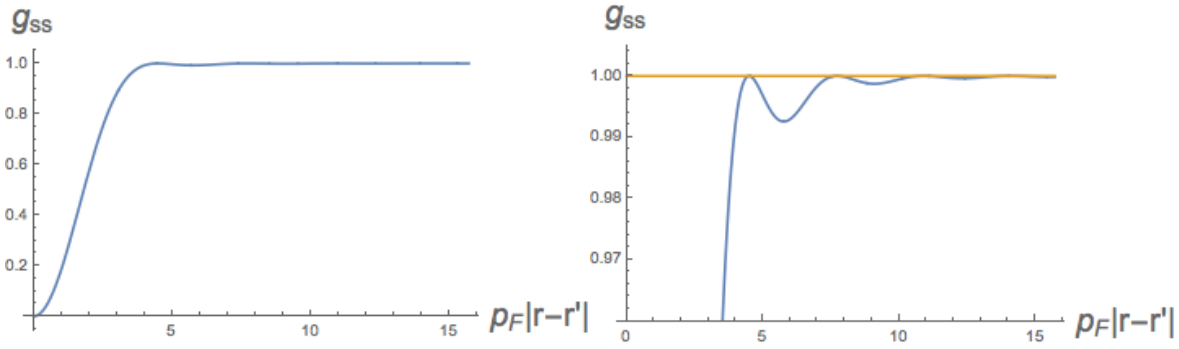
In the underbrace we used $\{\mathbf{a}_{ps}, \mathbf{a}^\dagger_{qs}\} = \delta_{p,q}$. But the contribution from $p = q$ cancels between the two terms by Fermi statistics. Therefore for like spins,

$$\left(\frac{n}{2}\right)^2 g_{ss}(r-r') = \frac{1}{V^2}\sum_{pq}\left(1 - e^{-\mathbf{i}(p-q)\cdot(r-r')}\right) n_{ps}n_{qs} = \left(\frac{n}{2}\right)^2 - (G_s(r-r'))^2 \quad (1.85)$$

and therefore

$$g_{ss}(r-r') = 1 - \frac{9}{x^6}\left(\sin x - x\cos x\right)^2, \quad x \equiv p_F|r-r'|,$$

which is plotted below:



In the right plot, we zoom in to show the oscillations with period π/p_F. The key point, though, is that there is a big trough around $r = r'$ which is a consequence of the Pauli principle combined with the kinetic energy wanting to make the wavefunctions smooth.

Compare this plot to the analogous plot for a perfect solid. In that case $g(r)$ would have peaks whenever $|r|$ = a lattice vector, and zero otherwise. This is because the location of one atom determines all the rest. Now consider a liquid made of particles with short-range repulsion. Then again $g(r) = 0$ when $r < R$ where R is the hard core radius of the particles. There will be a peak in $g(r)$ just past R, since the particles are trying to be close together in a liquid. After some wiggles, the answer will approach the uniform answer because the correlations between the positions are only short-ranged. It generally looks like the plot above! Fermions achieve such correlations without any interactions.

1.9.2 Easy problems versus hard problems

There is more to say about correlation functions of the form we've been discussing, to illustrate the contrast between bosons and fermions. But first an important general comment which will also establish some notation.

Non-interacting/Gaussian/Free systems. So far, we have been studying a very special class of quantum many-body systems, where the Hamiltonian is of the

form

$$\mathbf{H} = \sum_{ij}^{D} \mathbf{a}_i^\dagger \mathbf{a}_j h_{ij} \qquad (i,j = 1 \cdots D = \dim \mathcal{H}_1) \tag{1.86}$$

in terms of some creation and annihilation operators

$$[\mathbf{a}_i, \mathbf{a}_j^\dagger]_\pm \equiv \mathbf{a}_i \mathbf{a}_j^\dagger \mp \mathbf{a}_j^\dagger \mathbf{a}_i = \delta_{ij}.$$

The fact that $\mathbf{H}$ is quadratic in these operators means that it is solvable by diagonalizing the (hermitian, if $\mathbf{H}$ is hermitian) matrix h. That is, find the eigenvectors $u_\alpha(i)$ so that $h_{ij} u_\alpha(i) = \epsilon_\alpha u_\alpha(i)$. Then[18], if we let $\mathbf{a}_i = \sum_\alpha u_\alpha(i) \mathbf{a}(u_\alpha)$ in terms of a new set of (normal) modes $\mathbf{a}(u_\alpha)$, then

$$\mathbf{H} = \sum_\alpha \epsilon_\alpha \mathbf{a}^\dagger(u_\alpha) \mathbf{a}(u_\alpha)$$

decomposes into a sum of independent oscillators. The eigenstates of $\mathbf{H}$ are then of the form

$$|\psi\rangle \equiv \mathbf{a}^\dagger(u_1) \cdots \mathbf{a}^\dagger(u_n) |0\rangle, \quad \text{where } \mathbf{a}(u_\alpha) |0\rangle = 0 \tag{1.87}$$

with

$$\mathbf{H} |\psi\rangle = \sum_{\alpha=1}^{n} \epsilon_\alpha |\psi\rangle .$$

In the case of fermions, all the u_α must be distinct to get a nonzero state, in the case of bosons, not.

Now you might say, well, any $\mathbf{H}$ you can write is just a big matrix, and we can solve the system by diagonalizing it. Yes, but notice that the matrix h_{ij} here is a $D \times D$ matrix, where D is the size of the single-particle Hilbert space. This size is in stark contrast to the size of $\mathbf{H}$ as a matrix on the many-body Hilbert space. Even if we fix the number of particles to be N, it is a matrix whose size grows exponentially in N (almost like D^N). The third section of the notes is called Hard Problems, and the subject is all the other Hamiltonians which we can't solve by diagonalizing a single-particle Hamiltonian.

Notice, by the way, that (1.86) is not necessarily translation invariant. If it's not, it makes the $D \times D$ matrix harder to diagonalize, but it is still generally doable.

[End of Lecture 9]

1.9.3 Wick's theorem

The calculation we did of the pair correlation function is a special case of a very useful fact about correlation functions of free fermions (but not free bosons, as we'll see).

[18] Notice that $u_\alpha^i \equiv u_\alpha(i)$ is a unitary matrix since the eigenvectors are orthonormal.

Consider correlation functions in a state $|\psi\rangle$ of the form (1.87), which is an eigenstate of our free Hamiltonian (not necessarily the groundstate). Here $\mathbf{a}_x \equiv \psi(x)$ is just another name for the field operator, but could be in an arbitrary basis; α labels the eigenbasis of h_{xy}.

$$G_\psi(x,y) = \langle\psi|\, \mathbf{a}_x^\dagger \mathbf{a}_y \,|\psi\rangle = \sum_{\alpha\beta} \underbrace{\langle\psi|\, \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta \,|\psi\rangle}_{=\delta_{\alpha\beta} n_\alpha} u_\alpha^\star(x) u_\beta(y) = \sum_{\alpha\in\psi} u_\alpha^\star(x) u_\alpha(y).$$

This is only nonzero if we put back what we take out, so $\alpha = \beta$. What I mean by $\alpha \in \psi$ is that the state α is one of the single-particle states $\{1 \cdots n\}$ that are occupied in the state $|\psi\rangle$.

Now a more general 2-particle correlator:

$$C \equiv \langle\psi|\, \mathbf{a}_x^\dagger \mathbf{a}_{x'}^\dagger \mathbf{a}_y \mathbf{a}_{y'} \,|\psi\rangle = \sum_{\alpha\beta\gamma\delta} \langle\psi|\, \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\gamma \mathbf{a}_\delta \,|\psi\rangle\, u_\alpha^\star(x) u_\beta^\star(x') u_\gamma(y) u_\delta(y').$$

To evaluate it, we expand the field operators in terms of the single-particle eigenstates. To be nonzero, again we must put back what we took out, so we need $\alpha = \gamma, \beta = \delta$ or $\alpha = \delta, \beta = \gamma$, and for fermions we must have $\alpha \neq \beta$. Therefore

$$\begin{aligned}
C = \sum_{\alpha\neq\beta} \Big(& \langle u_1 \cdots u_n|\, \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\alpha \mathbf{a}_\beta \,|u_1 \cdots u_n\rangle\, u_\alpha^\star(x) u_\beta^\star(x') u_\alpha(y) u_\beta(y') && (1.88)\\
& + \langle u_1 \cdots u_n|\, \mathbf{a}_\alpha^\dagger \mathbf{a}_\beta^\dagger \mathbf{a}_\beta \mathbf{a}_\alpha \,|u_1 \cdots u_n\rangle\, u_\alpha^\star(x) u_\beta^\star(x') u_\beta(y) u_\alpha(y') \Big) && (1.89)\\
& = \sum_{\alpha\neq\beta\in\psi} \big(-u_\alpha^\star(x) u_\alpha(y) u_\beta^\star(x') u_\alpha(y') + u_\alpha^\star(x) u_\alpha(y') u_\beta^\star(x') u_\alpha(y) \big) \\
& = -\left(\sum_{\alpha\in\psi} u_\alpha^\star(x) u_\alpha(y)\right)\left(\sum_{\beta\in\psi} u_\beta^\star(x') u_\beta(y')\right) + \left(\sum_{\alpha\in\psi} u_\alpha^\star(x) u_\alpha(y')\right)\left(\sum_{\beta\in\psi} u_\beta^\star(x') u_\beta(y)\right) && (1.90)\\
& = \left\langle \mathbf{a}_x^\dagger \mathbf{a}_{y'} \right\rangle_\psi \left\langle \mathbf{a}_{x'}^\dagger \mathbf{a}_y \right\rangle_\psi - \left\langle \mathbf{a}_x^\dagger \mathbf{a}_y \right\rangle_\psi \left\langle \mathbf{a}_{x'}^\dagger \mathbf{a}_{y'} \right\rangle_\psi && (1.91)
\end{aligned}$$

where in the step (1.89) we used the sneaky trick of adding back in the term with $\alpha = \beta$ because it cancels between the two terms.

This was a complicated calculation, but now that we've done it, the structure of the answer is simple to understand and to generalize to arbitrary n-point functions:

A correlation function of fermion operators (in a state of the form ψ) is equal to the sum of *contractions*, weighted by a $(-1)^{\#\text{ of crossings}}$.

A contraction is just a way of pairing up the creation and annihilation operators in the correlator: draw a line connecting each pair ij, and replace the pair by its two-point function in the same state, $\left\langle \mathbf{a}_i^\dagger \mathbf{a}_j \right\rangle_\psi$. By the number of crossings, I mean the number of times these lines cross each other on the piece of paper; this is the number of times we must move fermionic operators through each other.

In this example, we have

$$\left\langle \mathbf{a}_x^\dagger \mathbf{a}_{x'}^\dagger \mathbf{a}_y \mathbf{a}_{y'} \right\rangle_\psi = \left\langle \overbrace{\mathbf{a}_x^\dagger \mathbf{a}_{x'}^\dagger} \mathbf{a}_y \mathbf{a}_{y'} \right\rangle_\psi + \left\langle \overbrace{\mathbf{a}_x^\dagger \mathbf{a}_{x'}^\dagger} \mathbf{a}_y \mathbf{a}_{y'} \right\rangle_\psi .$$

The second contraction involves one crossing, and so comes with a (-1), and this reproduces (1.91).

This is a generalization to fermions of the familiar idea that in a gaussian ensemble, all correlations are products of two-point functions ('covariances').

In what sense is the state $|\psi\rangle$ gaussian? Well, correlations in the state $|\psi\rangle$, are the same as

$$\langle \psi | O | \psi \rangle = \mathrm{tr} O \rho \tag{1.92}$$

where $\rho = \lim_{\beta\to\infty} e^{-\beta \mathbf{H}}/Z$, and $\mathbf{H}$ is a quadratic operator.

1.9.4 Correlators of bosons

Now let's ask the same questions about a collection of bosons, again in a state of the form

$$|\psi\rangle \equiv \frac{1}{\prod_\alpha \sqrt{n_\alpha^\psi!}} \mathbf{b}^\dagger(u_1) \cdots \mathbf{b}^\dagger(u_n) |0\rangle , \quad \text{where } \mathbf{b}(u_\alpha)|0\rangle = 0. \tag{1.93}$$

To emphasize the difference, I've called the bosonic mode operators $\mathbf{b}$. In the case of bosons, some of the u_α in the state $|\psi\rangle$ may be the same; I'll call n_α^ψ the occupation number of the mode α in the state ψ, *i.e.*

$$\mathbf{N}_\alpha |\psi\rangle = \mathbf{b}_\alpha^\dagger \mathbf{b}_\alpha |\psi\rangle = n_\alpha^\psi |\psi\rangle . \tag{1.94}$$

The factor $\frac{1}{\prod_\alpha \sqrt{n_\alpha!}}$ is required in order that the state be normalized; recall that $|n\rangle = \frac{\left(\mathbf{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle$. Recall that $0! = 1$.

First let's think about two-point functions:

$$\left\langle \mathbf{b}_x^\dagger \mathbf{b}_y \right\rangle_\psi \equiv \langle \psi | \mathbf{b}_x^\dagger \mathbf{b}_y |\psi\rangle = \sum_{\alpha\beta} u_\alpha^\star(x) u_\beta(y) \underbrace{\langle \psi | \mathbf{b}_\alpha^\dagger \mathbf{b}_\beta |\psi\rangle}_{\overset{(1.94)}{=} \delta_{\alpha\beta} n_\alpha^\psi} = \sum_\alpha u_\alpha^\star(x) u_\alpha(y) n_\alpha^\psi .$$

This is just like the fermion case above, with the only difference that n_α can be larger than one.

Let's do the general case first:

$$B \equiv \langle\psi|\, \mathbf{b}_x^\dagger \mathbf{b}_{x'}^\dagger \mathbf{b}_y \mathbf{b}_{y'}\, |\psi\rangle = \sum_{\alpha\beta\gamma\delta} \langle\psi|\, \mathbf{b}_\alpha^\dagger \mathbf{b}_\beta^\dagger \mathbf{b}_\gamma \mathbf{b}_\delta\, |\psi\rangle\, u_\alpha^\star(x) u_\beta^\star(x') u_\gamma(y) u_\delta(y') \ . \tag{1.95}$$

Now there are three ways to put back what we took out:
(i) $\alpha = \beta = \gamma = \delta$
(ii) $\alpha \neq \beta, \alpha = \gamma, \beta = \delta$
(iii) $\alpha \neq \beta, \alpha = \delta, \beta = \gamma$. This leads to three terms

$$\begin{aligned} B = &\sum_\alpha \underbrace{\langle\psi|\, \left(\mathbf{b}_\alpha^\dagger\right)^2 \left(\mathbf{b}_\alpha\right)^2 |\psi\rangle}_{=n_\alpha^\psi(n_\alpha^\psi - 1)} u_\alpha^\star(x) u_\alpha^\star(x') u_\alpha(y) u_\alpha(y') \qquad \text{(i)} \\ &+ \sum_{\alpha\neq\beta} \underbrace{\langle\psi|\, \mathbf{b}_\alpha^\dagger \mathbf{b}_\beta^\dagger \mathbf{b}_\alpha \mathbf{b}_\beta\, |\psi\rangle}_{=n_\alpha^\psi n_\beta^\psi} u_\alpha^\star(x) u_\beta^\star(x') u_\alpha(y) u_\beta(y') \qquad \text{(ii)} \\ &+ \sum_{\alpha\neq\beta} \underbrace{\langle\psi|\, \mathbf{b}_\alpha^\dagger \mathbf{b}_\beta^\dagger \mathbf{b}_\beta \mathbf{b}_\alpha\, |\psi\rangle}_{=n_\alpha^\psi n_\beta^\psi} u_\alpha^\star(x) u_\beta^\star(x') u_\beta(y) u_\alpha(y') \qquad \text{(iii)} \ . \end{aligned}$$

Each of the second and third terms are of the form

$$\sum_{\alpha\neq\beta} n_\alpha n_\beta f_{\alpha\beta} = \sum_{\alpha\beta} n_\alpha n_\beta f_{\alpha\beta} - \sum_\alpha n_\alpha^2 f_{\alpha\alpha}. \tag{1.96}$$

Therefore

$$\begin{aligned} B = &\underbrace{\left(\sum_\alpha n_\alpha u_\alpha^\star(x) u_\alpha(y)\right)}_{=\left\langle \mathbf{b}_x^\dagger \mathbf{b}_y \right\rangle_\psi} \underbrace{\left(\sum_\beta n_\beta u_\beta^\star(x') u_\beta(y')\right)}_{=\left\langle \mathbf{b}_{x'}^\dagger \mathbf{b}_{y'} \right\rangle_\psi} + \underbrace{\left(\sum_\alpha n_\alpha u_\alpha^\star(x) u_\alpha(y')\right)}_{=\left\langle \mathbf{b}_x^\dagger \mathbf{b}_{y'} \right\rangle_\psi} \underbrace{\left(\sum_\beta n_\beta u_\beta^\star(x') u_\beta(y)\right)}_{=\left\langle \mathbf{b}_{x'}^\dagger \mathbf{b}_y \right\rangle_\psi} \\ &- \sum_\alpha n_\alpha(n_\alpha + 1) u_\alpha^\star(x) u_\alpha^\star(x') u_\alpha(y) u_\alpha(y'). \end{aligned} \tag{1.97}$$

The first line is from terms (ii) and (iii), and the second line is from (i) plus the second term in (1.96). The first line would be the result from the naive bosonic version of Wick's theorem. The second line is an extra term which is not present for fermions. So Wick's theorem is not true for a general permanent of bosons. An important exception correlations in the *vacuum*, where all the $n_\alpha = 0$; then the extra term vanishes. (This special case comes up a lot in relativistic QFT.)

Pair correlator for (spinless) bosons. A special case of the expression $B = B(x, y, x', y')$ is the pair correlation function, when the eigenmodes (for which so far

we've been using the abstract labels $\alpha, \beta...$) are momentum eigenstates. So consider a state of (non-interacting) spinless bosons in free space, in a box,

$$|\Phi\rangle = |n_{p_0} n_{p_1} \cdots\rangle$$

specified by the occupation number of each momentum mode, with density

$$\rho(x) = \langle\Phi| \mathbf{b}_x^\dagger \mathbf{b}_x |\Phi\rangle = \frac{1}{V}\sum_p n_p = n.$$

By the same argument as above, the pair correlator (proportional to the probability of finding a particle at y given that we already found one at x) is

$$n^2 g_B(x-y) \equiv \langle\Phi| \mathbf{b}_x^\dagger \mathbf{b}_y^\dagger \mathbf{b}_y \mathbf{b}_x |\Phi\rangle \tag{1.98}$$

$$= \frac{1}{V^2}\sum_{pp'qq'} e^{-\mathbf{i}(p-p')\cdot x - \mathbf{i}(q-q')\cdot y} \langle\Phi| \mathbf{b}_p^\dagger \mathbf{b}_q^\dagger \mathbf{b}_{q'} \mathbf{b}_{p'} |\Phi\rangle \tag{1.99}$$

The matrix element is

$$\begin{aligned}\langle\Phi| \mathbf{b}_p^\dagger \mathbf{b}_q^\dagger \mathbf{b}_{q'} \mathbf{b}_{p'} |\Phi\rangle &= \delta_{pq}\delta_{pp'}\delta_{qq'} \left\langle \left(\mathbf{b}_p^\dagger\right)^2 \mathbf{b}_p^2 \right\rangle && \text{(i)} \\ &+ (1-\delta_{pq})\delta_{pp'}\delta_{qq'} \left\langle \mathbf{b}_p^\dagger \mathbf{b}_q^\dagger \mathbf{b}_p \mathbf{b}_q \right\rangle && \text{(ii)} \\ &+ (1-\delta_{pq})\delta_{pq'}\delta_{qp'} \left\langle \mathbf{b}_p^\dagger \mathbf{b}_q^\dagger \mathbf{b}_q \mathbf{b}_p \right\rangle && \text{(iii)} \\ &= (1-\delta_{pq})\left(\delta_{pp'}\delta_{qq'} + \delta_{pq'}\delta_{qp'}\right) n_p n_q + \delta_{pq}\delta_{pp'}\delta_{qq'} n_p(n_p-1). \end{aligned} \tag{1.100}$$

The labelling of terms is the same as in the calculation above. The $1-\delta_{pq}$s are there to avoid overcounting. So

$$n^2 g_B(x-y) = \frac{1}{V^2}\left(\sum_p n_p \sum_q n_q + \sum_p n_p e^{-\mathbf{i}p\cdot(x-y)} \sum_q n_q e^{-\mathbf{i}q\cdot(y-x)} - \sum_p n_p(n_p+1)\right) \tag{1.101}$$

$$= n^2 + \left|\frac{1}{V}\sum_p n_p e^{-\mathbf{i}p\cdot(x-y)}\right|^2 - \frac{1}{V^2}\sum_p n_p(n_p+1). \tag{1.102}$$

Comparing this expression with the result for fermions (1.85), there are two differences. The oscillating (second) term has a plus sign for bosons, and there is an extra additive constant, the correction relative to the Wick result.

To see some physical consequences, consider two example states:

1. In the groundstate of free bosons, all N bosons are in the same (the lowest-energy) single-particle level, $|\Phi\rangle = |n_{p_0} = N\rangle$. Then we get

$$n^2 g_B(x-y) = n^2 + n^2 - \frac{N(N+1)}{V^2} = \frac{N(N-1)}{V^2}.$$

Notice that if we take $V \to \infty$ at fixed density n, we can ignore the correction to Wick. Later we will see some dramatic physical consequences of such states.

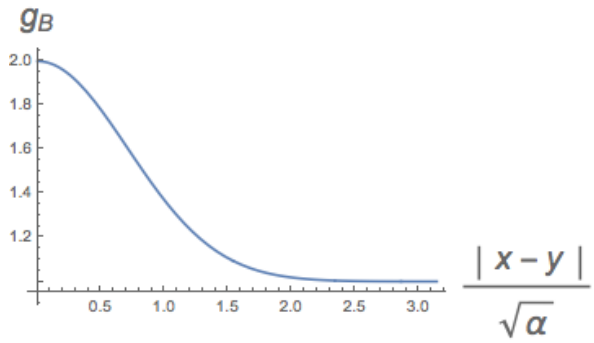
2. Consider a *beam* of particles. This is accomplished by

$$n_p = ce^{-\alpha(p-p_0)^2/2}$$

for some constants c, p_0, α. Normalization determines c in terms of the average density $n = \int đ^3 p n_p$. Again consider the thermodynamic limit ($V \to \infty$ at fixed density n):

$$g_B(x-y) \simeq \frac{1}{n^2}\left(n^2 + |\int đ^3 p n_p e^{-\mathbf{i}p\cdot(x-y)}|^2\right) = 1 + e^{-(x-y)^2/\alpha}.$$

It looks like this:



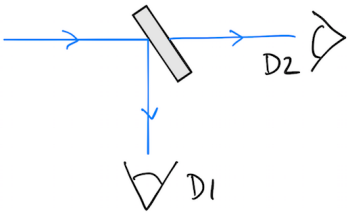
Independent of the width α of the beam, the value at $x = y$ is *twice* the value for distinguishable particles. Bosons tend to clump together!

1.9.5 Intensity interferometry

Ingredients:

- A beam of incoherent light. That means a bunch of photons of various wavelengths, emitted at at various times. A good example to think about is a distant star.
- A beam-splitter, aka a half-silvered mirror. Let us suppose that we have a device with the property that the amplitude for light (of any wavelength) to pass through it is $\frac{1}{\sqrt{2}}$, and the amplitude for it to be reflected is also $\frac{1}{\sqrt{2}}$.
- Two detectors, which we'll call detector 1 and detector 2.

Recipe: The arrangement of detectors and beam-splitter is shown at right. Measure (by sampling) the probability of observing a photon with detector 2 at time $t+\tau$ given that we have seen a photon with detector 1 at time t:



$$\text{Prob}\left(\text{observe a photon at detector 2 at time } t+\tau \;\middle|\; \text{observe a photon at detector 1 at time } t\right) \propto I_1(t)I_2(t+\tau).$$

Here $I_{1,2}$ are the intensities of the beam at the two detectors. τ is a time delay that we get to pick. When collecting samples over some time interval, the thing we actually measure is the time average

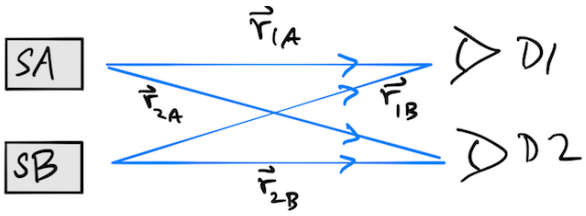
$$\overline{I_1 I_2} \equiv \int dt I_1(t)I_2(t+\tau) = g_B(c\tau).$$

I claim that this will take the form of the pair correlator we calculated above for a beam of bosons.

This is because light is a beam of bosons.

In case you don't believe that argument, here is a more direct calculation, in a model that also includes some information about the source. Suppose there are two sources (for example, two locations on the star) A and B, each of which emits a plane wave of wavenumber $k_{A/B}$ with a *random phase*. This random phase accounts for the fact that the photons are coming from totally uncorrelated, incoherent sources. The amplitudes of light at the two detectors are then

$$\begin{aligned}\mathcal{A}_{\text{at }1} &= \alpha_1 e^{\mathbf{i}k_A\cdot r_{1A}} + \beta_1 e^{\mathbf{i}k_B\cdot r_{1B}} \\ \mathcal{A}_{\text{at }2} &= \alpha_2 e^{\mathbf{i}k_A\cdot r_{2A}} + \beta_2 e^{\mathbf{i}k_B\cdot r_{2B}} \end{aligned} \qquad (1.103)$$



where the vectors are indicated in the figure.

The intensities at the detectors are then

$$I_{i=1,2} = |\mathcal{A}_{\text{at }i}|^2 = |\alpha|^2 + |\beta|^2 + 2\text{Re}\,\alpha^\star\beta e^{\mathbf{i}(k_B\cdot r_{iB} - k_A\cdot r_{iA})}.$$

The time-averaged intensities are then just

$$\overline{I_i} = |\alpha|^2 + |\beta|^2$$

because the random phases α, β depend on time and so any term not of the form $|\alpha|^2$ or $|\beta|^2$ averages to zero.

Consider instead

$$I_1 I_2 = |\mathcal{A}_1 \mathcal{A}_2|^2 = \left|\alpha^2 e^{\mathbf{i}k_A(r_{1A}+r_{2A})} + \beta^2 e^{\mathbf{i}k_B(r_{1B}+r_{2B})} + \alpha\beta\left(e^{\mathbf{i}k_A r_{1A}+\mathbf{i}k_B r_{2B}} + e^{\mathbf{i}k_B r_{1B}+\mathbf{i}k_A r_{2A}}\right)\right|^2 .$$

Some words: the α^2 term is the amplitude for both photons to come from A, the β^2 is where both come from B. The interesting $\alpha\beta$ term is where one photon comes from A and one comes from B; since photons are indistinguishable bosons, there are two ways for this to happen ($A \to 1, B \to 2$ or $A \to 2, B \to 1$), and these two paths interfere. Now time-average:

$$\overline{I_1 I_2} = |\alpha|^4 + |\beta|^4 + |\alpha\beta|^2 \left|e^{\mathbf{i}k_A r_{1A}+\mathbf{i}k_B r_{2B}} + e^{\mathbf{i}k_B r_{1B}+\mathbf{i}k_A r_{2A}}\right|^2 \tag{1.104}$$

$$= \overline{I_1}\cdot\overline{I_2} + 2|\alpha|^2|\beta|^2 \cos\left(k_B(r_{1B}-r_{2B}) - k_A(r_{1A}-r_{2A})\right) \tag{1.105}$$

$$\overset{r_{1A}-r_{2A}\simeq r_{1B}-r_{2B}\equiv r}{\simeq} \overline{I_1}\cdot\overline{I_2} + 2|\alpha|^2|\beta|^2 \cos\left((k_B-k_A)r\right). \tag{1.106}$$

In the last step, we considered the case where the two sources are close together compared to their separation from the detectors, as in the case of parts of a distant star. Suppose that the sources emit plane waves $\alpha_k e^{\mathbf{i}k\cdot r}$ with amplitude $|\alpha_k| = |\beta_k|$, with probability $p(k) = ce^{-\alpha k^2/2}$ (normalization fixes c). Then we should average over the colors in the beam:

$$\int \mathrm{d}^3k_A p(k_A) \int \mathrm{d}^3k_B p(k_B) \frac{\overline{I_1 I_2}}{\overline{I_1}\cdot\overline{I_2}} = c^2 \int \mathrm{d}^3k_A \int \mathrm{d}^3k_B e^{-\alpha k_A^2/2 - \alpha k_B^2/2}\left(1 + \frac{1}{4}\mathrm{Re}\, e^{\mathbf{i}(k_B-k_A)\cdot r}\right) = 1 + \frac{1}{2}e^{-r^2/\alpha}$$

as promised.

More generally, if instead of two discrete sources, we have a distribution of sources $\rho(r)$, the result is

$$\frac{\overline{I_1 I_2}}{\overline{I_1}\cdot\overline{I_2}} = 1 + \left|\int d^3r \rho(r) e^{\mathbf{i}(\vec{k}_1-\vec{k}_2)\cdot\vec{r}}\right|^2 .$$

The fact that this is (absolute value of the) the Fourier transform of the source distribution means that we can learn about the source distribution!

Notice that we could have replaced this whole discussion with a classical one. Instead of amplitudes in (1.103) I could have written electric field strengths $\vec{E}_\perp$. The calculations are continuously connected because Bose statistics allows for coherent states.

This beautiful idea was first used by Hanbury-Brown and Twiss to measure the sizes of very distant stars by varying the distance between two radio telescopes. A nice review of its many applications (including in high energy physics and in condensed matter) is this one by Baym. This method has been used to measure, for example, the size of viruses. [End of Lecture 10]

2 Interference phenomena

2.1 Path integrals, briefly

Some of the things I've said above are unified by the description of quantum mechanics in terms of path integral. It is the quantum mechanical analog of Lagrangian mechanics. It describes, for example, the propagator, as a sum of phases, each associated with a possible path. The phase for a path is $e^{\frac{\mathbf{i}}{\hbar}S[\text{path}]}$, where $S = \int dtL$ is the action.

Why should there be such a representation? It is the logical conclusion of the double-slit experiment. A wall with a double-slit restricts a particle to pass through one of two locations. The conclusion of the experiment is that the amplitude is the sum of the contributions of the two paths, each of which is a complex number.

Now suppose that instead of the detector, we put another wall with two slits. To find the probability amplitude for a detector placed after the second wall, we would have two sums, one over the path through first wall, and another over the path through the second wall. You see that we can keep adding walls.

Now suppose instead of two slits, each wall has three slits. Then there would be three terms in each sum.

Now imagine adding more walls, each with more holes.

Finally, imagine that the world is totally full of walls and that *all the walls are totally full of holes*. Even if there is no wall, we must sum over the paths. [19]

The more precise derivation of this statement is straightforward, in that it involves inserting lots of resolutions of the identity, but it is a little annoying and takes most of a lecture. Here are some payoffs:

- Classical mechanics is the stationary phase approximation.
- The fact that the vector potential term in the action is geometric makes the A-B effect very natural.
- It gives a straightforward way to derive the propagator for the harmonic oscillator.
- In quantum systems with many degrees of freedom, such as quantum field theories, the path integral is more useful, especially as an organizing device.
- Path integrals, with fewer factors of $\mathbf{i}$, are also useful in statistical physics. The derivation from quantum mechanics gives a useful perspective on them.

[19] This wonderful device is due to Feynman. Take a look at Volume III of the Feynman Lectures. A more elaborate treatment appears in Feynman and Hibbs, *Quantum Mechanics and Path Integrals*.

Propagator. Recall that the time evolution operator is the unitary $\mathbf{U}(t_b, t_a)$ that satisfies $\mathbf{U}(t_a, t_a) = \mathbb{1}$ and

$$\mathbf{i}\hbar\partial_{t_b}\mathbf{U}(t_b, t_a) = \mathbf{H}(t_b)\mathbf{U}(t_b, t_a).$$

If $\mathbf{H}(t) = \mathbf{H}$ is time-independent, then

$$\mathbf{U}(t_b, t_a) = \mathbf{U}(t_b - t_a) = e^{-\mathbf{i}(t_b - t_a)\mathbf{H}/\hbar}.$$

(More generally, we need to specify an ordering in the exponential.) The (position-space) propagator is its matrix elements in position-space:

$$K(x, t; x_a, t_a) = \langle x| \mathbf{U}(t, t_a) |x_a\rangle ,$$

the amplitude to propagate from x_a and time t_a to x at time t. It satisfies the Schrödinger equation:

$$\mathbf{i}\hbar\partial_t K(x, t; x_a, t_a) = \langle x| \mathbf{i}\hbar\partial_t \mathbf{U}(t - t_a) |x_a\rangle = \langle x| \mathbf{H}\mathbf{U}(t - t_a) |x_a\rangle .$$

For example, for a point particle, with $\mathbf{H}(\mathbf{x}, \mathbf{p}) \overset{e.g.}{=} \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$, we may replace $\langle x| \mathbf{H}(\mathbf{x}, \mathbf{p}) = \langle x| H(x, -\mathbf{i}\hbar\partial_x)$, so

$$\mathbf{i}\hbar\partial_t K(x, t; x_a, t_a) = H(x, -\mathbf{i}\hbar\partial_x)K(x, t; x_a, t_a).$$

The initial condition on this differential equation is

$$K(x, t_a; x_a, t_a) = \langle x|\mathbf{U}(t_a, t_a)|x_a\rangle = \delta(x - x_a).$$

For a free particle, $V = 0$, this is diffusion in imaginary time, and is solved by Fourier transform:

$$\mathbf{i}\hbar\partial_t K(x, t; x_a, t_a) = -\frac{\hbar^2\partial_x^2}{2m}K(x, t; x_a, t_a) \quad \Longrightarrow \quad K(x, t; x_a, t_a) = \sqrt{\frac{m}{2\pi\mathbf{i}t}}e^{\frac{\mathbf{i}m(x-x_a)^2}{2t}}$$

(I set $\hbar = 1$ in the last expression.)

Since waiting a bit and waiting some more is the same as waiting a lot, the time evolution operators satisfy a nice composition property:

$$\mathbf{U}(t_b, t_a) = \mathbf{U}(t_b, t)\mathbf{U}(t, t_a)$$

for any t (which need not even be in between t_b, t_a). If $\mathbf{H}$ is time independent, this just comes from adding the exponents. But we can stick a resolution of the identity in between the two factors on the RHS:

$$\mathbf{U}(t_b, t_a) = \int dx \mathbf{U}(t_b, t)|x\rangle\langle x|\mathbf{U}(t, t_a)$$

and make a sandwich of the whole thing:

$$K(x_b,t_b;x_a,t_a)=\int dx K(x_b,t_b;x,t)K(x,t;x_a,t_a).$$

This is the operation of placing a wall full of holes along the path of the particle.

Path integral representation of propagator. Now do this $N-1$ times: divide the interval into N equal segments of (tiny) size $\Delta t=\frac{t_b-t_a}{N}$:

$$K(x_b,t_b;x_a,t_a)=\int dx_1\cdots dx_{N-1}K(x_b,t_b;x_{N-1},t_{N-1})\cdots K(x_1,t_1;x_a,t_a).$$

Writing $\mathbf{H}=\mathbf{T}(\mathbf{p})+\mathbf{V}(\mathbf{x})$, the propagator for a tiny step is

$$\begin{aligned}K(x_j,t_j;x_{j-1},t_{j-1}) &= \langle x_j|\, e^{-\mathbf{i}\Delta t\mathbf{T}-\mathbf{i}\Delta t\mathbf{V}}\,|x_{j-1}\rangle\\ &= \langle x_j|\, e^{-\mathbf{i}\Delta t\mathbf{T}}e^{-\mathbf{i}\Delta t\mathbf{V}}\,|x_{j-1}\rangle+\mathcal{O}(\Delta t^2)\\ &= \int đp_j\,\langle x_j|\, e^{-\mathbf{i}\Delta t\mathbf{T}}\,|p_j\rangle\,\langle p_j|\, e^{-\mathbf{i}\Delta t\mathbf{V}}\,|x_{j-1}\rangle+\mathcal{O}(\Delta t^2)\\ &= \int đp_j\; e^{-\mathbf{i}T(p_j)\Delta t-\mathbf{i}V(x_{j-1})\Delta t}e^{\mathbf{i}p_j(x_j-x_{j-1})}+\mathcal{O}(\Delta t^2).\\ &= \sqrt{\frac{m}{2\pi\mathbf{i}\Delta t}}\exp\left(\mathbf{i}\Delta t\left(\frac{m}{2}\frac{(x_j-x_{j-1})^2}{\Delta t^2}-V\left(\frac{x_j+x_{j-1}}{2}\right)\right)\right)+\mathcal{O}(\Delta t^2).\end{aligned}$$

In the last step we used $\int_{-\infty}^{\infty}dp\; e^{-\mathbf{i}ap^2}=\sqrt{\frac{\pi}{\mathbf{i}a}}$. Assembling the whole thing,

$$\begin{aligned}K(x_b,t_b;x_a,t_a) &= A^N\int\prod_{j=1}^{N-1}dx_j\exp\left(\mathbf{i}\sum_{j=1}^{N-1}\frac{\Delta t}{\hbar}L\left(t_j,\frac{x_j+x_{j-1}}{2},\frac{x_j-x_{j-1}}{\Delta t}\right)\right)\\ &\equiv \int[dx]_{x(t_a)=x_a}^{x(t_b)=x_b}e^{\frac{\mathbf{i}}{\hbar}\int_{t_a}^{t_b}dtL(t,x,\dot{x})}\;. \qquad (2.1)\end{aligned}$$

with $L(t,x,\dot{x})=\frac{1}{2}m\dot{x}^2-V(x)$. We see that the true role in life of $\hbar$ is to make up the units of action in this expression. The first expression here defines what we mean by the path integral $\int[dx]$. It includes horrible things which are not differentiable at all (they have $\Delta x\sim\sqrt{\Delta t}$, not $\Delta x\sim\Delta t$); when this matters, you need to use the discretization to make it well-defined.

Stationary phase and classical mechanics. The path integral *explains* the special role of configurations that solve the equations of motion. Recall that

$$I=\int dx\; e^{-Nf(x)}=e^{-Nf(x_0)}\int dy e^{-\frac{N}{2}f''(x_0)y^2+\cdots}\simeq e^{-Nf(x_0)}\sqrt{\frac{2\pi}{Nf''(x_0)}}$$

where $f'(x_0)=0$ and $y\equiv x-x_0$. This is called saddle point approximation, and it holds because other contributions are suppressed by $e^{-N\Delta f}$. If instead we have

$$\tilde{I}=\int dx\; e^{\mathbf{i}Nf(x)}=e^{-\mathbf{i}Nf(x_0)}\int dy e^{\mathbf{i}\frac{N}{2}f''(x_0)y^2+\cdots}\simeq e^{-\mathbf{i}Nf(x_0)}\sqrt{\frac{2\pi\mathbf{i}}{Nf''(x_0)}}$$

where $f'(x_0) = 0$ and $y \equiv x - x_0$, this is called stationary phase. It holds because other contributions add destructively. With more variables:

$$\int dx_1 \cdots dx_N \; e^{\mathbf{i}Nf(x_1 \cdots x_N)} \simeq e^{\mathbf{i}Nf(\underline{x})} \sqrt{\det_{ij} \left(\frac{\pi}{\mathbf{i}N \partial_i \partial_j f} \right)}.$$

where

$$0 = \partial_{x_j} f(x)|_{x=\underline{x}} \forall j. \tag{2.2}$$

The path integral is just of the previous form with $\hbar = \frac{1}{N}$ and $f(x) = S[x] = \int dt L(t, x, \dot{x})$, the action functional. The square brackets indicate that the argument x is a whole function, rather than just a finite collection of numbers, but basically it just means that N is big. The saddle point condition (2.2) can be rewritten in the fancy notation:

$$0 = \frac{\delta}{\delta x(t)} S[\underline{x}] \quad , \forall t. \tag{2.3}$$

What is this when $S[x] = \int ds \left(\frac{1}{2} m \dot{x}^2(s) - V(x(s)) \right)$? The key ingredient is the 'fundamental rule of variational calculus', which in words is different independent variables are independent:

$$\frac{\partial x_j}{\partial x_i} = \delta_{ij} \qquad \leftrightarrow \qquad \frac{\delta x(s)}{\delta x(t)} = \delta(t - s).$$

$$\begin{aligned} \frac{\delta S}{\delta x(t)} &= \int ds \left(m \partial_s x(s) \partial_s \delta(s - t) - \frac{\partial V(x(s))}{\partial x(s)} \delta(t - s) \right) \\ &\overset{\text{IBP}}{=} \int ds \left(-m \partial_s^2 x(s) - \partial_{x(s)} V(x(s)) \right) \delta(t - s) \\ &= -m \ddot{x} - \partial_x V \end{aligned} \tag{2.4}$$

which is an equation due to Newton.

Evaluate for free particle (in a way that is useful for non-free particles). For $V = 0$, the classical path is a straight line:

$$\ddot{\underline{x}} = 0 \quad \Longrightarrow \quad \underline{x}(t) = x_a + (t - t_a) \frac{x_b - x_a}{t_b - t_a}.$$

$$S[\underline{x}] = \int_{t_a}^{t_b} L dt = \int \frac{m}{2} \dot{\underline{x}}^2 = \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}.$$

The fluctuations about the classical path are

$$y_j \equiv \delta x_j = x_j - \underline{x}(t_j).$$

The endpoints $x_0 = x_a, x_N = x_b$ don't fluctuate. The path integral is actually gaussian:

$$K(x_b, t_b; x_a, t_a) = \left(\frac{m}{2\pi \mathbf{i} \Delta t} \right)^{N/2} \int dx_1 \cdots dx_{N-1} \prod_{j=1}^{N} \exp \left(\mathbf{i} \frac{m}{2} \frac{(x_j - x_{j-1})^2}{\Delta t} \right)$$

Now plugging in $x_j = \underline{x}_j + y_j$,

$$(x_j - x_{j-1})^2 = \underbrace{(\underline{x}(t_j) - \underline{x}(t_{j-1}))^2}_{\to S[\underline{x}]} + (y_j - y_{j-1})^2 + \text{terms linear in } \delta x_j$$

we can ignore the terms linear in δx because they are zero by definition of the classical path.

$$K(x_b, t_b; x_a, t_a) = \left(\frac{m}{2\pi \mathbf{i} \Delta t}\right)^{N/2} e^{\frac{\mathbf{i}}{\hbar} S[\underline{x}]} \underbrace{\int dy_1 \cdots dy_{N-1} e^{\mathbf{i} \sum_{jk} y_j M_{jk} y_k}}_{= \frac{\pi^{\frac{N-1}{2}}}{\sqrt{\det(-\mathbf{i}M)}}}$$

where the $N-1 \times N-1$ matrix M is the discrete laplacian (recall the homework)

$$M_{jk} = \frac{m}{2\Delta t} \begin{pmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & & \ddots & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}_{jk}$$

We need to compute its determinant. We've seen that $[M, T] = 0$ where $T = \begin{pmatrix} 0 & 1 & 0 & & \\ 0 & 0 & 1 & & \\ & & & \ddots & \end{pmatrix}$ is the discrete translation operator. Its eigenstates are plane waves: $v_j(p) = ae^{\mathbf{i}pj} + be^{-\mathbf{i}pj}$; the boundary conditions $y_0 = y_N = 0$ determine $v_j(p) = \sin pj$, $p = p_n = \frac{2\pi n}{N}$ So we could try to compute $\det M = \prod_{n=1..N-1}(2 - \cos p_n)$. Instead, here's a trick, whereby we'll solve a slightly more general problem: let

$$M_N(u) \equiv \begin{pmatrix} 2\cosh u & -1 & & & & & \\ -1 & 2\cosh u & -1 & & & & \\ & -1 & 2\cosh u & -1 & & & \\ & & & \ddots & & & \\ & & & -1 & 2\cosh u & -1 & \\ & & & & -1 & 2\cosh u & \end{pmatrix}.$$

and $d_N \equiv \det M_N$. The recursion relation

$$\det M_N = 2\cosh u \det M_{N-1} - \det M_{N-2}(-1)^2$$

follows from the block structure of the matrix. For $u = 0$, it's just $d_N = 2d_{N-1} - d_{N-2}$. We need two initial conditions to solve this two-step recursion: $\det M_1 = 2\cosh u \to 2$

for $u \to 0$. $\det M_2 = 4\cosh^2 u - 1 \to 3$ for $u \to 0$. The solution for $u = 0$ is simple: $d_{N-1} = d_{N-2} + 1$, hence $d_{N-1} = N$. (For general u, it is $d_N = \frac{\sinh(N+1)u}{\sinh u}$.)

$$\begin{aligned} K(x_b, t_b; x_a, t_a) &= \left(\frac{m}{2\pi \mathbf{i}\Delta t}\right)^{N/2} e^{\frac{\mathbf{i}}{\hbar}S[\underline{x}]} \frac{\pi^{\frac{N-1}{2}}}{\sqrt{\det(-\mathbf{i}M)}} \\ &= \left(\frac{m}{2\pi \mathbf{i}\Delta t}\right)^{N/2} e^{\frac{\mathbf{i}}{\hbar}S[\underline{x}]} \left(\frac{m}{2\pi \mathbf{i}\Delta t}\right)^{-(N-1)/2} N^{-1/2} \\ &= \sqrt{\frac{m}{2\pi(t_b - t_a)\mathbf{i}}} e^{\frac{\mathbf{i}}{\hbar}S[\underline{x}]}. \end{aligned} \tag{2.5}$$

[End of Lecture 11]

Coherent state path integral. The position basis resolution on the identity does not have a monopoly here; we can use whatever resolution we like. We can even use coherent states! This representation is very useful in quantum many-body physics.

So suppose $\mathcal{H} = \mathcal{H}_{\text{SHO}} = \text{span}\{|0\rangle, |1\rangle \cdots\}$ where $\mathbf{a}^\dagger \mathbf{a} |n\rangle = n |n\rangle$, $[\mathbf{a}, \mathbf{a}^\dagger] = 1$. We need not take $\mathbf{H} = \hbar\omega\left(\mathbf{a}^\dagger \mathbf{a} + \frac{1}{2}\right)$, but we will.

Recall that coherent states have $\mathbf{a}|\alpha\rangle = \alpha|\alpha\rangle$. The coherent-state representation of the propagator is

$$K(\alpha_b, t_b; \alpha_a, t_a) \equiv \langle \alpha_b | \mathbf{U}(t_b, t_a) | \alpha_a \rangle .$$

They resolve the identity by

$$\mathbb{1} = \int \frac{d\text{Re}\alpha d\text{Im}\alpha}{\pi} |\alpha\rangle \langle\alpha|$$

and their overlaps are

$$\langle \alpha | \alpha' \rangle = e^{-\frac{1}{2}\left(|\alpha|^2 + |\alpha'|^2\right) + \alpha^\star \alpha'}.$$

So sticking $N-1$ walls full of holes in the coherent state basis:

$$K(\alpha_b, t_b; \alpha_a, t_a) = \int \frac{d^2\alpha_1 \cdots d^2\alpha_{N-1}}{\pi^{N-1}} K(\alpha_b, t_b; \alpha_{N-1}, t_{N-1}) \cdots K(\alpha_1, t_1; \alpha_a, t_a)$$

where the small step is

$$K(\alpha_j, t_j; \alpha_{j-1}, t_{j-1}) = \langle \alpha_j | e^{-\frac{\mathbf{i}}{\hbar}\Delta t \mathbf{H}} | \alpha_{j-1} \rangle \ .$$

This is useful if $\mathbf{H}$ acts nicely on the coherent states, as is the case when it can be written in terms of creation and destruction operators. For simplicity consider the (cop out!) case of the SHO:

$$\begin{aligned} K(\alpha_j, t_j; \alpha_{j-1}, t_{j-1}) &= \langle \alpha_j | e^{-\mathbf{i}\Delta t \omega \mathbf{a}^\dagger \mathbf{a}} | \alpha_{j-1} \rangle \\ &= e^{-\mathbf{i}\Delta t \omega \alpha_j^\star \alpha_{j-1}} \langle \alpha_j | \alpha_{j-1} \rangle + \mathcal{O}(\Delta t^2) \end{aligned}$$

$$= e^{-\mathbf{i}\Delta t\omega\alpha_j^\star\alpha_j+\mathcal{O}(\Delta t^2)}\exp\quad \underbrace{\left(-\frac{1}{2}|\alpha_j|^2-\frac{1}{2}|\alpha_{j-1}|^2+\alpha_j^\star\alpha_{j-1}\right)}_{=\frac{1}{2}\alpha_j^\star\underbrace{(\alpha_j-\alpha_{j-1})}_{=\dot\alpha\Delta t}+\frac{1}{2}\alpha_{j-1}\underbrace{\left(-\alpha_{j-1}^\star+\alpha_j^\star\right)}_{=-\dot\alpha^\star\Delta t}} \tag{2.6}$$

$$\begin{aligned} K(\alpha_b,t_b;\alpha_a,t_a) &= \int\prod_{j=1}^{N-1}\frac{d^2\alpha_j}{\pi}e^{\mathbf{i}\int_{t_a}^{t_b}dt\left(\frac{\mathbf{i}}{2}(\alpha^\star\dot\alpha-\alpha\dot\alpha^\star)-\omega\alpha^\star\alpha\right)} \\ &= \int[d\alpha]e^{\mathbf{i}\int dtL(\alpha,\dot\alpha)} \end{aligned} \tag{2.7}$$

with $L=p\dot x-H$.

For the special case of the SHO, recall that we know the answer since coherent states remain coherent under time evolution by the SHO hamiltonian:

$$\mathbf{U}(t)\left|\alpha\right\rangle = \mathcal{N}_\alpha\underbrace{\mathbf{U}(t)e^{\mathbf{a}^\dagger\alpha}\mathbf{U}^\dagger(t)}_{=e^{\mathbf{a}^\dagger\alpha e^{-\mathbf{i}\omega t}}}\underbrace{\mathbf{U}(t)\left|0\right\rangle}_{=e^{-\mathbf{i}\omega t/2}|0\rangle} = e^{-\mathbf{i}\omega t/2}\left|\alpha e^{-\mathbf{i}\omega t}\right\rangle.$$

So

$$K(\alpha_b,t_b;\alpha,0)=\left\langle\alpha_b\right|\mathbf{U}(t)\left|\alpha\right\rangle = e^{-\mathbf{i}\omega t/2}\left\langle\alpha_b|\alpha e^{-\mathbf{i}\omega t}\right\rangle = e^{-\mathbf{i}\omega t/2}e^{-|\alpha_b|^2/2-|\alpha|^2/2+\alpha_b^\star\alpha e^{-\mathbf{i}\omega t}}.$$

The situation when this comes into its own is when we have a collection of SHOs:

$$\mathbf{H}=\sum_k\hbar\omega_k\left(\mathbf{a}_k^\dagger\mathbf{a}_k\right)+\cdots$$

where the $\cdots$ represents some interactions that may be treated as small.

Euclidean-time path integral. Above I wrote a formula for the real-time propagator. Euclidean path integrals are also very useful, because they compute ground-state expectation values. Here's why:

The vacuum can be prepared by starting in an arbitrary state and acting with e^{-TH} for some large T, and then normalizing (as usual when discussing path integrals, it's best to not worry about the normalization and only ask questions which don't depend on it),

$$|0\rangle = \mathcal{N}e^{-\mathbf{H}T}\left|\text{any}\right\rangle.$$

To see this, just expand in the energy eigenbasis. This 'imaginary time evolution operator' $e^{-\mathbf{H}T}$ has a path integral representation just like the real time operator, by nearly the same calculation

$$e^{-\mathbf{H}T}=\int[Dq]e^{-\int_{-T}^0 d\tau L(q(\tau),\dot q(\tau))}.$$

Doing the same thing to prepare $\langle 0|$, making a sandwich of $e^{q(0)\cdot k} = e^{\int d\tau q(\tau)\cdot k\delta(\tau)}$, and taking $T \to \infty$ we can forget about the arbitrary states at the end, and we arrive at

$$\langle 0|\, \hat{\mathcal{O}}(\mathbf{q},\mathbf{p})\, |0\rangle = \frac{1}{Z}\int [Dq] e^{-\int_{-\infty}^{\infty} d\tau L(q(\tau),\dot{q}(\tau)} \mathcal{O}(q(0), m\dot{q}(0)). \tag{2.8}$$

On the LHS $\hat{\mathcal{O}}$ is some operator; on the RHS $\mathcal{O}$ is just a function of the integration variables. Z is a normalization factor chosen so that $\langle 0|0\rangle = 1$.

For example, consider the case of our chain of balls on springs:

$$\left\langle e^{\mathbf{i}K\mathbf{q}} \right\rangle_0 = \frac{1}{Z}\int \prod_i dq_i \; e^{-q_i D_{ij} q_j} e^{\mathbf{i}Kq_0} \tag{2.9}$$

with $Z = \int \prod_i dq_i \; e^{-q_i D_{ij} q_j}$. Here i, j are discrete time labels, and D_{ij} is the matrix which discretizes the action. Repeated indices are summed.

Notice that in this way we can find a path integral representation for the thermal partition function $\mathrm{tr} e^{-\beta \mathbf{H}}$: simply impose periodic boundary conditions on the configurations over which we sum: $q(\tau) = q(\tau + \beta)$:

$$Z = \mathrm{tr} e^{-\beta \mathbf{H}} = \oint [Dq]_{q(0)=q(\beta)} e^{-\int_0^\beta d\tau L}. \tag{2.10}$$

A fancy way of describing this is to say that putting the system at finite temperature is accomplished by making the imaginary time direction into a circle.

2.2 Wave mechanics of charged particles

When we talked about the radiation field I mentioned that one motivation for introducing the electromagnetic potentials, $\Phi, \vec{A}$, such that

$$\vec{E} = -\vec{\nabla}\Phi - \frac{1}{c}\partial_t \vec{A}, \quad \vec{B} = \vec{\nabla} \times \vec{A},$$

is that they are required to discuss the quantum mechanics of a charged particle moving in an electromagnetic field $(\vec{E}, \vec{B})$.

You will recall that the form of E, B is preserved by a *gauge transformation*,

$$\vec{A} \to \vec{A} - \vec{\nabla}\lambda, \quad \Phi \to \Phi - \frac{1}{c}\partial_t \lambda. \tag{2.11}$$

These expressions are nicely packaged in terms of the four-vector potential $A_\mu \equiv (\vec{A}, c\Phi)_\mu \to A_\mu - \partial_\mu \lambda$, but we will not consider any relativistic situation here. This ambiguity may make it seem like the vector potential is not real. Some of the vector

potential is indeed an artifice, but notice that $\oint_C \vec{A} \cdot d\vec{x}$ is not changed by the gauge transformation (2.11). We will now see how this quantity arises physically, because of quantum mechanics.

It is useful to think about the Lagrangian description of the charged particle, which has

$$L = \frac{1}{2} m\dot{x}^2 - e\Phi - \frac{e}{c}\dot{\vec{x}} \cdot \vec{A} \, . \tag{2.12}$$

Notice that the extra term in the action $S = \int dt L$ from the vector potential is *geometric*, in the sense that $\int dt \dot{\vec{x}} \cdot \vec{A} = \int d\vec{x} \cdot \vec{A}$ depends only on the path of the particle, not on how quickly the path traversed.

The canonical momentum deduced from the Lagrangian L is

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i - \frac{e}{c} A_i$$

and now differs from the *mechanical momentum* $m\dot{x}_i$. Legendre transformation gives the Hamiltonian

$$H = \frac{1}{2m}\left(p - \frac{e}{c}A\right)^2 + e\Phi.$$

Let's consider time-independent EM fields for simplicity. The Schrödinger equation in position space is then

$$\mathbf{i}\hbar\partial_t \psi(x,t) = \langle x|\mathbf{H}|\psi(t)\rangle = \frac{1}{2m}\left(-\mathbf{i}\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(x)\right)^2 \psi(x,t) + e\Phi(x)\psi(x,t). \tag{2.13}$$

The probability density is still $\rho(x,t) = |\psi(x,t)|^2$. Is it still conserved? In fact $\partial_t \rho + \vec{\nabla} \cdot \vec{j}_A = 0$ but where

$$\vec{j}_A \equiv \frac{\hbar}{2m\mathbf{i}}\left(\psi^\star \vec{\nabla}\psi - \psi\vec{\nabla}\psi^\star\right) - \frac{e}{mc}\psi^\star\psi\vec{A}$$

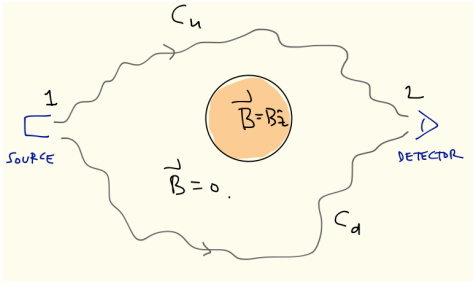
has an extra term. This depends very explicitly on $\vec{A}$! Is it gauge invariant? Only if the gauge transformation acts on the wavefunction:

$$\vec{A} \to \vec{A} + \vec{\nabla}\lambda, \quad \psi \to e^{-\mathbf{i}\frac{e\lambda}{\hbar c}}\psi \, .$$

Now we turn to showing that the vector potential (or at least its integral around closed curves) is real, via the Aharonov-Bohm effect.

2.2.1 Aharonov-Bohm effect

Consider the following situation. A infinite solenoid extends in the z direction. The figure depicts the xy-plane. The $\vec{B}$ field is only nonzero inside the solenoid and points out of the page $\vec{B} = \hat{z}B$. We treat it here as a fixed background field.



We send quantum mechanical charged particles from the source at left to the detector at right. They cannot enter the solenoid, but are otherwise free to proceed as they like. So they never move in a region where $\vec{B} \neq 0$. But we will show that the field affects them.

The path integral is very helpful here: We can group the possible paths (over which we integrate to find *e.g.* the amplitude Z for the particle to hit the detector) into two disconnected components: they either go above the solenoid or below it[20]:

$$Z = \int [dx] ... = \int [dx]_u ... + \int [dx]_d ...$$

The ... here is $e^{\frac{\mathbf{i}}{\hbar} S[x]}$ with $S[x]$ the action for a charged particle above, $S = \int dt L$, with L from (2.12). In particular it has a term

$$S_A = \frac{e}{c} \int_1^2 A \equiv \frac{e}{c} \int_1^2 \vec{A}(x) \cdot d\vec{x} = \frac{e}{c} \int_{t_1}^{t_2} A_i \frac{dx^i}{dt} dt$$

The vector potential is curl-free $\vec{\nabla} \times \vec{A} = 0$ in the region outside the solenoid – this is what it means that $\vec{B} = 0$. This means that the line integral S_A is *path-independent.* [21] For all the paths that go above the solenoid, the phase factor resulting from the $\int A$ term in the action is the same:

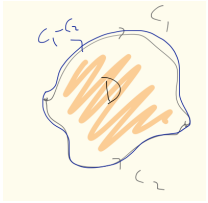
$$e^{\mathbf{i} \frac{e}{\hbar c} \int_{C_u} A}$$

for some fixed reference path C_u (in the figure). Similarly, all the paths below give a phase factor $e^{\mathbf{i} \frac{e}{\hbar c} \int_{C_d} A}$. But these phase factors from above and below are not the same: if we deform the path through the solenoid, we have to go through the region with $\vec{B} \neq 0$.

The probability of a particle hitting the detector is then

$$P = |Z_u e^{\mathbf{i} \frac{e}{\hbar c} \int_{C_u} A} + Z_d e^{\mathbf{i} \frac{e}{\hbar c} \int_{C_d} A}|^2 = |Z_u|^2 + |Z_d|^2 + \left(Z_u Z_d^\star e^{\mathbf{i} \frac{e}{\hbar c} \left(\int_{C_u} A - \int_{C_d} A \right)} + c.c. \right)$$

[20] Actually there are also paths that wind around the solenoid some number of times. These have very large action and we will ignore them here.



[21] Recall that the difference between two paths is

$$\int_{C_1} \vec{A} \cdot d\vec{x} - \int_{C_2} \vec{A} \cdot d\vec{x} = \int_{C_1 - C_2} A = \int_D \vec{\nabla} \times \vec{A} \cdot d\vec{a} = \int_D \vec{B} \cdot d\vec{a}$$

by Stokes' theorem, where D is the region bounded by the paths. So as long as the $\vec{B}$-field vanishes in D, we can change the path without changing the phase.

where $Z_{u,d}$ don't depend on the EM field at all.

But now

$$\left(\int_{C_u} A - \int_{C_d} A\right) = \int_{C_u - C_d} A = \int_{\text{inside}} \vec{B} \cdot d\vec{a} = B_z A \equiv \Phi \ .$$

So, for a simple example, if we arrange things symmetrically so that $Z_d = Z_u \equiv Z$, then

$$P = 2|Z|^2 \left(1 + \cos \frac{e\Phi}{\hbar c}\right) \ .$$

By varying B_z and hence the flux Φ, we can vary the intensity of particles hitting the detector! For example, we could choose $\frac{e\Phi}{\hbar c} = \pi$ to do total destructive interference.

But the particles never went near the region where the magnetic field was nonzero! They only know about it because of the vector potential. Score one more for quantum mechanics.

(Notice that if $\frac{e\Phi}{\hbar c} = 2\pi n, n \in \mathbb{Z}$, you can't detect the field this way.)

2.2.2 AB effect without the path integral

[I skipped this discussion in lecture.]

Here is a useful mathematical nugget: Suppose we know the solution $u_0(t)$ in $\mathbf{i}\hbar\partial_t u_0 = H_0 u_0$ for some H_0. Suppose we want to solve $\mathbf{i}\hbar\dot{\psi} = H\psi$ with $H \equiv H_0 + V(t)$, where $V(t)$ is a c-number function when acting on u_0. Then let $\psi = f(t)u_0$ and

$$Hu_0 f = \mathbf{i}\hbar\left(u_0\dot{f} + \dot{u}_0 f\right) \quad \Longrightarrow \quad \frac{\dot{f}}{f} = -\frac{\mathbf{i}}{\hbar}V(t)$$

$$\Longrightarrow \quad f(t) = f(0)e^{-\frac{\mathbf{i}}{\hbar}\int_0^t V(s)ds}. \tag{2.14}$$

Next, let's consider a double-slit experiment, where a particle may follow two possible paths from a source to a detector, which we'll call u(pper) and l(ower). The intensity at position x on the detector is

$$I_x = |\psi_u(x) + \psi_l(x)|^2$$

where $\psi_{u/l}(x)$ is the amplitude for the case where the l/u path is blocked.

Now here's the real thing. Consider a charged particle traversing the same double-slit experiment, where now the (completely impenetrable) wall between the slits contains a (perfect) solenoid, with

$$\vec{B} = \begin{cases} B\check{z}, & \text{inside} \\ 0, & \text{outside} \end{cases} \ .$$

The Schrödinger equation is

$$-\mathbf{i}\hbar\partial_t\psi(x,t) = \frac{1}{2m}\left(-\mathbf{i}\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(x)\right)^2\psi(x,t) + V(x)\psi(x,t) \tag{2.15}$$

where V includes the walls of the barrier, and $\vec{\nabla}\times\vec{A} = \vec{B}$. Notice that the wavefunction vanishes wherever the magnetic field is nonzero (since the walls are impenetrable ($V = \infty$ inside the walls)) and the magnetic field vanishes wherever the wavefunction is nonzero (since the solenoid is perfect ($B = 0$ outside the solenoid)).

Now, suppose we know the solution u_0 for $\vec{A} = 0$:

$$-\mathbf{i}\hbar\partial_t u_0(x,t) = \frac{1}{2m}\left(-\mathbf{i}\hbar\vec{\nabla} + 0\right)^2 u_0(x,t) + V(x)u_0(x,t)\ . \tag{2.16}$$

This might be quite difficult to find, but we don't need to find it. I claim that the solution to (2.15) is

$$\psi = e^{\mathbf{i}\frac{e}{\hbar c}\int_{x_0}^{x} d\vec{\ell}\vec{A}(\ell)}u_0 \equiv e^g u_0.$$

Notice the similarity with (2.14). To check this, let's differentiate:

$$\left(-\mathbf{i}\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\psi(x) \overset{\text{FTC}}{=} -\mathbf{i}\hbar\left(\vec{\nabla}u_0\right)e^g - \mathbf{i}\hbar u_0\left(\frac{\mathbf{i}e}{\hbar c}\vec{A}\right)e^g - \frac{e}{c}\vec{A}u_0e^g.$$

Doing it again:

$$\frac{1}{2m}\left(-\mathbf{i}\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2(u_0e^g) = \frac{1}{2m}\left(\left(-\mathbf{i}\hbar\vec{\nabla}\right)^2 u_0\right)e^g.$$

Notice that we didn't have to choose a path in $\int^x A$.

The combination $D \equiv \left(-\mathbf{i}\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)$ is sometimes called a *covariant derivative*, because it preserves the gauge transformation properties of the function it acts on:

$$\psi \to e^{\mathbf{i}\lambda}\psi \implies (D\psi) \to e^{\mathbf{i}\lambda}(D\psi).$$

Without $\vec{B}$, the probability amplitude at the location x on the detector is $u_0^u(x) + u_0^l(x)$. With $\vec{B}$, it is

$$\begin{aligned}\psi(x) &= \psi^u(x) + \psi^l(x)\\ &= u_0^u(x)e^{\frac{\mathbf{i}e}{\hbar c}\int_{C_u}\vec{A}(\ell)\cdot d\vec{\ell}} + u_0^d(x)e^{\frac{\mathbf{i}e}{\hbar c}\int_{C_l}\vec{A}(\ell)\cdot d\vec{\ell}}\\ &= e^{\frac{\mathbf{i}e}{\hbar c}\int_{C_u}\vec{A}(\ell)\cdot d\vec{\ell}}\left(u_0^u(x) + u_0^l(x)e^{\frac{\mathbf{i}e}{\hbar c}\oint_{C_l-C_u}\vec{A}(\ell)\cdot d\vec{\ell}}\right)\ .\end{aligned} \tag{2.17}$$

The relative phase between the two terms is changed by the integral of $\vec{A}$ over a *closed* path:

$$\frac{e}{\hbar c}\oint_{C_l - C_u} \vec{A}(\ell)\cdot d\vec{\ell} \overset{\text{Stokes}}{=} \frac{e}{\hbar c}\int_S \underbrace{\vec{\nabla}\times\vec{A}}_{=\vec{B}}\cdot \underbrace{d\vec{a}}_{\equiv \hat{n}d^2x} \equiv \frac{e}{\hbar c}\Phi_B(S)\ .$$

Here S is any surface bounded by $\partial S = C_l - C_u$, and the magnetic flux through the surface is $\Phi_B(S) = BA$ in the situation above.

Notice that Φ_B is gauge invariant. And this is good because the measured result depends on it: The probability of seeing the particle hit the location x is

$$P_x = |\psi(x)|^2 = \left|u_0^u + u^l e^{\mathbf{i}\frac{e}{\hbar c}\Phi_B}\right|^2$$

– if we turn the knob controlling the current through the solenoid, the interference pattern will shift! (Notice that the pattern returns to itself when $\frac{e}{\hbar c}\Phi_B$ changes by 2π.)

[End of Lecture 12]

The observability of this kind of phase was used brilliantly by Dirac to show that if magnetic monopoles exist with magnetic charge g, then the combination eg is quantized.

2.2.3 Magnetic monopoles and quantization of charge and angular momentum

[from Commins] A magnetic monopole is a point source of magnetic field, around which

$$\vec{B} = \frac{g}{R^2}\check{R}$$

where g is the magnetic charge, $\oint \vec{B}\cdot d\vec{a} = 4\pi g$. We can learn quite a lot by supposing one of these exists.

Consider also an electric charge, separated by $-\vec{a}$ from the location of the monopole, so

$$\vec{E} = \frac{e}{r^2}\check{r}, \quad \vec{R} \equiv \vec{r} - \vec{a}.$$

If neither moves, there is no force on either. But notice that $\vec{E}$ is not parallel to $\vec{B}$, so there is energy and momentum in the fields; the momentum density (in cgs) is

$$\begin{aligned}\vec{\wp} &= \frac{1}{4\pi c}\vec{E}\times\vec{B} \\ &= \frac{1}{4\pi c}\frac{ge}{R^3 r^3}\vec{r}\times\underbrace{\vec{R}}_{\vec{r}-\vec{a}} \\ &= -\frac{1}{4\pi c}\frac{ge}{R^3 r^3}\vec{r}\times\vec{a}\end{aligned} \tag{2.18}$$

The angular momentum density about the origin is

$$\vec{j} = \vec{r} \times \vec{\wp} = \frac{1}{4\pi c} \frac{ge}{r^3 R^3} \vec{r} \times (\vec{a} \times \vec{r}) \, .$$

The total angular momentum is

$$\vec{S} = \int \vec{j} d^3 v \ ;$$

this must be interpreted as the spin of the charge-monopole pair.

What is $\vec{S}$? It must point along $\vec{a}$, since there is azimuthal symmetry about the $\vec{a}$ axis. And if $\vec{S}$ points along $\vec{a}$, then a configuration where we put charges $e/2$ at $\vec{a}$ and $-\vec{a}$ must have zero angular momentum. Starting from that configuration, we can find $\vec{S}$ by integrating the torque $\vec{\tau} = \partial_t \vec{S}$ necessary to put the charges together: $\vec{S} = \Delta \vec{S} = \int dt \vec{\tau}$. Move the charge along an arc of radius $|\vec{a}|$. The Lorentz force on the charge is $\vec{F} = \frac{e}{2} \frac{\vec{v}}{c} \times \vec{B} = \frac{e}{2c} v B \check{z}$ (where $\check{z}$ is out of the board). We must exert $-\vec{F}$ to keep the charge moving along the circle (other forces such as Coulomb repulsion don't contribute to the torque along $\check{a}$). The component of the torque along $\vec{a}$ is

$$\vec{\tau} \cdot \check{a} = \left(\vec{r} \times \vec{F} \right) \cdot \check{a} = a \sin\theta \frac{vB}{c} \frac{e}{2}.$$

Along the arc, $vdt = d\ell = ad\theta$, so $dt = \frac{ad\theta}{v}$ and

$$S \equiv |\vec{S}| = \int dt \tau = \int_0^\pi \frac{d\theta a^2}{v} \sin\theta \frac{vB}{c} \frac{e}{2} = a^2 \frac{g}{a^2} \frac{e}{2c} \underbrace{\int_0^\pi \sin\theta d\theta}_{=2} = \frac{eg}{c}.$$

But angular momentum is quantized in units of $\frac{\hbar}{2}$. (You learned this in the 'bootstrap' discussion of 212A.) This means that $S = \frac{eg}{c} = \frac{\hbar}{2} n, n \in \mathbb{Z}$. Therefore electric charges only come in integer multiples of $\frac{\hbar c}{2g}$.

Here is another point of view on this result, which is called Dirac quantization. Since $\vec{\nabla} \cdot \vec{B} = 0$ away from $R = 0$, we can still find a vector potential, though it will be singular at $R = 0$.

$$\vec{B} = \frac{g}{R^2} \check{R} = \vec{\nabla} \times \vec{A} = \frac{1}{R \sin\theta} \left(\partial_\theta \left(\sin\theta A_\varphi \right) - \partial_\varphi A_\theta \right) \check{R} + \ldots$$

$$\implies \frac{g}{R^2} = \frac{1}{R \sin\theta} \left(\partial_\theta \left(\sin\theta A_\varphi \right) - \partial_\varphi A_\theta \right)$$

We can set $A_\theta = 0$ by azimuthal symmetry, so we need

$$\frac{g}{R} \sin\theta = \partial_\theta \left(\sin\theta A_\varphi(R, \theta) \right)$$

Integrating gives

$$-g\frac{\cos\theta}{R}+\frac{K(R)g}{R}=\sin\theta A_\varphi \quad\Longrightarrow\quad A_\varphi=\frac{g}{R\sin\theta}\left(K(R)-\cos\theta\right).$$

(Vanishing of the other components of $\vec{\nabla}\times\vec{A}$ will tell us that $K(R)=k$ is constant.)

Even for $R\neq 0$, this solution A_φ will be singular when $\sin\theta=0$, *i.e.* at the poles $\theta=0,\pi$. We can avoid this by choosing k:

$$k=+1:\ A_\varphi^{(+)}=\frac{g}{R}\left(\frac{1-\cos\theta}{\sin\theta}\right)=\frac{g}{R}\frac{2\sin^2\frac{\theta}{2}}{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}}=\frac{g}{R}\tan\frac{\theta}{2}$$

is singular at $\theta=\pi$, but not $\theta=0$.

$$k=-1:\ A_\varphi^{(-)}=\frac{g}{R}\left(\frac{-1-\cos\theta}{\sin\theta}\right)=-\frac{g}{R}\frac{2\cos^2\frac{\theta}{2}}{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}}=\frac{g}{R}\cot\frac{\theta}{2}$$

is singular at $\theta=0$, but not $\theta=\pi$. So we can make a vector potential which is nonsingular everywhere (except the origin) by patching together solutions: use $k=1$ in the northern hemisphere, and $k=-1$ in the southern hemisphere.

This is possible because the two solutions are related by a gauge transformation $A^{(+)}-A^{(-)}=\vec{\nabla}\lambda$ where the gauge function $\lambda=2g\varphi$ is well-defined enough around the equator. For this to work, answers for physics around the equator must agree. Let's do the Aharonov-Bohm experiment, sending two charged-particle beams in circular paths around the equator of a sphere surrounding the magnetic monopole. The relative phase shift between the two paths is $e^{\mathrm{i}\delta^\pm}$ with

$$\delta^\pm=\frac{e}{\hbar c}\oint\vec{A}^{(\pm)}\cdot d\vec{\ell}=\frac{e}{\hbar c}\cdot 2\pi R\cdot\frac{\pm g}{R}=\pm\frac{2\pi eg}{\hbar c},$$

where the $\pm$ indicates whether we use the northern gauge or the southern gauge. The difference is unobservable only if it is an integer mutliple of 2π :

$$\frac{2\pi eg}{\hbar c}=2\pi n-\frac{2\pi eg}{\hbar c}\quad\leftrightarrow\quad\frac{eg}{\hbar c}4\pi=2\pi n\quad\leftrightarrow\quad eg=\frac{\hbar c}{2}n$$

where $n\in\mathbb{Z}$. This the same condition as we found from angular momentum quantization.

2.3 Integer Quantum Hall Effect

[Wen, Quantum Field Theory of Many-Body Systems] As a synthesis of several of the things we've studied so far (free fermions, charged particle in an electromagnetic field, the notion of states of matter), I want to discuss an interesting state of matter that can be realized by subjecting a 2d electron gas to a large magnetic field. This state can be understood without worrying about interactions.

It is interesting for several reasons. One is that it seems like a vegetable (*e.g.* it has a unique groundstate with an energy gap, and breaks no symmetries), but if it has a boundary, it has gapless edge modes that move in only one direction (a *chiral* edge mode). Recall that when we studied the groundstate of non-interacting fermions in one dimension, we always found an *even* number of Fermi points (values of p where $\epsilon(p) = \epsilon_F$). Here is a way to get an odd number.

The second reason it is interesting gives it its name. The Hall effect is when, in the presence of a magnetic field, an applied electric field E_x makes a current in the y direction: $J_y = \sigma^{xy} E_x$. This can happen classically, and in such a description the *Hall conductivity*, σ^{xy}, is proportional to B and to the density of electrons and can vary arbitrarily. But in an integer quantum Hall state, $\sigma^{xy} = \nu \frac{e^2}{h}$, where ν is an *integer* and e^2 and h are fundamental constants of nature.

Consider one (for now) electron constrained to move in the xy plane under the influence of a uniform magnetic field of magnitude B oriented in the $+\hat{z}$ direction. We're going to ignore its spin, because the magnetic field polarizes it to point in the $\hat{z}$ direction. The Hamiltonian for this electron is

$$\mathbf{H} = \frac{1}{2m}\left(\left(\mathbf{p}_x - \frac{e}{c}A_x\right)^2 + \left(\mathbf{p}_y - \frac{e}{c}A_y\right)^2\right) \tag{2.19}$$

where m and e are the mass and charge of the electron, and c is the speed of light, which I will set to one.

Let $z = x + \mathbf{i}y, \bar{z} = x - \mathbf{i}y$, so $\partial_z = \frac{1}{2}(\partial_x - \mathbf{i}\partial_y), \partial_{\bar{z}} = \frac{1}{2}(\partial_x + \mathbf{i}\partial_y)$. Let's choose symmetric gauge: $(A_x, A_y) = \frac{B}{2}(-y, x)$, where $B = \partial_x A_y - \partial_y A_x$ here is a constant. Then acting on a single particle position-space wavefunction,

$$H = -\frac{1}{2m}\sum_{i=x,y}(\partial_i - \mathbf{i}eA_i)^2 = -\frac{1}{m}(D_z D_{\bar{z}} + D_{\bar{z}} D_z) \tag{2.20}$$

where $D_z = \partial_z - \frac{eB}{4}\bar{z}, \quad D_{\bar{z}} = \partial_{\bar{z}} + \frac{eB}{4}z$. An intermediate step here, which we'll use later is:

$$L_z = \mathbf{i}(y\partial_x - x\partial_y) = z\partial_z - \bar{z}\partial_{\bar{z}} \tag{2.21}$$

the angular momentum of the particle.

When $\hbar = c = 1$, a magnetic field has dimensions of length^{-2}:

$$\ell_B^2 \equiv \left|\frac{c\hbar}{eB}\right| \propto \frac{1}{B}, \tag{2.22}$$

ℓ_B is called the magnetic length.

Now I'll do something mysterious-seeming that will solve this problem. On the homework you'll see that (in a different gauge) it can be written as a single harmonic oscillator. Let $\varphi \equiv e^{-\frac{|z|^2}{4\ell_B^2}}$. Then it is useful to observe that if $eB > 0$,

$$H = \varphi\left(-\frac{1}{m}\left(\tilde{D}_z\tilde{D}_{\bar{z}} + \tilde{D}_{\bar{z}}\tilde{D}_z\right)\right)\varphi^{-1}, \tag{2.23}$$

where

$$\begin{aligned}\tilde{D}_z &= \varphi^{-1}D_z\varphi = \partial_z - \frac{eB}{4}\bar{z} - \frac{eB}{4}\bar{z} = \partial_z - \frac{eB}{2}\bar{z},\\ \tilde{D}_{\bar{z}} &= \varphi^{-1}D_{\bar{z}}\varphi = \partial_{\bar{z}}.\end{aligned} \tag{2.24}$$

This can be rewritten as

$$H = \varphi\left(-\frac{2}{m}\left(\partial_z - \frac{1}{2\ell_B^2}\bar{z}\right)\partial_{\bar{z}}\right)\varphi^{-1} + \frac{1}{2}\hbar\omega_c \tag{2.25}$$

where $\omega_c = \frac{eB}{mc}$ is the cyclotron frequency. In this form we can immediately read off the eigenstates. States of the form at left have the energy at right:

$$\begin{aligned}\Psi_0(z) &= e^{-\frac{|z|^2}{4\ell_B^2}}f(z) && E_0 = \frac{1}{2}\hbar\omega_c && \text{lowest Landau level}\\ \Psi_1(z) &= e^{-\frac{|z|^2}{4\ell_B^2}}\tilde{D}_z f(z) && E_1 = E_0 + \hbar\omega_c && \text{second Landau level}\\ \Psi_n(z) &= e^{-\frac{|z|^2}{4\ell_B^2}}\tilde{D}_z^n f(z) && E_n = E_0 + n\hbar\omega_c && .\end{aligned} \tag{2.26}$$

Here $f(z)$ is an arbitrary *holomorphic* function, meaning that it depends only on z and not on $\bar{z}$, and it is well-behaved. [End of Lecture 13]

There are many such functions! A nice basis of them is the polynomials:

$$\psi_m^{(0)}(z) = z^m e^{-\frac{|z|^2}{4\ell_B^2}} \tag{2.27}$$

is a lowest Landau level (LLL) state with angular momentum (2.21) equal to m. It has support in a ring centered at the origin, with a maximum at $r_m = \sqrt{2m}\ell_B$:

$$|\psi_m^{(0)}(z)| \propto e^{m\log z - \frac{|z|^2}{4\ell_B}}. \tag{2.28}$$

The orbit of such an electron has area $\pi r_m^2 = 2\pi\ell_B^2 m$ and therefore in a constant magnetic field it encloses m flux quanta: $\int_m B \cdot da = B\pi r_m^2 = m\frac{hc}{e}$.

Therefore, there is one state in the LLL for each flux quantum. This means that if the number of electrons per flux quantum $\nu = 1$, the free fermion groundstate will completely fill the lowest Landau level, and not at all involve states in the second Landau level. There's an energy gap $\hbar\omega_c$. The groundstate wavefunction takes a beautiful form:

$$\Psi_{\nu=1}(z_1 \cdots z_N) = \det_{ij} \psi^{(0)}_{m_i}(z_j) = (-1)^N \prod_i \varphi(z_i) \begin{vmatrix} 1 & 1 & \cdots \\ z_1 & z_2 & \cdots \\ z_1^2 & z_2^2 & \cdots \\ \vdots & \vdots & \ddots \end{vmatrix} = \prod_{i<j} (z_i - z_j) e^{-\sum_{i=1}^N |z_i|^2/(4\ell_B^2)}. \tag{2.29}$$

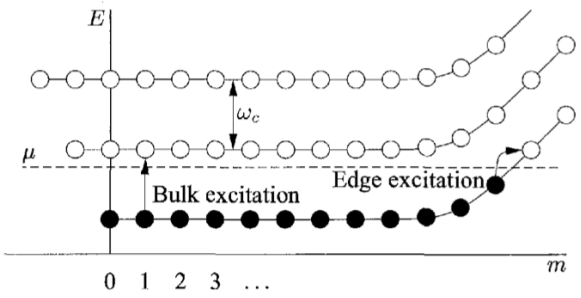
Now, there's something slightly awkward about what I said above: how can we have a uniform magnetic field everywhere, and one electron per flux quantum, and a finite number N of electrons? We could use periodic boundary conditions, but then we couldn't use polynomials z^n. In real life, what happens is that the Hall droplet has a boundary. Suppose that the electrons are confined to some region of space (where B is uniform, so the analysis above applies) by a smoothly-varying (electrostatic) potential $V(r)$. We can write the full hamiltonian as

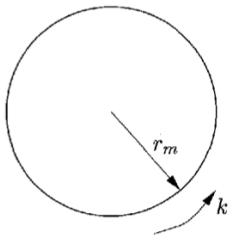
$$H = H_{\text{above}} + V(r) \tag{2.30}$$

and think of $V(r)$ as a perturbation. This perturbs the energies of the LLL states above by

$$E_m \approx \frac{1}{2}\hbar\omega_c + V(r_m). \tag{2.31}$$

But here $r_m = \sqrt{2m}\ell_B$. The excitations with small m lie in the bulk and have energy gap $\hbar\omega_c$. But for large enough m, r_m reaches the boundary of the sample, where the state $m+1$ is unfilled, and we can make an excitation by moving the particle from m to $m+1$.





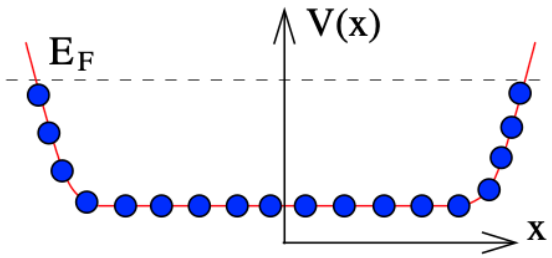
[fig from XG Wen]

The angular momentum m of an excitation at radius r_m is $m = r_m k$, where k is its linear momentum in the angular direction, $k = m/r_m$. So we can eliminate $\sqrt{m} = \sqrt{2}k\ell_B$ and regard (2.31) as a dispersion relation

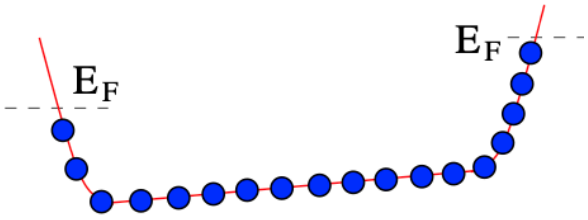
$$E_m \approx \frac{1}{2}\hbar\omega_c + V(2\ell_B^2 k) \tag{2.32}$$

for the edge excitations. The energy above the groundstate of the excitation is $\delta\omega = 2\ell_B^2 V'\delta k$. This is an excitation with velocity $2\ell_B^2 V'$, and there is no excitation with the opposite velocity. It is a gapless chiral edge excitation. And it will be there no matter what the potential is.

Using this picture we can also calculate the Hall conductivity. Let's think about a Hall droplet which is a strip extended in the y direction. In this geometry it's nicer to use Landau gauge, where $A_y = Bx$ (as you'll do on the homework) so that p_y is a conserved quantity. These states are labelled by the Landau level index n and the y-momentum k. The state labelled k is centered at $x = -k\ell_B^2$. (This relation is just like our relation for r_m above.) The groundstate looks like this [figure from David Tong]:



We'll apply an electric field in the x direction. Then the state looks like this:



The current in the y direction is

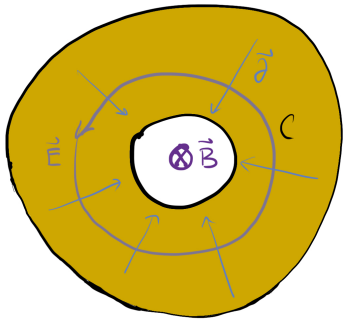
$$I_y = -e\int_{\text{filled states}} đk v_y(k) \simeq -\frac{e}{2\pi}\int \frac{dx}{\ell_B^2}\left(-\frac{1}{eB}\partial_x V\right) \overset{\text{FTC}}{=} \frac{e}{h}\Delta V = \frac{e^2}{h}\phi \tag{2.33}$$

where ϕ is the applied voltage across the sample in the x direction. So $\sigma_{xy} = \frac{I_y}{\phi} = \frac{e^2}{h}$. If we filled n Landau levels, we would find $\sigma_{xy} = n\frac{e^2}{h}$. Notice that this result is really robust: even if the potential were all wiggly, we would get the same answer.

Robustness of quantum Hall plateaux. The value of $\sigma_{xy}\frac{h}{e^2}$ is measured to be an integer to many decimal places. But we have not yet explained why it keeps the same value of B is varied away from the value where the filling fraction is exactly an integer. The fact that there is an energy gap suggests that not much can happen, because getting a different state would require some involvement of higher Landau levels. But in fact the extreme precision which with the Hall conductivity remains an integer requires one more ingredient. Ironically, it is actually a consequence of disorder. Imagine that the electrons are moving in a smooth but random electrostatic potential (this is what I mean by disorder). Our calculation above shows that classically electrons move along equipotential contours. As we vary the filling, the Hall fluid of electrons is like a rising sea, filling up more of the landscape. One effect of the disorder is to broaden each Landau level into a band of energies. The states at the top and bottom of each of these bands are associated with orbits that go around minima or maxima of the potential – these orbitals are *localized*, and do not contribute to the conductivity. Only special contours, which are in the middle of the bands, are extended across the sample. The key point is that only when the fermi level passes through one of these extended states does the Hall conductivity change.

General arguments about quantum Hall states. Actually there is a very general argument that a state with nonzero Hall conductivity $\sigma_{xy} = \nu\frac{e^2}{h}$ and an energy gap in the bulk must have gapless edge modes. The idea is to consider a cylinder geometry.

Consider the system on an annulus (sometimes called, in this context, the 'Corbino geometry'). Adiabatically thread a unit flux quantum $\Phi_0 = \frac{hc}{e}$ worth of magnetic field into (a solenoid in) the hole in the annulus. This means we slowly vary the magnetic field in the hole, so that the change in flux is the unit flux quantum $\Phi_0 \equiv \frac{hc}{e} = 2\pi$. This is called *flux-threading*.



$$\Phi_0 = \Delta\Phi = \int \mathrm{d}t\partial_t \left(\int_{\text{hole}} \mathrm{d}\vec{a}\cdot\vec{B}\right) \overset{\text{Faraday}}{=} -c\int \mathrm{d}t \oint_C \vec{E}\cdot\mathrm{d}\vec{\ell} \overset{j_r=\sigma_{xy}E_\varphi}{=} -\frac{c}{\sigma_{xy}}\underbrace{\int \mathrm{d}t j_r}_{=\Delta Q}$$

where C is a curve going around the hole. We conclude that an amount of charge

$$\Delta Q = \frac{\Phi_0}{c}\sigma_{xy} = \nu e \tag{2.34}$$

(e is the charge of the electron) is transferred from one edge of the cylinder to the other.

Moreover, the initial and final Hamiltonians are related by a gauge gransformation:

$$H(\Phi = 0) \cong H(\Phi = 2\pi).$$

They have the same spectrum. Moreover, the work done on the system is $\int I d\Phi \propto \int dt \left(\frac{d\Phi}{dt}\right)^2$ which goes to zero in the thermodynamic limit (make both inner and outer radius of the cylinder large), if our process is adiabatic. Therefore the initial and final states must be degenerate in the thermodynamic limit.

We've identified two different states related by the flux threading whose energies become degenerate in the thermodynamic limit. Since we've assumed the bulk is gapped, we conclude that there must be gapless edge states.

These two states differ in that an amount of charge ν has been moved from one boundary to the other. If charge is carried only by electrons, localized objects with integer charge, we conclude $\mathbb{Z} \ni \nu = \Delta Q/e = \sigma_{xy}$, the Hall conductivity must be an integer in units of $\frac{e^2}{h}$.

Amazingly, the innocent-looking assumption "if charge is carried only by electrons" can be violated. There are *fractional quantum Hall states*, where the bulk is gapped, but $\sigma_{xy} = \nu\frac{e^2}{h}$ with ν a fraction! The loophole is that these states have excitations that carry fractional charge – in such a medium, the electron splits apart. Such states cannot be understood without interactions. For more on this subject, you might try reading chapter 2 here. For more on quantum Hall states in general, I recommend David Tong's notes.

[End of Lecture 14]

Part 2:
Hard Problems

I have already emphasized that so far we've been studying very special many-body systems that can be solved by diagonalizing a one-particle Hamiltonian. Now it is time to look at the rest of the world. The problem is that such Hamiltonians are hard to solve. They are hard to solve numerically, because they involve matrices of size V^N where N is the number of particles and V is the volume of space. This grows very quickly with N and the best we can do with exact diagonalization is usually on the order of $N \sim 10^1$ particles and $V \sim 10^1$ lattice sites.

In general, they are also hard to solve analytically. There are a few examples where various tricks allow us to solve exactly, mostly only in $d = 1$. Otherwise we must use our wits. That is, we have to analyze extreme limits of couplings, where the problem simplifies, and we have to use mean field theory when we can. And we have to come up with new ideas. To illustrate these techniques in action, we will spend a little time on an example which is not obviously made of particles hopping around. Rather it is a model of a magnet.

3 A simple magnet

The Hilbert space is simply $\otimes_x \mathcal{H}_{\frac{1}{2}}$ where $\mathcal{H}_{\frac{1}{2}} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$ is the Hilbert space of a single qbit, that is, a spin-one-half. Acting on each of these Hilbert spaces is a set of Pauli operators, which I will denote $\mathbf{X}_x, \mathbf{Y}_x, \mathbf{Z}_x$. Their matrix elements are the Pauli matrices. More precisely, *e.g.* by $\mathbf{X}_x$ I mean the operator that acts as the identity on all the factors except for the spin at x, on which it interchanges up and down

$$\mathbf{X}_x |\sigma_1\rangle \otimes \cdots |\sigma_x\rangle \cdots \otimes |\sigma_V\rangle = |\sigma_1\rangle \otimes \cdots |\bar{\sigma}_x\rangle \cdots \otimes |\sigma_V\rangle$$

where $\bar{\uparrow} = \downarrow, \bar{\downarrow} = \uparrow$. That is,

$$\mathbf{X}_x = \mathbb{1} \otimes \cdots \otimes \mathbf{X} \otimes \cdots \otimes \mathbb{1}$$

where the $\mathbf{X}$ appears in the xth entry.

Hardcore bosons. In case you are bothered by the apparent left turn our discussion has taken, let me show you that this same Hilbert space can actually be realized as that of many particles. Relabel the two states at each site $|\uparrow\rangle \equiv |1\rangle, |\downarrow\rangle \equiv |0\rangle$. Regard these as eigenstates of a number operator

$$\mathbf{n}_x |\{n_1 \cdots n_V\}\rangle = n_x |\{n_1 \cdots n_V\}\rangle . \tag{3.1}$$

That is, each site may contain either zero particles (like the Fock vacuum) or one particle. The operators

$$\sigma_x^{\pm} \equiv \frac{1}{2} (\mathbf{X}_x \pm \mathbf{i}\mathbf{Y}_x)$$

respectively create a particle from $|0\rangle_x$ or destroy a particle if it is present at x. So these particles are like fermions in that there can only be one or zero in each orbital. However, they *commute* at different sites

$$[\sigma_x^{\alpha}, \sigma_y^{\beta}] = 0, \quad \text{for } x \neq y$$

rather than anticommute, so they are not actually fermionic operators. These particles are called *hard-core bosons*. Even if we write a Hamiltonian which is quadratic in $\boldsymbol{\sigma}_x^{\alpha}$, it will not be exactly solvable, because the creation and annihilation operators do not satisfy the canonical algebra. Another warning about this representation for present purposes: the Hamiltonian we'll study, (3.2), will not conserve particle number.

Another way to think about how such a Hilbert space might arise is if we had a bunch of spin-half electrons, each of which got stuck, for some reason, at one of the sites

x. 'Stuck' means that their position degrees of freedom are frozen out, that is, it costs too much energy to get them to move. But their spin degeneracy is still there. These spins can then interact with each other. This is one way in which insulating magnets happen, called a *Mott insulator*. Later we'll make this description more quantitative.

Arrange the sites x into a lattice. Denote by $\langle xy \rangle$ a pair of neighboring sites, which share a link of the lattice. The Hamiltonian we will consider is called the *transverse field Ising model*:

$$\mathbf{H}_{\text{TFIM}} = -J \left(\sum_x g\mathbf{X}_x + \sum_{\langle xy \rangle} \mathbf{Z}_x \mathbf{Z}_y \right) . \tag{3.2}$$

Some of the things we say next will be true in one or more spatial dimensions.

Notice that J has units of energy; we could choose units where it's 1. In 1d (or on bipartite lattices), the sign of J does not matter for determining what state of matter we realize: if $J < 0$, we can relabel our operators: $\tilde{\mathbf{Z}}_j = (-1)^j \mathbf{Z}_j$ and turn an antiferromagnetic interaction into a ferromagnetic one. So let's assume $g, J > 0$.

Competition. One reason that this model is interesting is because of the competition between the two terms: the $\mathbf{X}_j$ term wants *each* spin (independently of any others) to be in the state $|{\rightarrow}\rangle_j$ which satisfies

$$\mathbf{X}_j |{\rightarrow}\rangle_j = |{\rightarrow}\rangle_j . \quad |{\rightarrow}\rangle_j = \frac{1}{\sqrt{2}} \left(|{\uparrow}\rangle_j + |{\downarrow}\rangle_j \right) .$$

In conflict with this are the desires of $-\mathbf{Z}_j \mathbf{Z}_{j+1}$, which is made happy (*i.e.* smaller) by the more cooperative states $|{\uparrow_j \uparrow_{j+1}}\rangle$, or $|{\downarrow_j \downarrow_{j+1}}\rangle$. In fact, it would be just as happy about any linear combination of these $a\,|{\uparrow_j \uparrow_{j+1}}\rangle + b\,|{\downarrow_j \downarrow_{j+1}}\rangle$ and we'll come back to this point.

Compromise? Another model that looks like it might have some form of competition is

$$\mathbf{H}_{\text{boring}} = \cos\theta \sum_j \mathbf{Z}_j + \sin\theta \sum_j \mathbf{X}_j , \quad \theta \in [0, \frac{\pi}{2}]$$

Why is this one boring? Notice that we can continuously interpolate between the states enjoyed by these two terms: the groundstate of $\mathbf{H}_1 = \cos\theta \mathbf{Z} + \sin\theta \mathbf{X}$ is

$$|\theta\rangle = \cos\frac{\theta}{2} |{\uparrow}\rangle + \sin\frac{\theta}{2} |{\downarrow}\rangle$$

– as we vary θ from 0 to $\pi/2$ we just smoothly rotate from $|{\uparrow_z}\rangle$ to $|{\uparrow_x}\rangle$.

How do we know the same thing can't happen in the transverse-field Ising chain? Symmetry. The Ising model has a $G = \mathbb{Z}_2$ symmetry which acts by $\mathbf{Z}_j \to \mathbf{S}\mathbf{Z}_j\mathbf{S}^\dagger = -\mathbf{Z}_j, \mathbf{X}_j \to \mathbf{S}\mathbf{X}_j\mathbf{S}^\dagger = +\mathbf{X}_j$, where the unitary $\mathbf{S}$ commutes with $\mathbf{H}_{\text{TFIM}}$: $\mathbf{S}\mathbf{H}_{\text{TFIM}}\mathbf{S}^\dagger =$

$\mathbf{H}_{\text{TFIM}}$. More explicitly, $\mathbf{S} = \prod_x \mathbf{X}_x$. It is a $\mathbb{Z}_2$ symmetry in the sense that $\mathbf{S}^2 = \mathbb{1}$ (since $\mathbf{X}^2 = 1$). The difference with $\mathbf{H}_{\text{boring}}$ is that $\mathbf{H}_{\text{TFIM}}$ has two phases in which G is realized differently on the groundstate.

$\boxed{g = \infty}$: First, let's take g so big that we may ignore the ZZ ferromagnetic term, so

$$\mathbf{H}_{g\to\infty} = -\sum_j \mathbf{X}_j \ .$$

(The basic idea of this discussion will apply in any dimension, on any lattice.) Since all terms commute, the groundstate is the simultaneous groundstate of each term:

$$\mathbf{X}_j \left|\text{gs}\right\rangle = +\left|\text{gs}\right\rangle, \quad \forall j, \qquad \Longrightarrow \ \left|\text{gs}\right\rangle = \otimes_j \left|\rightarrow\right\rangle_j .$$

Notice that this state *preserves the symmetry* in the sense that $\mathbf{S}\left|\text{gs}\right\rangle = \left|\text{gs}\right\rangle$. Such a symmetry-preserving groundstate is called a *paramagnet*.

$\boxed{g = 0}$: Begin with $g = 0$.

$$\mathbf{H}_0 = -J\sum_j \mathbf{Z}_j\mathbf{Z}_{j+1}$$

has groundstates

$$\left|+\right\rangle \equiv \left|\uparrow\uparrow\cdots\uparrow\right\rangle, \quad \left|-\right\rangle \equiv \left|\downarrow\downarrow\cdots\downarrow\right\rangle,$$

or any linear combination. Note that the states $\left|\pm\right\rangle$ are not symmetric: $\mathbf{S}\left|\pm\right\rangle = \left|\mp\right\rangle$, and so we are tempted to declare that the symmetry is broken by the groundstate.

You will notice, however, that the states

$$\left|\ \text{  }_{\pm}\right\rangle \equiv \frac{1}{\sqrt{2}}\left(\left|+\right\rangle \pm \left|-\right\rangle\right)$$

are symmetric – they are $\mathbf{S}$ eigenstates, so $\mathbf{S}$ maps them to themselves up to a phase. It gets worse: In fact, in finite volume (finite number of sites of our chain), with $g \neq 0$, $\left|+\right\rangle$ and $\left|-\right\rangle$ are *not* eigenstates, and $\left|\ \text{  }_{+}\right\rangle$ is the groundstate. **BUT:**

1. The two states $\left|+\right\rangle$ and $\left|-\right\rangle$ only mix at order N in perturbation theory in g, since we have to flip all N spins using the perturbing hamiltonian $\Delta\mathbf{H} = -gJ\sum_j \mathbf{X}_j$ to get from one to the other. The tunneling amplitude is therefore

$$T \sim g^N \left\langle -\right| \mathbf{X}_1\mathbf{X}_2\cdots\mathbf{X}_N \left|+\right\rangle \overset{N\to\infty}{\to} 0.$$

2. There's a reason for the symbol I used to denote the symmetric states: at large N, these 'cat states' are superpositions of macroscopically distinct quantum states. Such things don't happen, because of decoherence: if even a single dust particle in the room measures the spin of a single one of the spins, it measures the value of the whole chain. In general, this happens very rapidly.

3. Imagine we add a small symmetry-breaking perturbation: $\Delta\mathbf{H} = -\sum_j h\mathbf{Z}_j$; this splits the degeneracy between $|+\rangle$ and $|-\rangle$. If $h > 0$, $|+\rangle$ is for sure the groundstate. Consider preparing the system with a tiny $h > 0$ and then setting $h = 0$ after it settles down. If we do this to a finite system, $N < \infty$, it will be in an excited state of the $h = 0$ Hamiltonian, since $|+\rangle$ will not be stationary (it will have a nonzero amplitude to tunnel into $|-\rangle$). But if we take the thermodynamic limit *before* taking $h \to 0$, it will stay in the state we put it in with the 'training field' h. So beware that there is a singularity of our expressions (with physical significance) that means that the limits do not commute:

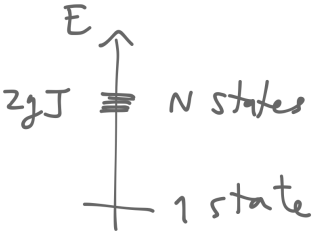
$$\lim_{N\to\infty}\lim_{h\to 0} Z \neq \lim_{h\to 0}\lim_{N\to\infty} Z.$$

   The physical one is to take the thermodynamic limit first.

The conclusion of this brief discussion is that spontaneous symmetry breaking actually happens in the $N \to \infty$ limit. At finite N, $|+\rangle$ and $|-\rangle$ are approximate eigenstates which become a better approximation as $N \to \infty$.

This state of a $\mathbb{Z}_2$-symmetric system that spontaneously breaks the $\mathbb{Z}_2$ symmetry is called a ferromagnet.

So the crucial idea I want to convey here is that there must be a sharp phase transition at some finite g: the situation cannot *continuously* vary from one unique, symmetric groundstate $\mathbf{S}\left|\mathrm{gs}_{g\ll 1}\right\rangle = \left|\mathrm{gs}_{g\ll 1}\right\rangle$ to two symmetry-breaking groundstates: $\mathbf{S}\left|\mathrm{gs}_{\pm}\right\rangle = \left|\mathrm{gs}_{\mp}\right\rangle$. We'll make this statement more precise when we discuss the notion of long-range order. First, let's see what happens when we try to vary the coupling away from the extreme points. For definiteness now, we focus on one dimension, a chain of N sites.



$\boxed{g \gg 1}$ An excited state of the paramagnet, deep in the phase, is achieved by flipping one spin. With $\mathbf{H} = \mathbf{H}_\infty = -gJ\sum_j \mathbf{X}_j$, this costs energy $2gJ$ above the groundstate. There are N such states, labelled by which spin we flipped:

$$|n\rangle \equiv \Big|\to\cdots\to \underbrace{\leftarrow}_{nth\ \text{site}} \to\cdots\Big\rangle, \qquad (\mathbf{H}_\infty - E_0)\,|n\rangle = 2gJ\,|n\rangle\,, \ \forall n$$

[End of Lecture 15]

When g is not infinite, we can learn a lot from (1st order) degenerate perturbation theory in the ferrmomagnetic term. The key information is the matrix elements of the perturbing hamiltonian between the degenerate manifold of states. Using the fact that $\mathbf{Z}_j |{\rightarrow}\rangle = |{\leftarrow}\rangle$, so,

$$\mathbf{Z}_j\mathbf{Z}_{j+1} |{\rightarrow_j\leftarrow_{j+1}}\rangle = |{\leftarrow_j\rightarrow_{j+1}}\rangle$$
$$\langle n \pm 1| \sum_j \mathbf{Z}_j\mathbf{Z}_{j+1} |n\rangle = 1,$$

the ferromagnetic term hops the spin flip by one site. Within the degenerate subspace, it acts as

$$\mathbf{H}_{\text{eff}} |n\rangle = -J\left(|n+1\rangle + |n-1\rangle\right) + (E_0 + 2gJ) |n\rangle .$$

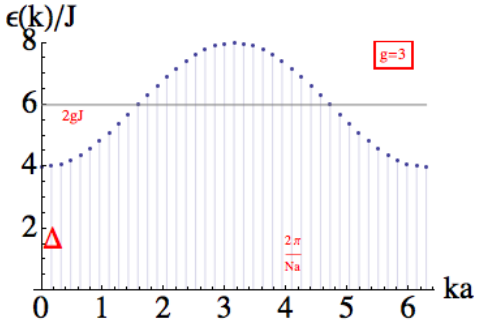
It is a kinetic, or 'hopping' term for the spin flip.

Let's see what this does to the spectrum. Assume periodic boundary conditions and N sites total. Again this is a translation invariant problem (in fact essentially the same one we've studied several times before), which we can solve by Fourer transform:

$$|n\rangle \equiv \frac{1}{\sqrt{N}} \sum_j e^{-\mathbf{i}kx_j} |k\rangle , \quad \begin{cases} x_j \equiv ja, \\ k = \frac{2\pi m}{Na}, \quad m = 1..N \end{cases} .$$

On the momentum states, we have

$$(H - E_0) |k\rangle = (-2J\cos ka + 2gJ) |k\rangle .$$



The dispersion of these spinon particles is

$$\epsilon(k) = 2J(g - \cos ka) \overset{k\to 0}{\sim} \Delta + J(ka)^2 \qquad (3.3)$$

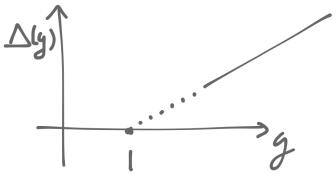
with $\Delta = 2J(g-1)$ – there is an energy gap (notice that Δ does not depend on system size). So these are *massive* particles, with dispersion $\epsilon = \Delta + \frac{k^2}{2M} + ...$ where Δ is the energy to create one at rest (notice that the rest energy is not related to its inertial mass $M^{-1} = 2Ja^2$).

A particle at j is created by the creation operator $\mathbf{Z}_j$:

$$|j\rangle = \mathbf{Z}_j |\text{gs}_\infty\rangle .$$

And it is annihilated by the annihilation operator $\mathbf{Z}_j$ – you can't have two spin flips at the same location! These particles are their own antiparticles.

The *number* of such particles is counted by the operator $\sum_j (-\mathbf{X}_j)$. The number of particles is only conserved modulo two, however.



What happens as g gets smaller? The gap to creating a spin flip at large g looks like $2J(g-1)$. If we take this formula seriously, we predict that at $g=1$ it costs zero energy to create spin flips: they should *condense* in the vacuum. An excitation is said to be *condensed* in a state $|\psi\rangle$ if $\langle\psi|\mathcal{O}|\psi\rangle \neq 0$, where $\mathcal{O}$ is the operator that creates the excitation. Condensing spin flips means $\langle Z\rangle \neq 0$, so the state is magnetized. (We shouldn't take this $g=1$ prediction too seriously because it's just first order in perturbation theory, but it turns out to be exactly right.)

It's possible to develop some more evidence for this picture and understanding of the physics of the paramagnetic phase in the Ising chain by doing more perturbation theory, and including states with two spin flips. Notice that for a state with two spin-flip particles, the total momentum k no longer uniquely determines the energy, since the two spin-flips can have a relative momentum; this means that there is a *two-particle continuum* of states, once we have enough energy to make two spin flips. For more on this, see *e.g.* Sachdev (2d ed) §5.2.2. In particular the two spin-flips can form boundstates, which means there are two-particle states with energies slightly below 2Δ.

$\boxed{g \ll 1}$ Now let's consider excitations of the ferromagnet, about the state $|+\rangle = |\uparrow\uparrow\cdots\uparrow\rangle$. It is an eigenstate of $\mathbf{H}_0 = -J\sum_j \mathbf{Z}_j\mathbf{Z}_{j+1}$ and its (groundstate) energy is $E_0 = -JN$. We can make an excitation by flipping one spin:

$$|\cdots\uparrow\ \uparrow\ \uparrow\cdot\downarrow\cdot\uparrow\ \uparrow\ \uparrow\cdots\rangle$$

This makes two bonds unhappy, and costs $2J+2J=4J$. But once we make it, there are many such states: the hamiltonian is the same amount of unhappy if we also flip the next one.

$$|\cdots\uparrow\ \uparrow\ \uparrow\cdot\downarrow\ \downarrow\cdot\uparrow\ \uparrow\cdots\rangle$$

The actual elementary excitation is a *domain wall* (or *kink*), which only costs $2J$. The domain wall should be regarded as living between the sites. It is not entirely a local object, since with periodic boundary conditions, we must make two, which can then move independently. To create two of them far apart, we must change the state of many spins.

At $g=0$ the domain walls are *localized* in the sense that a domain wall at a fixed position is an energy eigenstate (just like the spinons at $g=\infty$), with the same energy for any position. But now the paramagnetic term $-\sum_j g\mathbf{X}_j$ is a kinetic term for the domain walls:

$$\mathbf{X}_{j+1}\underbrace{|\cdots\uparrow\uparrow\uparrow_j\cdot\downarrow_{j+1}\downarrow\downarrow\cdots\rangle}_{|\bar{j}} = \underbrace{|\cdots\uparrow\uparrow\uparrow_j\uparrow_{j+1}\cdot\downarrow_{j+2}\downarrow\cdots\rangle}_{=|\bar{j}+1\rangle}.$$

Just like in our $g \gg 1$ discussion, acting on a state with an even number of well-separated domain walls

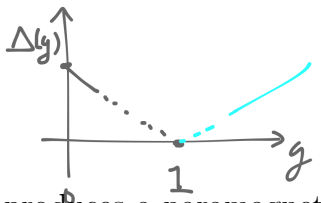
$$(H_{\text{eff}} - E_0)\,|\bar{j}\rangle = -gJ\,(|\bar{j}+1\rangle + |\bar{j}-1\rangle) + 2J\,|\bar{j}\rangle$$

where the diagonal term is the energy cost of one domain wall at rest. Again this is diagonalized in k-space with energy

$$\epsilon_{\text{one dwall}}(k) = 2J(1 - g\cos ka)$$

Again, this calculation is almost ridiculously successful at predicting the location of the phase transition:

$$\Delta_{DW} = 2J(1-g) \overset{g\to 1}{\to} 0.$$



We predict that for $g > 1$, the domain walls condense; this produces a paramagnetic state.

Notice that although our discussion of the paramagnetic state $g \gg 1$ can be applied in any $d \geq 1$, the physics of domain walls is very dimension-dependent.

3.0.1 Mean field theory

So far we have used perturbation theory about $g = 0$ and $g = \infty$ to delicately inch our way toward the interior of the phase diagram of the TFIM in one dimension (3.2). Here we take a plunge and try to guess the groundstate for all g. The nice thing about trying to guess the groundstate is the Rayleigh-Schrödinger hedge: the energy expectation in any state is an upper bound for the groundstate energy; minimizing the energy within a class of guesses is called a 'variational approach'.

The name for the particular guess we'll make is 'mean field theory', which means that we completely ignore entanglement between different sites, and suppose that the state is a product state

$$|\text{MFT}\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \cdots |\psi_j\rangle \cdots \ldots$$

If we further assume translational invariance then the state at every site is the same and we have one bloch sphere to minimize over for each g:

$$|\check{n}\rangle = \otimes_j\, |\uparrow_{\check{n}}\rangle_j = \otimes_j \left(\cos\frac{\theta}{2} e^{\mathbf{i}\varphi/2}\,|{\to}\rangle + \sin\frac{\theta}{2} e^{-\mathbf{i}\varphi/2}\,|{\leftarrow}\rangle\right)_j .$$

(Here θ is the angle $\check{n}$ makes with the x axis, and φ is the azimuthal angle in the yz plane, from the z-axis.) To evaluate the energy expectation in this state, we only need to know single-qbit expectations:

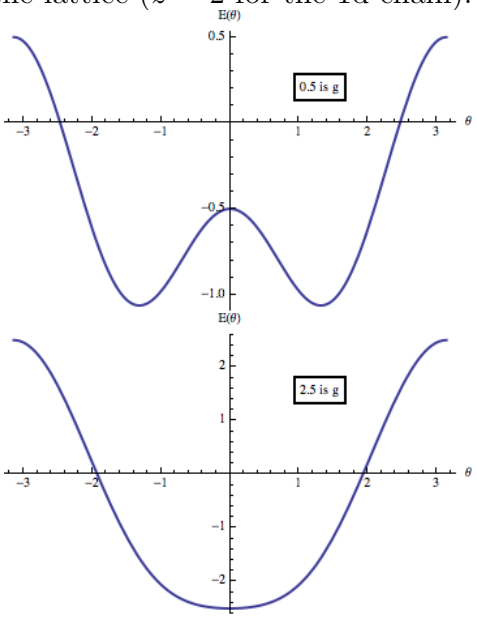
$$\langle\uparrow_{\check{n}}|\,\mathbf{X}\,|\uparrow_{\check{n}}\rangle = \cos\theta, \quad \langle\uparrow_{\check{n}}|\,\mathbf{Z}\,|\uparrow_{\check{n}}\rangle = \sin\theta\cos\varphi.$$

So the energy expectation is

$$E(\theta,\varphi) = -NJ\left(\frac{z}{2}\sin^2\theta\cos^2\varphi + g\cos\theta\right)$$

where z is the number of neighbors of each site of the lattice ($z = 2$ for the 1d chain). This is extremized when $\varphi = 0, \pi$ and when

$$0 = \partial_\theta E = NJ\sin\theta\,(z\cos\theta - g)\,.$$



Notice that when $\theta = 0$, the two solutions of φ are the same, since the φ coordinate degenerates at the pole. The solutions at $\cos\theta = g/z$ only exist when $g/z < 1$. In that case they are minima (see the figure) since $\partial_\theta^2 E|_{\cos\theta = g/z} > 0$, while $\partial_\theta^2 E|_{\theta=0} = NJ(g-z)$ is negative for $g < 2$. (Notice that $\varphi = \pi$ can be included by allowing $\theta \in (-\pi, \pi]$, as in the figure.)

So mean field theory predicts a phase transition at $g = 2$, from a state where $\langle \mathbf{Z}_j \rangle = \sin\theta$ to one where $\langle \mathbf{Z} \rangle = 0$. It overestimates the range of the ordered phase because it leaves out fluctuations which tend to destroy the order.

Let's study the behavior near the transition, where θ is small. Then the energy can be approximated by its Taylor expansion

$$E(\theta) \simeq NJ\left(-z + \frac{g-z}{2}\theta^2 + \frac{z}{8}\theta^4\right)$$

(where I have set $g = g_c = z$ except in the crucial quadratic term). This has minima at

$$\langle \mathbf{Z}_j \rangle = \sin\theta \simeq \theta = \pm\sqrt{g_c - g}\ . \tag{3.4}$$

The energy behaves like

$$\frac{E_{MFT}(g)}{NJ} = -g + \begin{cases} \frac{1}{2z}(g_c - g)^2\ , & g < g_c \\ \\ 0\ , & g \geq g_c \end{cases}$$

Notice that $\partial_g E$ is continuous at the transition. So mean field theory (correctly) predicts a continuous quantum phase transition between the ordered phase and the disordered phase. The location of the transition is wrong (mean field theory overestimates the size of the ordered region because it leaves out lots of order-destroying

fluctuations), and so are other properties, such as the exponent in (3.4), which should be 1/8 instead of 1/2.

Another point of view on mean field theory is: let's think about the experience of the world of a single spin. Much like a human during lockdown, its experience of the world is mediated by the behavior of its neighbors. We can write the Hamiltonian as

$$\mathbf{H} = -J\left(g\sum_i \mathbf{X}_i + \sum_i \mathbf{Z}_i\left(\frac{1}{2}\sum_{j,\text{ neighbors of } i}\mathbf{Z}_j\right)\right).$$

From the point of view of $\mathbf{Z}_i$, the object $\left(\frac{1}{2}\sum_{j,\text{ neighbors of } i}\mathbf{Z}_j\right) \equiv h_i$ just acts like an effective longitudinal magnetic field. A mean field theory arises by replacing the neighboring operators by their expectation values:

$$\mathbf{H}_{MF} = -J\left(g\sum_i \mathbf{X}_i + \sum_{\langle ij\rangle}\left(\mathbf{Z}_i\langle\mathbf{Z}_j\rangle + \langle\mathbf{Z}_i\rangle\mathbf{Z}_j - \langle\mathbf{Z}_i\rangle\langle\mathbf{Z}_j\rangle\right)\right).$$

Now this hamiltonian has the form of $\mathbf{H}_{\text{boring}}$ above, whose groundstate is just all the spins pointing in some direction $\theta(\langle\mathbf{Z}\rangle)$ between $\hat{x}$ and $\hat{z}$. This becomes slightly nontrivial if we demand that $\langle\mathbf{Z}\rangle$ comes out right when computed in the resulting groundstate. This self-consistency condition is

$$m \equiv \langle\mathbf{Z}\rangle = \frac{zJm}{\sqrt{(zJm)^2 + (gJ)^2}}$$

(where z is the number of neighbors of each site). This says $m = \pm\sqrt{1-\frac{g^2}{z^2}}$, reproducing our (approximate!) answer for the critical coupling $g = z$. (We would find the same condition by minimizing the groundstate energy over m.)

Notice that if we let the magnetization m in the mean field ansatz depend on space, we would get not just a Landau-Ginzburg potential, but a Landau-Ginzburg functional of m, involving derivative terms, like

$$\sum_{\langle ij\rangle} m_i m_j \simeq \int d^dx \vec{\nabla}m\cdot\vec{\nabla}m + \cdots. \tag{3.5}$$

But you can see that, as long as the sign in front is positive, we minimize the energy by taking m to be constant. (If the sign is the other way, we will make instead a density wave, where the sign of the magnetization oscillates in space, spontaneously breaking translation invariance. An antiferromagnet is an extreme example of this where the period of oscillation is a single lattice spacing, and where the approximation on the RHS of (3.5) is not valid.)

3.0.2 Correlation functions and long-range order

A useful set of physical (observable! as we'll discuss in a moment) quantities are the correlation functions of the spins:

$$C(r,r') \equiv \langle 0|\mathbf{Z}_r\mathbf{Z}_{r'}|0\rangle \quad .$$

Notice that this is an *equal-time* correlator. If the groundstate is translation invariant, this is only a function of the separation between the spins $C(r,r') = C(r-r')$. (Notice that I am using rs and js to label the positions interchangably, but $r = ja$, where a is the lattice spacing.) We can take further advantage of translation symmetry by thinking about the Fourier transform of this quantity, which is called the *static structure factor*:

$$S(q) \equiv \sum_r e^{-\mathbf{i}qr} C(r) \ ;$$

the sum over positions is over $r \in a\{1...N\}$, and (assuming periodic boundary conditions again) the argument $q \in \frac{2\pi}{Na}\{1...N\}$.

Correlations in the quantum Ising chain. At $g = \infty$, all the way in the paramagnetic phase,

$$\langle 0|\, \mathbf{Z}_j\mathbf{Z}_l \,|0\rangle\,|_{g=\infty} = \delta_{jl}$$

– different sites are totally uncorrelated. At finite but large $g \gg 1$ we have instead:

$$\langle 0|\, \mathbf{Z}_j\mathbf{Z}_l \,|0\rangle\,|_{g\gg 1} \overset{|x_j-x_l|\gg a}{\simeq} e^{-|x_j-x_l|/\xi} \tag{3.6}$$

[End of Lecture 16]

– the fluctuations of the spin flips communicate between the sites, but only over a short range, because the spin flips are massive[22].

In contrast, for $g \ll 1$, in the ferromagnetic phase,

$$\langle 0|\, \mathbf{Z}_j\mathbf{Z}_l \,|0\rangle\,|_{g\ll 1} \overset{|x_j-x_l|\gg a}{\simeq} N_0^2(g) \tag{3.7}$$

where $N_0^2(g) = 1$ for $g = 0$. $N_0 < 1$ for $g > 1$.

[22] To get a sense of where (3.6) comes from, let's represent Z_j as a scalar field, in terms of creation and annhilation operators for the spin-flip excitations: $Z_j = \sum_k \frac{1}{\sqrt{2\omega_k}}\left(\mathbf{a}_k e^{\mathbf{i}kaj} + h.c.\right)$. Then

$$\langle 0|\, \mathbf{Z}_j\mathbf{Z}_l \,|0\rangle \simeq \sum_k \frac{1}{2\omega_k} e^{\mathbf{i}ka(j-l)} \simeq \int \mathrm{d}^d k \frac{e^{\mathbf{i}kx}}{2\omega_k}$$

where $\omega_k = \Delta + \frac{k^2}{2M}$ is the dispersion relation for the spin flips and $x = a(j-l)$. This integral is doable and the answer goes like $e^{-\sqrt{2M\Delta}|x|}$ for large x. Notice that the long-wavelength behavior of ω_k is appropriate for large x, since then small k dominates the integral.

More simply, if we train the system appropriately (as we discussed in point 3), then we'll have

$$\langle 0|\, \mathbf{Z}_j \,|0\rangle = \pm N_0(g).$$

N_0 is the order parameter, the magnetization. Another way to state the issue about the order of limits of $h \to 0, N \to \infty$: in a finite system the magnetization is zero:

$$\lim_{N\to\infty}\lim_{h\to 0}\langle \mathbf{Z}_i\rangle = 0, \quad \text{but} \quad \lim_{h\to 0}\lim_{N\to\infty}\langle \mathbf{Z}_i\rangle = N_0 \ .$$

In this sense, the ferromagnet is said to have *long range order*.

OK but here's the simple important point: There's no smooth function of g that can interpolate between (3.6) and (3.7). A virtue of the notion of long-range order is it gives sharp distinctions between phases.

3.0.3 Physics of structure factors

Consider the limit where $N \to \infty$ so that the allowed momenta fill in a continuous Brillouin zone $q \in \frac{2\pi}{N}\{1..N\} \to (0, \pi] \simeq (-\pi, \pi]$. So the inverse Fourier transform is

$$C(R) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} S(q) e^{\mathbf{i}qR} \ .$$

When there is long range order,

$$C(R) \overset{R\to\infty}{\sim} N_0^2$$

what does $S(q)$ do? It means a singularity at $q = 0$:

$$S(q) = 2\pi\delta(q)N_0^2 + \text{regular} \tag{3.8}$$

where 'regular' means terms which are smooth at $q = 0$. This singularity is a sharp signature of the broken symmetry.

We can learn something by considering a spectral representation of $S(q)$, obtained by resolving the identity by energy eigenstates $|n\rangle$:

$$S(q) = \frac{1}{V}\langle 0|\, \mathbf{Z}_q \mathbf{Z}_{-q} \,|0\rangle = \frac{1}{V}\sum_n |\, \langle n|\, \mathbf{Z}_q \,|0\rangle \,|^2 \ . \tag{3.9}$$

Here I used $\mathbf{Z}_q \equiv \sum_r e^{-\mathbf{i}qr}\mathbf{Z}_r = \mathbf{Z}_{-q}^\dagger$.

A sum rule: $C(R = 0) = \langle 0|\, \mathbf{Z}_r\mathbf{Z}_r \,|0\rangle = \langle 0|0\rangle = 1$. But the (inverse) Fourier transform is

$$1 = C(R = 0) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} S(q) \ .$$

This is some short-distance information which remembers that the objects we're looking at square to one. Given the spectral interpretation, this sum rule means that as we vary parameters, the spectral weight can move around, but it can't go away. In particular, when the system orders as in (3.8), the $2\pi N_0^2$ contribution at $q = 0$ has to come from somewhere.

Dynamical structure factor.

$$C(r,t) \equiv \langle 0| \mathbf{Z}_r(t)\mathbf{Z}_0(0) |0\rangle .$$

This reduces to $C(r)$ if we set $t = 0$. It is useful to think of $\mathbf{Z}_r(t)$ in Heisenberg representation: $\mathbf{Z}_r(t) = e^{+\mathbf{i}\mathbf{H}t}\mathbf{Z}_r e^{-\mathbf{i}\mathbf{H}t}$. Its Fourier transform in time and space is the dynamical structure factor:

$$S(q,\omega) = \sum_r e^{-\mathbf{i}qr} \int_{-\infty}^{\infty} dt e^{+\mathbf{i}\omega t} C(r,t).$$

Notice that $S(q) = \int đ\omega S(q,\omega)$ (not $S(\omega = 0)$). The spectral representation of the dynamical structure factor is:

$$S(q,\omega) = \frac{1}{V}\sum_n |\langle n| \mathbf{Z}_q |0\rangle|^2 2\pi\delta(\omega + E_0 - E_n) . \tag{3.10}$$

So (3.9) is obtained by integrating over ω[23] which simply removes the ω dependence.

In words: $S(q,\omega)$ is the number of states of momentum q and energy ω, weighted by (the square of) their overlap with the state engendered upon the groundstate by the spin operator. This formula is crying out to be interpreted in terms of Fermi's Golden Rule.

Before we do that let's include finite temperature, too. Let

$$C(x,t;x't') = \frac{1}{Z}\mathrm{tr} e^{-\mathbf{H}/T}\mathbf{Z}(x,t)\mathbf{Z}(x't')$$

where again $\mathbf{Z}$ are Heisenberg picture operators and $Z = \mathrm{tr} e^{-\mathbf{H}/T}$. Its fourier transform is

$$S(q,\omega) = \frac{\int d^dx'}{V}\int d^dx \int_{-\infty}^{\infty} dt\ e^{\mathbf{i}\omega(t-t') - \mathbf{i}\vec{q}\cdot(\vec{x}-\vec{x}')} C(x,t;x't').$$

Notice that the time integral here is over real time, not euclidean time. To find the spectral representation, again, insert an energy eigenbasis $\mathbb{1} = \sum_n |n\rangle\langle n|$ in between each time evolution operator and each field, and do the space and time integrals. The result is:

$$S(q,\omega) = \frac{1}{ZV}\sum_{n,n'} e^{-E_{n'}/T} |\langle n| \mathbf{Z}(q) |n'\rangle|^2 2\pi\delta(\omega + E_{n'} - E_n) .$$

[23] With the usual $\frac{1}{2\pi}$ convention: $\int đ\omega S(q,\omega) = S(q)$.

V is the volume of space.

Now let's interpret this in terms of a transition rate in a scattering experiment, via Fermi's Golden Rule. Recall that the FGR says that the transition rate is

$$\Gamma = \sum_F |\langle F| \mathbf{H}_{\text{pert}} |I\rangle|^2;$$

more generally, if we are uncertain about the initial state, so it is described by a density matrix, $\rho = \sum_I p_I |I\rangle\langle I|$, then

$$\Gamma = \sum_{F,I} p_I |\langle F| \mathbf{H}_{\text{pert}} |I\rangle|^2.$$

In the problem above, the initial state is $|n'\rangle$ with probability $p_{n'} = e^{-E_{n'}/T}/Z$ given by the Boltzmann distribution. (In the $T \to 0$ limit, we return to (3.10), where the initial state is the groundstate with probability 1.) The perturbing hamiltonian is linear in the spin operator $\mathbf{H}_{\text{pert}} \propto \mathbf{Z}(q)$. With these assumptions, the transition rate per unit time is exactly $S(q,\omega)$. This explains the connection between the dynamical structure factor and experiments involving scattering of neutrons: a neutron couples to the spins via its magnetic dipole moment, which couples linearly to the spin operator; ω, q are the change in energy and momentum of the system. The transition probability (at zero temperature) is proportional to something like:

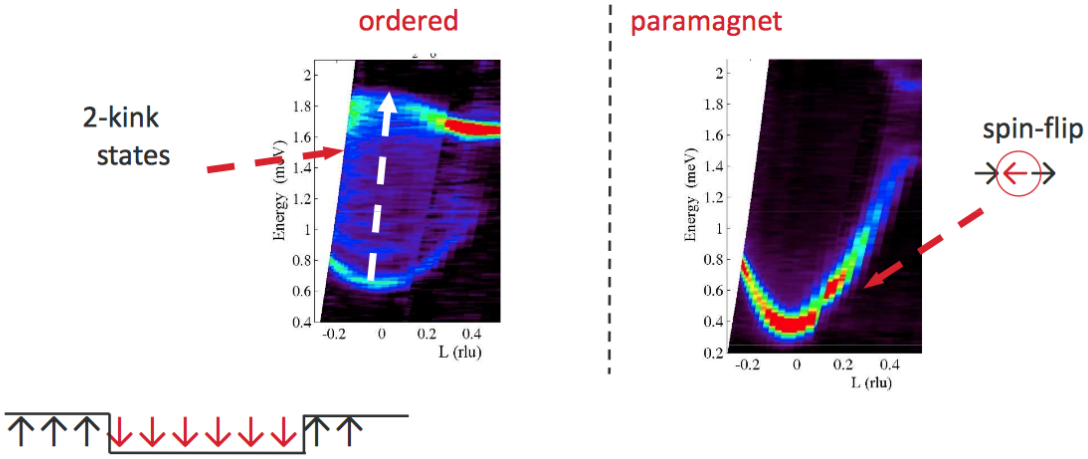
$$|\langle n| \otimes \left\langle \text{neutron, final}(E-\omega, \vec{k}-\vec{q}, \hat{z}) \right| \vec{\mathbf{S}}_{\text{neutron}} \cdot \vec{\boldsymbol{\sigma}} |0\rangle \otimes \left| \text{neutron, initial}(E, \vec{k}, \hat{z}) \right\rangle|^2 . \tag{3.11}$$

The (known) neutron states allow us to determine q, ω. You could ask me how we do an experiment that couples just to $\mathbf{Z}$, and not all of $\vec{\boldsymbol{\sigma}}$. We can do this if we can choose the initial and final spin states of the neutrons to be polarized along $\hat{z}$, as indicated in (3.11).

Given our understanding of the spectrum at large and small g, we have a prediction for the behavior of $S(q,\omega)$: at large g, the lowest-energy excitation is a single spin flip, which conveniently is created by $\mathbf{Z}$, and so contributes to $S(q,\omega)$. But it only contributes if q and ω are related in the right way, namely $\omega = \epsilon_q$. This means that there will be a sharp peak along this curve: for ω in the right range, $S(q,\omega) = Z\delta(\omega - \epsilon_q)$. For larger ω, we access the multi-particle continuum. In fact, $\mathbf{Z}|0\rangle$ only includes states with an odd number of particles, so the continuum in $S(q,\omega)$ starts near 3Δ. What happens at small g? At small g, the spin flip is not stable – it can decay into a pair of domain walls, which are free to move apart. Although these domain walls behave in many ways like particles, the operator $\mathbf{Z}_j$ cannot create a single domain wall. (In fact the domain wall creation operator is made of a string of $\mathbf{X}$s, since we must flip all the

spins on one side of the wall.) So the spectral function of $\mathbf{Z}$ has only a continuous mess at small g – a multiparticle continuum of domain walls, no sharp delta-function peak.

People[24] have done this experiment on a system that is well-described by the TFIM ($CoNb_2O_6$). It can be approximated as a collection of decoupled chains of spins with nearest-neighbor ferromagnetic Ising interactions. The transverse field term can be produced by applying a (surprise) transverse magnetic field, and hence g can be varied. Indeed at large g one sees a sharp single-particle peak, and at small g there is a featureless mess, *i.e.* a two-particle continuum. Here is a summary of the results of the experiment (from Ashvin Vishwanath):



A further feature of these experiments that I must mention is: if we apply a *longitudinal* field, $\Delta\mathbf{H} = \sum_j h_z \mathbf{Z}_j$, we *confine* the domain walls, in the following sense. This term means that a region of down-spins costs an energy proportional to its length. This is an interaction energy between the domain walls at the edges of the region which is linear in their separation, a constant attractive force between them. Their spectrum of boundstates is extremely interesting and represents a physical appearance of E_8 symmetry.

Confession. Actually it turns out that the TFIM in one dimension is one of the examples that can be solved exactly by cleverness. The cleverness is called the Jordan-Wigner transformation, and it relates the spin system to a model of fermions. And the hamiltonian is actually gaussian in those fermions! Actually, the discussion around (3.1) is the special case of it in $d = 0$, *i.e.* at a single site. But this is a story for another time (namely, the homework).

[24] Coldea et al, *Science* **327** (2010) 177.

4 Interacting bosons

[Leggett, *Quantum Liquids*] Recall that the groundstate of a collection of N non-interacting bosons is

$$\frac{\left(\mathbf{b}_{p_0}^\dagger\right)^N}{\sqrt{N!}}|0\rangle$$

where p_0 labels the mode with the lowest single-particle energy: $\epsilon(p_0)$ is the minimum of $\epsilon(p)$. The crucial feature of this state is that there is a macroscopic occupation of a single single-particle orbital. Let us tentatively call this phenomenon Bose-Einstein Condensation (BEC).

And recall briefly from statistical mechanics that this phenomenon survives to finite $T > 0$. For $0 \leq T \leq T_c$, the accounting of all N (still non-interacting) particles satisfies

$$N = N_0(T) + N\int_0^\infty \frac{\rho(\epsilon)d\epsilon}{e^{\beta\epsilon}-1}$$

where $\rho(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i)$ is the density of single-particle energy levels ($\{\epsilon_i\}$ is the spectrum of the single-particle hamiltonian h). T_c is the value of T for which $N_0(T)$ goes to zero. If $\rho(\epsilon) \propto \epsilon^{\alpha-1}$ then

$$N_0(T) = N\left(1 - \left(\frac{T}{T_c}\right)^\alpha\right), \quad T < T_c.$$

For a nonrelativistic gas in 3d free space, $\alpha = 3/2$; for a 3d harmonic trap, $\alpha = 3$. Notice that for 2d free space $\alpha = 1/2$ and the integral doesn't converge – there is no need to macroscopically occupy the lowest-energy state in this case.

This raises some questions for us:

1. Does this phenomenon (of macroscopic occupation of a single orbital) survive interactions?
2. How to even define it in that case?
3. Why does it matter if a single orbital is macroscopically occupied?

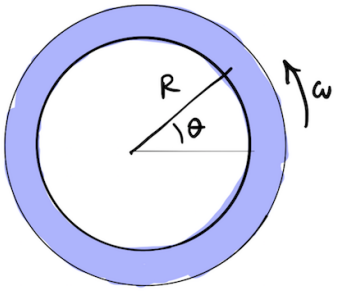
4.1 Phenomenology of super-flow

So what? Let us focus for a moment on question 3. The answer is associated with a collection of phenomena which are called *superfluidity* or *superconductivity*. The two names refer to two separate cases: the latter applies when the boson that is condensing

is *charged* under electromagnetism. Its condensation then has some important consequences for the behavior of the electric and magnetic fields and currents. The former case is when the boson is neutral, such as a ^{4}He atom. What are these phenomena? (We are going to indulge for the next several paragraphs in *phenomenology* – I will tell you some things that have been seen in experiments, and we'll come back and understand as many of them as possible as a consequence of the BEC phenomenon.)

Let us place our bosons in a ring-shaped container which can rotate. We can think of this as simply an external single-particle potential

$$U(\vec{r}) = U(r, z, \theta). \tag{4.1}$$



We assume that rotating the container at frequency ω means that the potential (4.1) becomes

$$U(r, z, \theta) \mapsto U(r, z, \theta - \omega t).$$

The classical moment of inertia of the particles is $I_{cl} = NmR^2$. $\omega_c \equiv \frac{\hbar}{mR^2}$ is a quantity with units of frequency, which since it has an $\hbar$ is like a quantum unit of angular velocity. In terms of it, the angular momentum of the particles at angular frequency ω is

$$L = I_{cl}\omega = N\hbar\frac{\omega}{\omega_c}.$$

We will consider two different but related experiments.

(1) Rotate the *fluid*. Do this just by stirring it: start by rotating the container at $\omega \gg \omega_c$. In fact, we can start stirring it when it's in the 'normal phase' at $T > T_c$. (In the case when the fluid is charged, we can do this by turning on a magnetic field, *i.e.* threading magnetic flux through the hole in the ring; by Faraday, this creates an EMF which will rotate the particles.) After it gets going at frequency ω, cool it below T_c.

If it were a normal system, the rotational motion would be transient. It gets damped by viscous drag with the walls of the container (in the case of a neutral fluid), or electrical resistance (in the case of a charged fluid). In the case of a superfluid, the rotation persists. In some cases it persists indefinitely. [End of Lecture 17]

Moreover, the angular momentum is given by

$$L = f_s(T) I_{cl}\tilde{\omega} \tag{4.2}$$

where (get ready) $\tilde{\omega}$ is the nearest integer to $\frac{\omega}{\omega_c}$ when the system cools below T_c. $f_s(T)$

is a function of temperature that is a property of the material. It satisfies

$$f_s(T) \to \begin{cases} 1, & T \to 0 \\ 0, & T \to T_c \end{cases}.$$

(4.2) therefore means that if we vary the temperature adiabatically, we can vary the angular momentum of the fluid reversibly.

(2) Consider first the neutral case. For the second experiment, we rotate the *container*. This means the hamiltonian is

$$\mathbf{H}_\omega = \mathbf{H} - \vec{\omega} \cdot \vec{L} = \mathbf{H} - \vec{\omega} \cdot \sum_{i=1}^{N} \vec{r}_i \times \vec{p}_i$$

where $\vec{p}_i$ is the lab-frame momentum of the ith particle, and $\mathbf{H}$ is the hamiltonian before we did any rotating.

A normal fluid will rotate along with the container, with $\vec{L} \sim I_{cl}\vec{\omega}$. In a superfluid (as long as the rotation isn't too fast, $\omega < \omega_c/2$), the angular momentum will instead satisfy

$$\vec{L} = (1 - f_s(T))I_{cl}\vec{\omega}, \tag{4.3}$$

with the same function f_s as above. It is as if the fraction f_s of the fluid simply refuses to participate, and doesn't contribute to the moment of inertia. Some names: $f_n(T) \equiv 1 - f_s(T)$ is sometimes called the 'normal fluid fraction'. This behavior (4.3) is called 'non-classical rotational inertia' or the London effect (after its theoretical predictor) or the Hess-Fairbanks effect (after its experimental discoverers).

Comparison between (1) and (2): Notice that (1) is *not* an equilibrium phenomenon. In fact, the groundstate of a system of non-relativistic particles *cannot* have angular momentum $L > N\hbar/2$. Suppose it did and call the wavefunction Ψ. Then consider the state with wavefunction $\Psi' \equiv e^{-\mathbf{i}\sum_{i=1}^{N}\theta_i}\Psi$ where θ_i is the angular position of the ith particle. This state has $\langle\Psi'|\, V\, |\Psi'\rangle = \langle\Psi|\, V\, |\Psi\rangle$ where V is any terms in the hamiltonian not involving derivatives. And if $K = \sum_i \frac{p_i^2}{2m}$ is the kinetic term, we have

$$\langle\Psi'|\, K\, |\Psi'\rangle = \langle\Psi|\, K\, |\Psi\rangle - \omega_c L + \frac{1}{2} I_{cl}\omega_c^2 = \langle\Psi|\, K\, |\Psi\rangle - \frac{\hbar^2}{mR^2}\left(L - N/2\right).$$

If $L > N\hbar/2$ this decreases the total $\langle\mathbf{H}\rangle$ which by the variational theorem contradicts our assumption that Ψ was the groundstate. Recall that we assumed that the initial frequency of rotation was $\omega \simeq \tilde{\omega} \gg \omega_c$ which means $L \gg \frac{1}{2}N\hbar$. On the other hand, the flow can last for 10^{15} years by some estimates. It is a very long-lived *metastable* state. In contrast (2) is a statement about the actual groundstate of $\mathbf{H}_\omega$.

The analog of (2) for charged fluids is the Meissner effect. And the analog of rotating the container is applying a magnetic field. This replaces $K+V$ with

$$\mathbf{H}_A = \frac{1}{2m}\sum_{i=1}^{N}\left(\vec{p}_i - e\vec{A}(r_i)\right)^2 + \sum_i U(r_i) + \sum_{i<j} V\left(r_{ij}\right).$$

For example, consider $e\vec{A}(r) = m\vec{\omega}\times\vec{r}$ for ω constant, and compare to $\mathbf{H}_\omega$ above. The microscopic current operator (participating in $\dot{\rho}+\vec{\nabla}\cdot\vec{j}=0$, with $\rho(r) = e\sum_i \delta^d(r-r_i)$) is

$$\vec{j}(r) = \frac{\delta \mathbf{H}_A}{\delta \vec{A}(r)} = \frac{e}{m}\sum_{i=1}^{N}\left(p_i - eA_i\right)\delta^d(r-r_i).$$

In the case of a normal conductor (charged fluid), there is no steady-state current. In the case of a superconductor, the current takes the form

$$\vec{j}(r) = -\Lambda(T)\vec{A}(r).$$

This is called the London equation. $\Lambda(T) = \frac{ne^2}{m^\star} f_s(T)$ where $f_s(T)$ is as above.

Its consequence is that a superconductor is diamagnetic: If we plug the London equation into Maxwell's equations (i.e. Faraday's law) $c^2\vec{\nabla}\times\vec{B} = \vec{J} + \partial_t\vec{E}$ in the way we would usually derive the wave equation for lightwaves in vacuum, we find that $\vec{A}$ satisfies

$$-\partial_t^2\vec{A}x + c^2\vec{\nabla}\times\vec{\nabla}\times\vec{A} = -\Lambda\vec{A}.$$

If we work in $\vec{\nabla}\cdot\vec{A}=0$ gauge, this becomes the massive wave equation. This has the consequence that if we apply a static magnetic field to such a system, it will fall off inside the sample like

$$B \sim e^{-x\sqrt{\Lambda}}$$

where the penetration depth $\frac{c}{\sqrt{\Lambda}}$ is something like 100 $\mathring{\text{A}}$.

Notice that the results of (both versions of) experiment (2) are intrinsically quantum mechanical: it is possible to prove that neither rotating the container, nor applying a uniform magnetic field can change the equilibrium properties of a *classical* system. (This is the Bohr-van Leeuwen theorem. For details see Appendix 1A of Leggett's book.)

4.2 Robust definition of BEC

(Question 2) Next we turn to a more robust definition of BEC. Suppose someone hands us an N-boson wavefunction $\Psi(r_1\cdots r_N)$. Without any notion of who is the single-particle hamiltonian, how would we decide whether it exhibits BEC?

More generally, suppose we are given a distribution of such wavefunctions Ψ_s, with probability p_s, that is, a density matrix

$$\rho = \sum_s p_s |\Psi_s\rangle\langle\Psi_s|.$$

Consider the one-particle density matrix (the reduced density matrix for a single particle, it doesn't matter which one):

$$\rho_1(r,r') = \sum_s p_s \sum_{r_2\cdots r_N} \Psi_s^\star(r,r_2\cdots r_N)\Psi_s(r',r_2\cdots r_N) = \frac{1}{N}\left\langle \psi^\dagger(r)\psi(r')\right\rangle = \frac{1}{N}\mathrm{tr}\rho\psi^\dagger(r)\psi(r').$$

This matrix (in the r,r' indices) is hermitian $\rho_1(r,r') = \rho_1^\star(r',r)$, *i.e.* $\rho_1 = \rho_1^\dagger$, and so it can be diagonalized:

$$N\rho_1(r,r') = \sum_i N_i \chi_i^\star(r)\chi_i(r').$$

Here χ_i are orthonormal eigenfunctions of ρ_1 ($\int d^d r \chi_i^\star(r)\chi_j(r) = \delta_{ij}$), and N_i/N are its eigenvalues. (If the Ψ_s depend on a parameter, such as time, then so do χ_i, N_i.)

I put a factor of N in front so that the normalization of the density matrix (assuming $\mathrm{tr}\rho = 1$) $\mathrm{tr}\rho_1 = 1$ implies that $\sum_i N_i = N$. We can regard these eigenvalues N_i as occupation numbers! The χ_i are an ON basis of single-particle states. *If* Ψ is of the form $\mathbf{b}_1^\dagger \cdots \mathbf{b}_N^\dagger |0\rangle$ of a gaussian state, then they are the single-particle orbitals that we filled, and the N_i are a histogram of their fillings.

If the N_i are all of order-one in N: $N_i = \mathcal{O}(N^0)$, we call this a *normal* state. If any $N_i = \mathcal{O}(N)$ is macroscopic, we call it BEC. (If exactly one is macroscopic, it is called 'simple' BEC. I will assume this always below for simplicity. There are some interesting things to say about the other case.) What I mean by saying something is $= \mathcal{O}(N^\alpha)$ is an asymptotic statement about a family of systems with different N: if $\lim_{N\to\infty} \frac{x}{N}$ is finite, then $x = \mathcal{O}(N)$; if it is zero (but $\lim_{N\to\infty} x$ is finite) then $x = \mathcal{O}(N^0)$. For example, for N non-interacting bosons at $T < T_c$, $\lim_{N\to\infty} \frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^\alpha$ is finite, so this agrees with our previous definition of BEC in this case.

Order parameter. Suppose $N_0 = \mathcal{O}(N)$. Then let $\Psi(r) \equiv \sqrt{N_0}\chi_0(r) \equiv |\Psi(r)|e^{\mathbf{i}\varphi(r)}$. This is the (superfluid) *order parameter*. It satisfies $\sum_r |\Psi|^2 = N_0$. The density and current associated with particles in the condensate are

$$\rho_c(r) = N_0|\chi_0|^2 = |\Psi|^2, \quad \vec{j}_c(r) = N_0\left(-\frac{\mathbf{i}\hbar}{2m}\chi_0^\star\vec{\nabla}\chi_0 + h.c.\right) = |\Psi|^2\frac{\hbar}{m}\vec{\nabla}\varphi.$$

Let

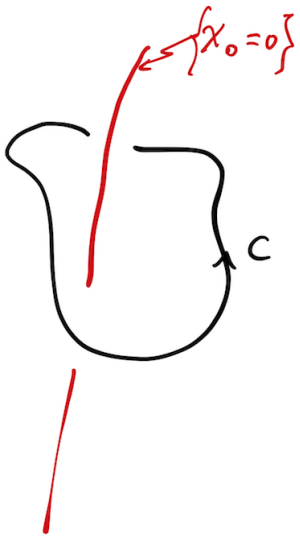
$$\vec{v}_s \equiv \frac{\vec{j}_c(r)}{\rho_c(r)} = \frac{\hbar}{m}\vec{\nabla}\varphi(r).$$

This is a quantity with dimensions of velocity, called the *superfluid velocity*. Two properties follow from the last expression:

$$\text{If } \chi_0(r) \neq 0, \text{ then:} \quad \vec{\nabla} \times \vec{v}_s = 0. \tag{4.4}$$

On the other hand, if we integrate over a closed curve C,

$$\oint_C \vec{v}_s \cdot d\vec{\ell} = \frac{nh}{m}, \quad n \in \mathbb{Z} \tag{4.5}$$



where n is an integer. This is because φ is only well-defined modulo shifts by $2\pi n$, so going in a closed path, the total change $\Delta\varphi = \oint_C \vec{\nabla}\varphi \cdot d\vec{\ell} = \frac{m}{\hbar}\oint_C \vec{v}_s \cdot d\vec{\ell}$ must be an integer multiple of 2π. This result is due to Feynman and Onsager. The integral (4.5) is only nonzero if $\chi_0 = 0$ inside the loop. Because of (4.4), the result of the integral doesn't change under small deformations of C that don't encounter a region with $\chi_0 = 0$, such as the hole in the ring studied above.

Regions with $\chi_0 = 0$ inside the sample are called *vortices*; in 3 spatial dimensions, they are strings.

In words, (4.5) says that the *vorticity* of the flow of a BEC is quantized. Why can't we always make such definitions? The answer is that the BEC is a compromise between quantumness and classicalness. Consider the following two extremes:

- Consider one particle in a box, say in one dimension. The lowest-energy state has wavefunction
$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \equiv e^{\mathbf{i}\varphi_1}|\psi_1|. \tag{4.6}$$
Nothing stops us from defining analogously the velocity
$$v_1 \equiv \frac{\hbar}{m}\vec{\nabla}\varphi_1. \tag{4.7}$$
This velocity (4.7) also satisfies (4.4) and (4.5). However: clearly it is just zero, since ψ_1 is real and positive. And if we actually tried to measure the velocity of the particle ($p/m = \frac{\mathbf{i}\hbar\partial_x}{m}$) we'll find $\pm\frac{\pi\hbar}{mL}$ each time with probability $\frac{1}{2}$. It is a highly fluctuating, very quantum, quantity with big fluctuations.

- At the other end of things, consider a normal fluid of many particles. Here too we can define a velocity
$$\vec{v}_{\text{hydro}} = \frac{\vec{j}_{\text{total}}}{\rho_{\text{total}}} = \frac{\hbar}{m}\left(\frac{\sum_i N_i|\chi_i|^2\vec{\nabla}\varphi_i}{\sum_j N_j|\chi_j|^2}\right).$$

In stark contrast to (4.7), this quantity is classical in the sense that its fluctuations go like $\frac{1}{\sqrt{N}}$ (I am appealing to the central limit theorem). However: it does *not* satisfy (4.4) or (4.5) (unless it is a simple BEC, $N_i = N\delta_{ij}$!).

The superfluid velocity has the best of both limits: it has small fluctuations (because of the macroscopic occupation of a single level), *i.e.* it behaves classically. For example, consider N free particles in the state (4.6). This has $\Delta v_s \sim \frac{\langle v_s \rangle}{\sqrt{N}}$, like a random walk with N steps.

On the other hand, it is quantum in the sense of exhibiting quantized vorticity. To reveal this property, we can put a hole in the box. I mean, we can consider a ring-shaped geometry as above. For simplicity, consider the limit where the ring is very narrow. The action of a particle fixed to move on such a ring of radius R is

$$S = \int dt \left(\frac{1}{2} m R^2 \dot{\theta}^2 + \omega m R^2 \dot{\theta} \right).$$

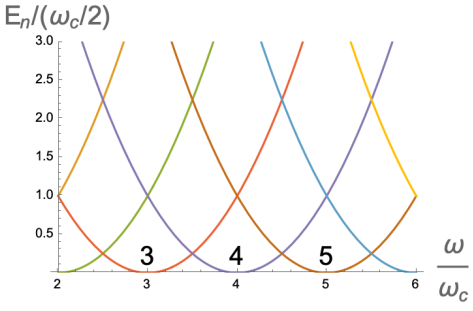
The second term is the effect of rotating the ring with frequency ω: $\vec{\omega} \times \vec{L} = \omega m R^2 \dot{\theta}$. Notice that this is a proof of the Bohr-van-Leeuwen theorem quoted above: this term is a total derivative, which therefore does not affect the equations of motion, or any other *classical physics*.

It does however make a big difference quantum mechanically, as you know from the homework. The associated single-particle hamiltonian is

$$H = \frac{\hbar^2}{2I} (\Pi - I\omega)^2, \quad I \equiv mR^2, \quad [\theta, \Pi] = \mathbf{i}\hbar.$$

The eigenstates are $e^{\mathbf{i}n\varphi}$ with $n \in \mathbb{Z}$ so that it is single-valued under $\theta \equiv \theta + 2\pi$. Acting on such a state, and writing H in terms of the quantum of angular velocity $\omega_c \equiv \frac{\hbar}{I}$ above, the spectrum is

$$E_n = \frac{\hbar\omega_c}{2} \left(n - \frac{\omega}{\omega_c} \right)^2.$$



Therefore, the groundstate is when $\pi/\hbar = n$ is the closest integer to ω/ω_c, as promised above. Notice that something special happens when $\omega \to \omega_c/2$ – there is a degeneracy in the spectrum since two values of n are equally close to ω_c.

If we put N bosons in this state, then the phase of the condensate wavefunction is $\varphi = n\theta$, and then $\vec{v}_s = \frac{\hbar}{m}\vec{\nabla}\varphi = \frac{n\hbar}{mR}\hat{\varphi}$. Notice that

$$\oint_{\text{ring}} \vec{v}_s \cdot d\vec{\ell} = \frac{n\hbar}{m} 2\pi = \frac{nh}{m}$$

in agreement with quantization of vorticity.

We haven't yet explained all of the super-flow phenomena, but already can see a basic reason for the robustness of the flow: The only way to get rid of it is to decrease the vorticity. But the integer n cannot change smoothly, it can only jump.

Relation to long-range order. Put the system in a very big box. Now consider the behavior of the single-particle density matrix when its arguments are far apart:

$$\lim_{|r-r'|\to\infty} N\rho_1(r,r') = \Psi^\star(r)\Psi(r') + N\tilde{\rho}_1(r,r').$$

The second term, $\sum_{i\neq 0} N_i\chi_i^\star(r)\chi_i(r')$ goes to zero for large $|r-r'|$. The non-vanishing of the $\Psi^\star\Psi$ term is another way to extract the order parameter. This is called *off-diagonal long-range order* (in this classic paper by CN Yang), in contradistinction to, for example, the order associated with a solid, which is visible in the diagonal matrix elements of the one-particle density matrix, $\rho_1(r,r) = n(r)$, *i.e.* the density.

[End of Lecture 18]

Relation to symmetry breaking. Yet another way to think about the order parameter is in terms of the field operator $\psi(r)$ (which we've often been calling $\mathbf{b}_r$ for bosons):

$$\Psi(r) = \langle \mathrm{gs}|\psi(r)|\mathrm{gs}\rangle\,.$$

In this sense, given my definition above that a particle condenses when there is an expectation value for its creation (or annihilation) operator, Ψ represents the condensate of bosons. This is consistent with the previous expression, because in the limit when the two operators are arbitrarily far apart, only the groundstate propagates between them:

$$N\rho_1(r,r') = \langle \mathrm{gs}|\,\psi^\dagger(r)\psi(r')\,|\mathrm{gs}\rangle \overset{|r-r'|\to\infty}{\to} \langle \mathrm{gs}|\psi^\dagger(r)|\mathrm{gs}\rangle\,\langle \mathrm{gs}|\psi(r)|\mathrm{gs}\rangle\,.$$

Think of this like the equation for the classical electric field:

$$\vec{E}_{\mathrm{classical}}(r) = \left\langle \vec{E}(r)\right\rangle$$

for example evaluated in a coherent state of the radiation field, $\mathbf{a}\,|z\rangle = z\,|z\rangle$.

There is, however, an important distinction from the case of the EM field. For photons, $E \to e^{\mathbf{i}\alpha}E$ is not a symmetry $[\mathbf{H}, \sum_k \mathbf{a}_k^\dagger\mathbf{a}_k] \neq 0$, and photons can come and go as they like. This means that $\left\langle \vec{E}\right\rangle \neq 0$ need break no symmetries (besides spatial symmetries like rotations). But suppose that $[\mathbf{H}, \underbrace{\sum_r \psi_r^\dagger\psi_r}_{\equiv\mathbf{N}}] = 0$. Here $[\mathbf{N},\psi] = -\psi$ (ψ

removes a particle). The existence of this conserved charge $\mathbf{N}$, by Noether's theorem, means a symmetry $\mathbf{U}_\theta = e^{-\mathbf{i}\theta\mathbf{N}}$, which acts on ψ by

$$\psi \to \mathbf{U}\psi\mathbf{U}^\dagger = e^{-\mathbf{i}\theta \mathrm{ad}_\mathbf{N}}\psi = e^{\mathbf{i}\theta}\psi$$

where $\mathrm{ad}_\mathbf{N}(\mathcal{O}) \equiv [\mathbf{N}, \mathcal{O}]$ is the *adjoint action* by $\mathbf{N}$. The last equation follows by Taylor expansion.

But now $\langle\alpha|\,\psi\,|\alpha\rangle \neq 0$ means that the state $|\alpha\rangle$ is not invariant under the particle-number symmetry $\mathbf{U}$. This is spontaneous symmetry breaking.

There is a problem with this picture, however. Acting with ψ changes the number of particles:

$$\psi(r)\,|n\text{-particle state}\rangle = |(n-1)\text{-particle state}\rangle\,.$$

This means that unless $|\alpha\rangle = \sum_n \alpha_n\,|n\rangle$ has an *indefinite* number of particles, *i.e.* is a superposition of states with different number of particles, we will find

$$\langle\alpha_n|\,\psi(r)\,|\alpha_n\rangle = 0$$

that Bose condensation, in this sense, is impossible.

Recall that even in the case of a magnet, SSB was a bit tricky to define. The best way to define it involved introducing a tiny (longitudinal) *training field* h which explicitly broke the $\mathbb{Z}_2$ symmetry, $\Delta\mathbf{H} = -h\sum_j \mathbf{Z}_j$. The analog of the training field here is something like

$$\Delta\mathbf{H} = -\lambda\int \psi^\dagger(r)d^dr + h.c.$$

which is a source and a sink for particles. Adding this term is a bit like coupling the system to a big reservoir of particles, except that we are not including the effects of the entanglement with the reservoir, since we're still treating the system as being in a pure state. Again the order of limits between $\lambda \to 0$ and $N \to \infty$ will matter.

A good practical way to think about the situation is: the zero-temperature grand-canonical ensemble is a convenient theoretical device. In this ensemble the $\mathsf{U}(1)$ symmetry is spontaneously broken. And in this ensemble, the fluctuations of the particle number are negligibly small $\Delta N/\langle N\rangle \sim \frac{1}{\sqrt{\langle N\rangle}}$ so don't worry about it. If N were not macroscopic, you would have to worry.

4.3 Interactions and BEC

(Question 1) [Feynman, *Statistical Mechanics* §11.3, Leggett] Now we can ask whether the BEC phenomenon survives interactions. We will approach this question in several

ways. For definiteness, let's think about an interacting system of bosons governed by a Hamiltonian such as

$$\mathbf{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} V(r_i - r_j). \tag{4.8}$$

We will take $V(r)$ to be short-ranged and strongly repulsive – it keeps the bosons from sitting on top of each other. They behave like hard spheres of some radius we'll call a. A good physical realization to keep in mind is ^{4}He.

What is the groundstate wavefunction $\Phi_0(r_1 \cdots r_N)$ of (4.8)? This is a Hard Question. But there are a few important things we can say about it without much work.

- Because it is a bosonic wavefunction, it is symmetric in its arguments.
- It can be chosen to be real. Look at the Schrödinger equation it satisfies:

$$\left(-\frac{\hbar^2}{2m} \sum_i \vec{\nabla}_i^2 + \sum_{i<j} V(r_{ij}) \right) \Phi_0 = E\Phi_0.$$

  Because there are no complex numbers involved besides Φ_0, $\Phi_0^\star$ satisfies the same equation. So $\Phi_0 + \Phi_0^\star$, the real part, also satisfies it. (If the real part happens to be zero, just take the imaginary part.) In fact this argument applies to all the eigenstates of $\mathbf{H}$, not just the groundstate. (It is a consequence of *time-reversal symmetry* of $\mathbf{H}$. More about that later if we have time.)
- The groundstate wavefunction Φ_0 has no nodes.

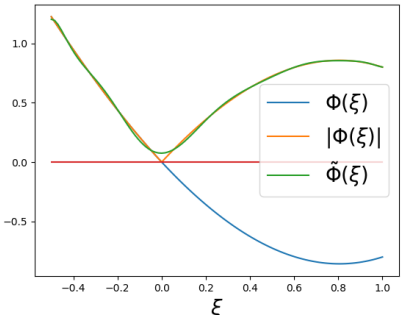
Suppose it were otherwise. For purposes of drawing, let $\Phi(\xi) = \Phi_0(r_1 \cdots \xi \cdots r_N)$ so ξ is the coordinate of one of the particles, it doesn't matter which one. The state with wavefunction $|\Phi|$ has the same values of $(\partial_\xi \Phi)^2, (\partial_{r_i} \Phi)^2, \Phi^2$ as Φ_0. Because $\mathbf{H}$ only involves first derivatives, this means that the energy expectation for $|\Phi|$,

$$E = \frac{\int |\Phi| \mathbf{H} |\Phi|}{\int |\Phi|^2} = \frac{\int \left(\frac{(\vec{\nabla}\Phi)^2}{2m} + V\Phi^2 \right)}{\int \Phi^2}$$

[25]

is the same as for Φ.

But now consider smoothing out the zero-crossings to make a new wavefunction $\tilde{\Phi}$, as in the figure. This *lowers* the kinetic energy, because the derivatives get smaller. So that state has an energy expectation lower than the groundstate, contradicting our assumption that there was a node.



- Φ_0 is non-degenerate. If it were degenerate with another orthonormal state Φ_1, then $c_0\Phi_0 + c_1\Phi_1$ would also be a solution, but by choosing the coefficients c_0, c_1 we could make a node. And anyway to make them orthogonal

  $$0 = \langle \Phi_0 | \Phi_1 \rangle = \int d^{dN} r \Phi_0(r) \Phi_1(r)$$

  requires one of them to be negative over some of the space.

- $\Phi_0(r_1, r_2 \cdots r_N) \simeq 0$ if $|r_1 - r_2| < a$ the size of the hard spheres determined by where V becomes large and positive. But furthermore in the groundstate the gradients of Φ_0 must be small. That means that Φ_0 must also be small if $|r_1 - r_2|$ is just a little bigger. So in a state where the average space per particle is not much bigger than a, the configurations where Φ_0 is appreciable will have the particles about equally spaced.

I will mention here a form of the wavefunction that builds in all these demands:

$$\Phi = e^{-\sum_{ij} f(r_{ij})} = \prod_{ij} F(r_{ij})$$

[25] You might worry that this argument assumes that the slope of $\Phi(\xi)$ is nonzero at the putative zero-crossing. However, if $\Phi(\xi)$ satisfies the schrodinger equation $-\partial_\xi^2 \Phi + (V - E)\Phi = 0$ then if there were some point ξ_0 where both $\Phi(\xi_0) = 0$ and $\partial_\xi \Phi(\xi_0) = 0$, then these two initial conditions would determine $\Phi(\xi) = 0$ everywhere. So this rules out a double zero $\Phi(\xi) \sim \xi^2$, or a zero-crossing with zero slope like $\Phi(\xi) \sim \xi^3$. This argument comes from this thesis.

with $F(r) \begin{cases} = 0, r < a \\ \stackrel{r\to a}{\to} 0 \\ \stackrel{r\to\infty}{\to} 1 \end{cases}$. An example of such a function is $1 - \frac{a}{r_{ij}}$ (for $r_{ij} > a$). You could imagine using this as a trial wavefunction, but it is not so easy to do the integrals.

Mean field theory in free space. One thing we can do is mean field theory. Here is a simple mean field ansatz: put every particle in a single-particle state $\chi(r)$, so that the order-parameter field is $\Psi(r) = \sqrt{N}\chi(r)$. Now evaluate the expectation value of the Hamiltonian. We will try to find the orbital χ that minimizes the expected energy. The answer will be a functional of Ψ which is invariant under (space-independent) shifts of the phase,

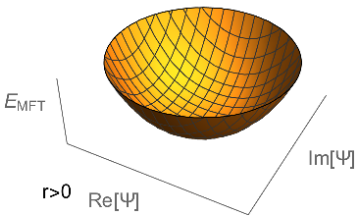
$$\Psi \to e^{i\alpha}\Psi. \tag{4.9}$$

It will inevitably have the form

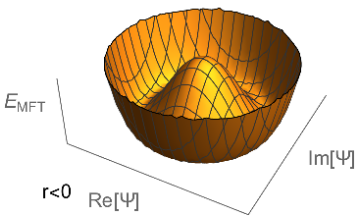
$$E[\Psi] = \int d^d r \left(r|\Psi|^2 + u|\Psi|^4 + \rho_s \vec{\nabla}\Psi^\star \cdot \vec{\nabla}\Psi + \cdots \right).$$

where the $\cdots$ is terms with more gradients or more powers of $|\Psi|^2$. Notice the similarity to the Landau-Ginzburg energy for a magnet; the only difference is that instead of a $\mathbb{Z}_2$ symmetry, we have a $\mathsf{U}(1)$ symmetry (4.9).

As long as $\rho_s > 0$, we lower the energy by making $\Psi(r)$ constant in space. As in the case of the magnet, there are two possible phases. One is where $r > 0$, in which case the minimum occurs when $\Psi = 0$. In this case, our ansatz isn't so good – the particles don't want to macroscopically occupy a single state. Notice that this solution is *invariant* under the $\mathsf{U}(1)$ symmetry (4.9). In that sense, such a state preserves the $\mathsf{U}(1)$ symmetry.



In contrast, if $r < 0$, this potential has a circle of degenerate minima. The points on these minima are swept out by the $\mathsf{U}(1)$ symmetry. In the same sense as for the ferromagnet, the $\mathsf{U}(1)$ symmetry is spontaneously broken by choosing one of these minima.



So you see that the description of superfluidity in terms of spontaneous breaking of the particle-number $\mathsf{U}(1)$ symmetry is pretty hard to resist, despite our earlier warnings.

Notice that the training field results in a tilt of the potential, which picks out a unique minimum determined by the phase of λ.

Variational estimate. Next we will broaden our space of trial wavefunctions a bit and see if the BEC still wins. Let's consider the special case where the potential is

so short-ranged that it can be approximated as a delta-function:

$$V(r_{ij}) = U_0 \delta^d(r_{ij}).$$

And let's focus for simplicity on the case of $N = 2$ particles. We'll make a variational ansatz, *i.e.* a trial wavefunction $\Psi(r_1, r_2) = \Psi(r_2, r_1)$. Its interaction energy is

$$E_{\text{int}} = \langle \Psi | \, \mathbf{H}_{\text{int}} \, | \Psi \rangle = U_0 \int d^d r_1 \int d^d r_2 \, \delta^d(r_1 - r_2) |\Psi(r_1, r_2)|^2 = U_0 \int d^d r |\Psi(r, r)|^2 = U_0 \int d^d r \rho_1(r, r).$$

Let $\chi_i(r)$ be a collection of orthonormal single-particle states. Let us compare the energies in two cases:

1. Put both particles in the same single-particle state: $\Psi(r_1, r_2) = \chi(r_1)\chi(r_2)$. This gives
$$E_{\text{int}} = U_0 \int d^d r |\chi(r)|^4.$$

2. Put the two particles in different, orthogonal states: $\Psi(r_1, r_2) = (\chi_1(r_1)\chi_2(r_2) + \chi_2(r_1)\chi_1(r_2))/\sqrt{2}$. This gives
$$E_{\text{int}} = U_0 \int d^d r \frac{1}{2} |\chi_1|^2 |\chi_2|^2 \times 4 = 2U_0 \int d^d r |\chi_1|^2 |\chi_2|^2. \tag{4.10}$$

First notice that (4.10) is twice the answer we would get for distinguishable particles. Furthermore, consider the case where $|\chi_1(r)| = |\chi_2(r)|$, such as for plane waves. In this case, $E_{\text{int}}(2) = 2E_{\text{int}}(1)$!

The generalization for $N \gg 2$ particles is

$$E_{\text{int}} \approx \frac{1}{2} U_0 \sum_{ij} N_i N_j (2 - \delta_{ij}) \int d^d r |\chi_i(r)|^2 |\chi_j(r)|^2 \tag{4.11}$$

where N_i is the occupation number of level i[26]. You see that, when the interaction is repulsive $U_0 > 0$, there is a big energy gain to be found by clumping the particles into

[26] A more precise expression is

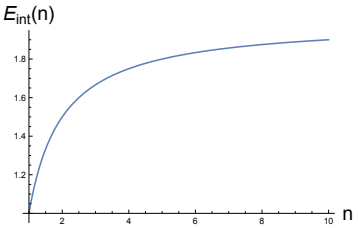
$$E_{\text{int}} \approx \frac{1}{2} U_0 \left(2 \sum_{i \neq j} N_i N_j \int d^d r |\chi_i(r)|^2 |\chi_j(r)|^2 + \sum_i N_i (N_i - 1) \int d^d r |\chi_i(r)|^4 \right).$$

In this expression, we are still ignoring some terms that average to zero in the $\int d^d r$. This is called

the same single-particle level, as compared to dividing them up into multiple levels. For example, for $N \gg 1$,

$$E_{\rm int}(N_i = 1) \simeq 4/3 E_{\rm int}(N_1 = N/2, N_2 = N/2, N_{i>2} = 0) = 2E_{\rm int}(N_1 = N, N_{i>1} = 0).$$

Suppose we divide up the particles into n equal groups. Then, assuming plane waves, $E_{\rm int}(n) = \frac{U_0}{2}\left(\frac{N}{n}\right)^2 \sum_{ij}^{n}(2-\delta_{ij}) = \frac{U_0}{2}\left(2-\frac{1}{n}\right)$, as plotted at right.



That is: repulsive interactions favor simple BEC over either the normal state or non-simple BEC. The opposite is true for attractive interactions. [End of Lecture 19]

Bose-Hubbard model. Restricting the positions of our bosons to a lattice can have a dramatic effect on the physics. Consider the following Hamiltonian (the *Bose-Hubbard model*):

$$\mathbf{H}_{\rm BH} = -t\sum_{\langle ij\rangle}(\mathbf{b}_i^\dagger \mathbf{b}_j + hc) + \sum_i U(\mathbf{n}_i - \bar{n})^2 \equiv H_t + H_u.$$

We'll focus on repulsive interactions $U > 0$. Here $\mathbf{n}_i \equiv \mathbf{b}_i^\dagger \mathbf{b}_i$ is the number of bosons at site i, and $\bar{n} > 0$ is a fixed number, a coupling constant. We will work in the grand canonical ensemble, so $\bar{n}$ behaves like a chemical potential, specifying the number of particles on average.

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the Hartree-Fock approximation. Let me give some explanation of what's involved. Write

$$\langle \mathbf{H}_{\rm int}\rangle = \frac{1}{2}\sum_{ijkl} V_{ijkl}\left\langle \mathbf{b}_i^\dagger \mathbf{b}_j^\dagger \mathbf{b}_k \mathbf{b}_l\right\rangle \tag{4.12}$$

where V_{ijkl} is the potential written in terms of the single-particle χ_i states (could be plane waves):

$$V_{ijkl} = \int d^d r_1 d^d r_2 \chi_i(r_1)\chi_j(r_2)V(r_1,r_2)\chi_j^\star(r_2)\chi_i^\star(r_1)\ . \tag{4.13}$$

The matrix element is of the form we studied earlier. The failure of Wick's theorem for bosons goes away in the thermodynamic limit, so let's ignore it. Then, for $i \neq j$,

$$\left\langle \mathbf{b}_i^\dagger \mathbf{b}_j^\dagger \mathbf{b}_k \mathbf{b}_l\right\rangle \simeq \left\langle \mathbf{b}_i^\dagger \mathbf{b}_j\right\rangle \left\langle \mathbf{b}_j^\dagger \mathbf{b}_k\right\rangle + \zeta \left\langle \mathbf{b}_i^\dagger \mathbf{b}_k\right\rangle \left\langle \mathbf{b}_j^\dagger \mathbf{b}_l\right\rangle \simeq N_i N_j\left(\delta_{il}\delta_{jl} + \zeta\delta_{ik}\delta_{il}\right).$$

On the other hand, if $i = j$, $\left\langle \left(\mathbf{b}_i^\dagger\right)^2 \mathbf{b}_k \mathbf{b}_l\right\rangle = N_i(N_i-1)\delta_{ik}\delta_{kl}$. This gives

$$\langle \mathbf{H}_{\rm int}\rangle \simeq \frac{1}{2}\sum_{i\neq j}\left(V_{ij,ij} + \zeta V_{ij,ji}\right) N_i N_j + \sum_i V_{ii,ii} N_i(N_i-1).$$

Taking all the N_i to be large, this gives the expression (4.11) when V is a contact potential.

As in the case of the TFIM, the two terms H_t and H_u do not commute and make differing demands on the low-energy states of the system. Again we'll make progress by considering limits of the couplings. Unlike the TFIM, this problem has *two* dimensionless couplings to play with: t/U and $\bar{n}$.

$\boxed{t/U \gg 1, \bar{n} \gg 1}$: Let $\mathbf{b}_i^\dagger = \sqrt{\mathbf{n}_i} e^{\mathbf{i}\varphi_i}$. Here $\mathbf{n}_i$ and φ_i are the number and phase operators. If they satisfy

$$[\varphi_i, \mathbf{n}_j] = -\mathbf{i}\delta_{ij} \tag{4.14}$$

then I claim that $[\mathbf{b}_i, \mathbf{b}_j^\dagger] = \delta_{ij}$ as usual. The idea is

$$[\mathbf{b}, \mathbf{b}^\dagger] = \sqrt{\mathbf{n}} \underbrace{[e^{\mathbf{i}\varphi}, \sqrt{\mathbf{n}}]}_{=\frac{e^{\mathbf{i}\varphi}}{2\sqrt{\mathbf{n}}}} e^{-\mathbf{i}\varphi} + \sqrt{\mathbf{n}} \underbrace{[\sqrt{\mathbf{n}}, e^{-\mathbf{i}\varphi}]}_{=\frac{e^{-\mathbf{i}\varphi}}{2\sqrt{\mathbf{n}}}} e^{\mathbf{i}\varphi} = 1.$$

We used the chain rule, *e.g.* $[\varphi, f(\mathbf{n})] = -\mathbf{i}f'(\mathbf{n})$. This works best when $\langle \mathbf{n} \rangle$ is large, so we don't divide by zero. Notice that (4.14) implies that there is an uncertainty relation between particle number $\mathbf{n}$ and the phase variable φ, they are conjugate variables like position and momentum.

In terms of these operators, the hamiltonian is

$$\mathbf{H}_{\rm BH} = -t \sum_{\langle ij \rangle} \sqrt{\mathbf{n}_i} e^{\mathbf{i}(\varphi_i - \varphi_j)} \sqrt{\mathbf{n}_j} + h.c. + \sum_i U(\mathbf{n}_i - \bar{n})^2.$$

When $\bar{n} \gg 1$, the dominant low-energy configurations will have $\langle \mathbf{n} \rangle \sim \bar{n} \gg 1$, and so we can write

$$\mathbf{n}_i = \bar{n} + \Delta\mathbf{n}_i, \quad \langle \Delta\mathbf{n}_i \rangle \ll \bar{n}$$

and expand $\mathbf{b}_i^\dagger \simeq \sqrt{\bar{n}} e^{\mathbf{i}\varphi_i}$. This gives

$$\mathbf{H}_{\rm BH} \simeq -2t\bar{n} \sum_{\langle ij \rangle} \cos(\varphi_i - \varphi_j) + U \sum_i (\Delta\mathbf{n}_i)^2 .$$

When $t \gg U$, we start by ignoring the U term. The cosine wants neighboring phases to be equal $\varphi_i = \varphi_j$, meaning $\varphi_i \simeq \varphi_j$ for all ij. This means

$$\left\langle \mathbf{b}_i^\dagger \right\rangle \simeq \sqrt{\bar{n}} \left\langle e^{\mathbf{i}\varphi_i} \right\rangle \neq 0.$$

This is a BEC.

What are the elementary excitations about this BEC state? When the fluctuations of φ_i are small (so that we can ignore the periodicity), we can expand the cosine about its minimum, $\cos(\varphi_i - \varphi_j) \simeq 1 - \frac{1}{2}(\varphi_i - \varphi_j)^2 + \cdots$, to find (dropping an additive constant)

$$\mathbf{H}_{\rm BH} \simeq t\bar{n} \sum_{\langle ij \rangle} (\varphi_i - \varphi_j)^2 + U \sum_i (\Delta\mathbf{n}_i)^2 , \quad [\Delta\mathbf{n}_i, \varphi_j] = -\mathbf{i}\delta_{ij}.$$

Where have we seen such a thing before? This has exactly the form of the harmonic lattice

$$\mathbf{H} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m\omega_0^2 \sum_{\langle ij \rangle} (\mathbf{q}_i - \mathbf{q}_j)^2$$

with the replacements $\mathbf{p} \to \Delta\mathbf{n}, \mathbf{q} \to \varphi, U \to \frac{1}{2m}, \frac{1}{2}m\omega_0^2 \to t\bar{n}$. This means in particular that there is a phonon-like state (called the phonon) which is gapless and has a linear dispersion relation,

$$\omega_k = \omega_0 |\sin(ka/2)| \overset{ka \ll 1}{\simeq} \omega_0 a|k|/2$$

(in the case of a chain) with $\omega_0 = 2\sqrt{t\bar{n}U}$. Notice that without the interaction term, there is no dispersion, the sound velocity $v_s = \sqrt{t\bar{n}U}a$ goes to zero.

Another virtue of the symmetry-breaking interpretation of BEC is that we can interpret the phonon here as a Goldstone mode for the spontaneously-broken $\mathsf{U}(1)$ symmetry, which acts by $\varphi_i \to \varphi_i + \alpha$: rotating all the phases φ_i costs no energy; therefore making a long-wavelength variation in φ_i will cost a small energy.

$\boxed{t/U \ll 1}$: This discussion will be valid for any $\bar{n}$, even say $\bar{n} = 1$. If $t = 0$, $\mathbf{H}_{\mathrm{BH}} = U\sum_i (\mathbf{n}_i - \bar{n})^2$ wants $n_i = N$, the integer closest to $\bar{n}$. This is unique, unless $\bar{n} = N + \frac{1}{2}, N \in \mathbb{Z}$ is a half-integer. In that case, there are two optimal states of each site, with $\mathbf{n}_i = N$ or $\mathbf{n}_i = N + 1$.

Assume for a moment that $\bar{n}$ is not a half-integer. Then there is a unique ground-state

$$|\mathrm{gs}\rangle = \prod_i \frac{\left(\mathbf{b}_i^\dagger\right)^N}{\sqrt{N!}} |0\rangle \tag{4.15}$$

which is a simple product state where we put N bosons at each site (in the figure, we have $N = 1$). The first excited state is where we take one of the bosons from site x and put it in site y, so that there are only $N - 1$ bosons at site x and an extra $N + 1$ at site y:

This state has energy above the groundstate by an amount proportional to U, independent of system size – there is a gap. This has two consequences: it means that small t can't dramatically change the groundstate, it will just broaden the degeneracy of the gapped excited states into a band, as in the TFIM. And it means that this state is an *insulator* – it costs a finite amount of energy to move the particles around by

even a small amount. It is a new kind of insulator, compared the band insulator of fermions that we discovered above. It is called a *Mott insulator*. In some sense it is much simpler and less quantum mechanical than the band insulator. It is just like a traffic jam – the particles can't move because there are other particles in the way, and they don't want to sit on top of each other.

We saw above that the number operator $\mathbf{n}_i$ at each site is conjugate to the phase operator φ_i, like $\mathbf{q}$ and $\mathbf{p}$. The Mott insulator groundstate (4.15) is an eigenstate of $\mathbf{n}_i$. By the usual logic of Heisenberg uncertainty principle, this means that the value of φ_i is maximally uncertain. This means that $\left\langle \mathbf{b}_i^\dagger \right\rangle \propto \left\langle e^{\mathbf{i}\varphi_i} \right\rangle = 0$, since the variable φ_i wanders all around between 0 and 2π. So the $\mathsf{U}(1)$ symmetry is not broken in the Mott insulator phase, as we knew it couldn't be because there is a gap, and hence no Goldstone boson.

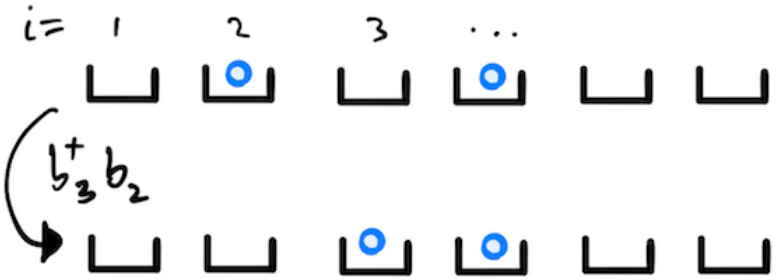
This means that at some intermediate value of t/U, something dramatic has to happen, because the superfluid-ordered gapless state at $t \gg U$ cannot continuously turn into the boring, dead Mott insulator state at $t \ll U$. One way to understand this is that the former breaks the $\mathsf{U}(1)$ symmetry and the latter does not. The drama could be a direct phase transition between them; it could also in principle be some intervening more interesting phase of matter.

$\boxed{\bar{n} = N + \frac{1}{2}}$: If $\bar{n} = N + \frac{1}{2}$, the story is more interesting. Now there are 2^N degenerate groundstates, associated with the choice between N and $N+1$ particles at each site. A small perturbation by H_t can make a big difference in splitting this degeneracy. The degeneracy is exactly like a spin system, under the identification $|\downarrow\rangle_x = |N \text{ particles at } x\rangle, |\uparrow\rangle_x = |N+1 \text{ particles at } x\rangle$. Under this identification, $S_i^+ = P\mathbf{b}_i^\dagger P, S_i^- = P\mathbf{b}_i P$ are the raising and lowering operators. Here P is the projector onto the degenerate subspace. $(S_i^+)^2 = 0$, while $(\mathbf{b}^\dagger)^2$ is not zero; but acting with $\mathbf{b}^\dagger$ twice inevitably removes one from the degenerate subspace. The perturbing Hamiltonian is

$$P\mathbf{H}_t P = P\left(-t\sum_{\langle ij\rangle} \mathbf{b}_i^\dagger \mathbf{b}_j + h.c.\right) P = -t\sum_{\langle ij\rangle} S_i^+ S_j^- + h.c.$$

What does this operator do? In the boson language, it hops the particles around (as

long as they don't go on top of each other), as in the figure.

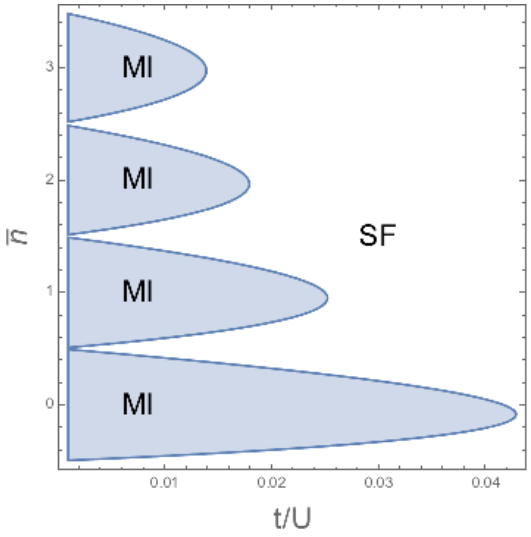


In the spin language, it's a ferromagnetic interaction (because of the minus sign) like you studied on the homework, which makes the spins want to align in the xy plane. The groundstates are $\otimes_x |\rightarrow\rangle_x$ and its images under spin rotations about the z axis:

$$e^{\mathbf{i}\theta \sum_i S_i^z} \otimes_x |\rightarrow\rangle_x .$$

This state has $\langle S_i^+ \rangle \neq 0$. In the boson language, this is a superfluid state, $\left\langle \mathbf{b}_i^\dagger \right\rangle \neq 0$.

So at half-integer $\bar{n}$, the Mott insulator is immediately unstable to superfluidity, at arbitrarily small t/U. As you'll see from mean field theory on the homework, the full phase diagram in the t/U and $\bar{n}$ plane looks like the figure at right (SF = superfluid, MI = Mott insulator).



Absence of low-lying modes. The key to the phenomenology of superfluids is their *absence* of low-lying excitations. A superfluid has the linearly-dispersing phonon mode that we found and *no other* low energy excitations. With a classical pile of (*e.g.* non interacting) bosons in the normal state, a chunk of moving fluid can donate some small momentum $\vec{k}$ to a single boson at energy cost $\frac{(\hbar\vec{k})^2}{2m}$. A quadratic dispersion means more modes at small k than a linear one (the density of states is $N(E) \propto k^{D-1}\frac{dk}{dE}$).

With only a linearly dispersing mode at low energies, however, there is a critical velocity below which a non-relativistic chunk of fluid cannot give up any momentum [Landau]: conserving momentum $M\vec{v} = M\vec{v}' + \hbar\vec{k}$ says the change in energy (which must be negative for this to happen on its own) is (eliminate $v' = v - \hbar k/M$):

$$\frac{1}{2}M(v')^2 + \hbar\omega(k) - \frac{1}{2}Mv^2 = -\hbar|k|v + \frac{(\hbar k)^2}{2M} + \hbar\omega(k) = (-v+v_s)|k| + \frac{(\hbar k)^2}{2M} .$$

For small k, this is only negative when $v > v_s$.

You can ask: an ordinary liquid also has a linearly dispersing sound mode; why doesn't Landau's argument mean that it has superfluid flow? The answer is that it has *other* modes with softer dispersion (so more contribution at low energies), in particular, we can excite a single-particle state which has $\omega \propto k^2$.

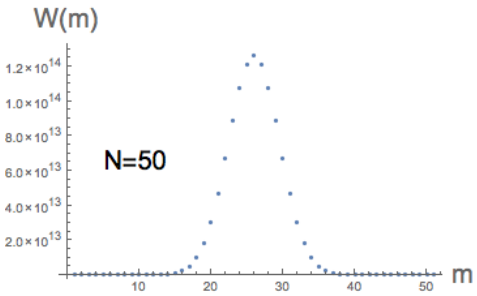
Landau's argument actually overestimates the critical velocity. Actually, the linearly-dispersing mode in Helium doesn't stay linear forever, but rather the dispersion relation has a minimum at finite k; the associated excitation is called a *roton*. A good way to think about this minimum is that it is trying to get to $\omega = 0$, in which case it would describe solidification. More precisely, it would describe an instability of the density at that wavevector. The momentum space then becomes periodic; this new zero would be the image under an inverse lattice vector of the zero at $k = 0$! I'll say more about the roton minimum below.

The absence of other low-lying modes in the superfluid can be traced directly to the indistinguishable nature of bosons. Here are two points of view.

(1) First consider the following comparison between the number of states of bosons and distinguishable particles. The problem of placing N particles in s single-particle states $i = 1..s$ is like putting N objects in s boxes.

First consider the case when the objects are distinguishable and take $s = 2$. Then

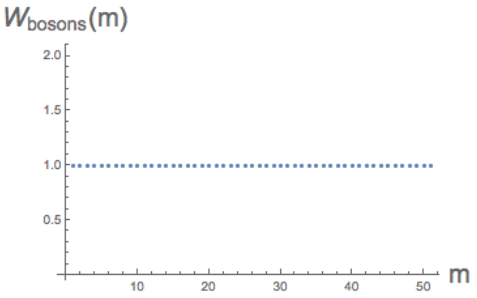
$$2^N = \sum_{m=0}^{N} \binom{N}{m} \equiv \sum_{m=0}^{N} W(m)$$



where $W(m) = \binom{N}{m} = \frac{N!}{m!(N-m)!}$ is the number of ways of placing m of the objects in to the first box (and $N - m$ in the other. This function $W(m)$ is highly-peaked about a typical configuration where $m \sim N/2$; the extreme configurations where all the particles are in one box or another $W(m \sim 0) \sim W(m \sim N) \ll W(m \sim N/2)$ are hugely suppressed. The generalization to s orbitals is

$$s^N = \sum_{\{m_i\}} \frac{N!}{\prod_{i=1}^{s} m_i!}.$$

Now consider the case of bosons with $s = 2$. In this case $W_{\text{bosons}}(m) = 1$ – there is only *one* way to place m bosons in one of the boxes and $N - m$ in the other! For general s, $W_{\text{bosons}}(\{m_i\}) = 1$ for each possible choice of ways of distributing the bosons. As you can see at right, this is a dramatic difference! All ways of distributing the bosons have the same weight $W(m)$ as the equally-distributed case.

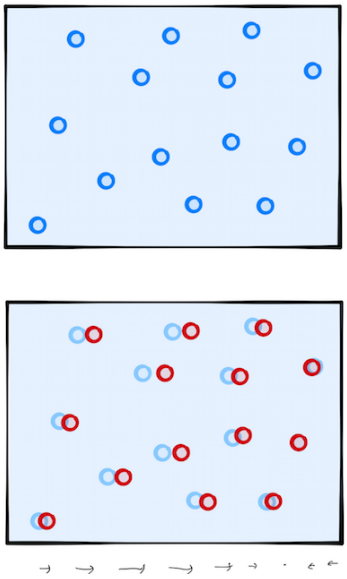


This means that even an infinitesimal energetic preference for one such state (say where all bosons are in the same single-particle state, such as we've seen above) will lead that state to completely win.

Notice that this mechanism breaks down when $s \gg N$ and the distinction between bosons and distinguishable particles goes away, because they can be distinguished by their single-particle label. This is a way to predict T_c, by estimating the number of accessible orbitals s as the number of states with $\epsilon < k_B T$.

(2) Now here is a more subtle but more informative argument due to Feynman. (His papers on this subject are fun to read.)

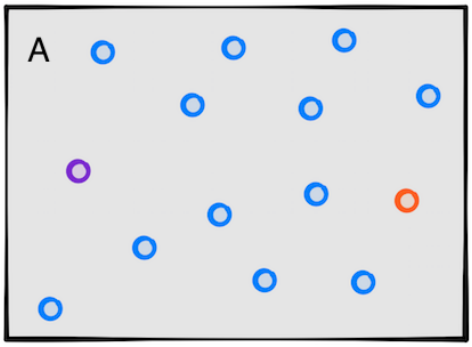
Let's return to the discussion of the form of the wavefunction from the beginning of this subsection. We want to understand why there are no low-lying excitations besides phonons. What is a phonon excitation in this language? A phonon is a compression wave. It's a state involving small displacements of each atom, as a result of which the density varies. For the low-energy phonons, the variation has a large wavelength. At right I compare a large-amplitude configuration in the groundstate, and a large-amplitude configuration in a phonon state of definite $\vec{k} \propto \hat{x}$ (with a wavelength of order the size of the box I've drawn).



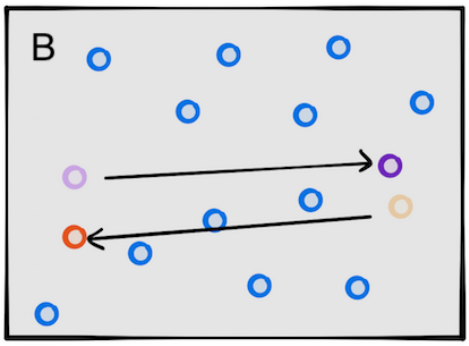
Consider the wavefunction of the first excited state Φ_1. Again it can be taken to be real. If our system were in one dimension, it would have to have "a single node". That is, for each coordinate $\psi(\xi) \equiv \Phi_1(\xi, x_2 \cdots x_N)$, the space can be divided into two regions of ξ, one where $\psi(\xi) > 0$, and one where $\psi(\xi) < 0$. This is required by $0 = \langle \Phi_1 | \Phi_0 \rangle = \int \Phi_1 \Phi_0$.

Now suppose that Φ_1 is *not* a phonon state. This means that it has to be orthogonal to all the phonon states also. But that means its sign has to be different in configurations which differ by long-wavelength changes of the density. In order for the sign of Φ_1 to vary *slowly* (required in order for Φ_1 to have low energy), it must change sign when the atoms are moved by a large distance.

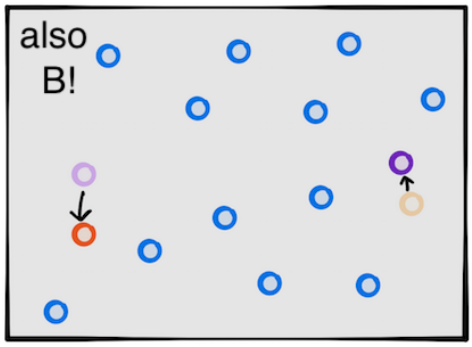
So the problem becomes to find a way to rearrange the atoms in a given configuration (say the configuration A where Φ_1 is largest, at right) so that they are still approximately uniformly spaced and non-overlapping, but the atoms move a long distance compared to their separation.



Let's try to identify the configuration B where Φ_1 is most negative and compare to configuration A. Making Φ_1 low-energy requires making A and B as different as possible. How to do this? Suppose for a moment the particles were distinguishable. Take some atoms from the left of configuration A and put them on the right. This leaves a hole on the left. To fix that, we have to take some other atoms from the right and put them on the left.



Now you can see why Bose statistics comes in. The atoms are all the same. We can accomplish the same rearrangement simply by rearranging the atoms on the left and right individually by small amounts. But either that's a phonon (if the sign doesn't change between these configurations) or it's a high energy state (if the sign does change). There's nothing else.



[End of Lecture 20]

Excitation spectrum. [Feynman, *Statistical Mechanics*, §11.5] I can't resist saying a little bit more about the spectrum of excitations. Following Feynman, we take a variational approach (now called the *single-mode approximation*). We make an ansatz for the excited-state wavefunction of the form:

$$\psi = \sum_i f(r_i)\Phi_0 \equiv F\Phi_0. \tag{4.16}$$

The idea is we want to excite one of the particles by multiplying by $f(r_i)$ (and the rest of the particles are just doing what they would do in the groundstate), but we have to symmetrize, so we sum over i. And we can use the variational principle for excited states. One way to think about it is that this state has a different momentum from the groundstate, and the variational principle works within each momentum sector.

A little bit of work shows that

$$\langle\psi|\,\mathbf{H}\,|\psi\rangle = \frac{\int d^{dN}r\left(\sum_i \frac{\hbar^2}{2m}|\vec{\nabla}_i\psi|^2 + V|\psi|^2\right)}{\int d^{dN}r|\psi|^2} = E_0 + \frac{\sum_i \frac{\hbar^2}{2m}\int d^{dN}r|\vec{\nabla}_i F|^2\Phi_0^2}{\int d^{dN}r|F|^2\Phi_0^2} \equiv E_0 + \epsilon. \tag{4.17}$$

Here $\mathbf{H}\Phi_0 = E_0\Phi_0$ and the trick is to integrate by parts enough to use this equation.

So far this works for general F; now we set $F = \sum_i f(r_i)$. The variational quantity is $\epsilon \equiv \frac{\mathcal{N}}{\mathcal{D}}$. The numerator is

$$\mathcal{N} = \sum_j \frac{\hbar^2}{2m}\int |\vec{\nabla}_i f(r_i)|^2\Phi_0^2(r_1\cdots r_N)d^{dN}r = N\frac{\hbar^2}{2m}\int |\vec{\nabla}_1 f(r_1)|^2\Phi_0^2(r_1\cdots r_N)d^{dN}r. \tag{4.18}$$

Now we use

$$\int d^d r_2\cdots d^d r_N\Phi_0^2(r_1\cdots r_N) = \rho_1(r_1,r_1) = \frac{1}{N}\left\langle\psi^\dagger(r_1)\psi(r_1)\right\rangle = \frac{1}{N}\left\langle\rho(r_1)\right\rangle = \frac{1}{N}\rho_0 = \frac{1}{V}$$

where ρ_1 is the one-particle density matrix and we used the fact that the groundstate is translation invariant, so the density is equal to the average density $\rho_0 = N/V$. Then

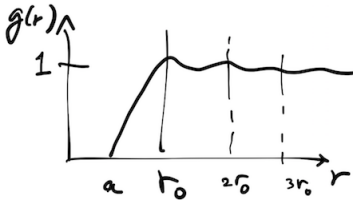
$$\mathcal{N} = \frac{\hbar^2}{2m}\rho_0\int |\vec{\nabla} f(r)|^2 d^d r. \tag{4.19}$$

The denominator involves the two-particle density matrix.

$$\mathcal{D} = \sum_{ij} \int d^{dN} r f^\star(r_i) f(r_j) \Phi_0^2 = \rho_0 \int d^d r_1 d^d r_2 f^\star(r_1) f(r_2) g(r_{12}) \tag{4.20}$$

where

$$\rho_0 g(r_{12}) \equiv \sum_{ij} \int d^{dN} r' \Phi_0^2 \delta^d(r_i' - r_1) \delta^d(r_j' - r_2). \tag{4.21}$$



Notice that i and j may be the same. This quantity we have met before: it is proportional to the probability of finding a particle at r_2 given that one has been found at r_1, the pair correlator. The pair correlator for bosons with short-range repulsive interactions is sketched at right.

Now we minimize ϵ over the choice of function f:

$$0 \stackrel{!}{=} \frac{\delta \epsilon[f]}{\delta f^\star(r)} = \frac{\delta}{\delta f^\star(r)} \left(\frac{\mathcal{N}}{\mathcal{D}} \right) \tag{4.22}$$

$$= \frac{-\frac{\hbar^2}{2m} \vec{\nabla}^2 f}{\mathcal{D}} - \frac{\mathcal{N}}{\mathcal{D}^2} \int d^d r_2 f(r_2) g(r - r_2) \tag{4.23}$$

$$= \frac{1}{\mathcal{D}} \left(-\frac{\hbar^2}{2m} \vec{\nabla}^2 f - \epsilon \int d^d r' g(r - r') f(r') \right). \tag{4.24}$$

This is an integrodifferential equation, a bit scary, but it's linear (if we treat ϵ as a constant). And it's translation invariant. So can you guess what the solution is? Trying the ansatz $f(r) = e^{\mathbf{i} k \cdot r}$, we learn that

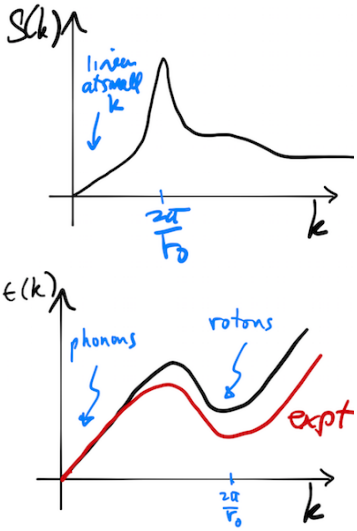
$$\epsilon(k) = \frac{\hbar^2 k^2}{2mS(k)} \tag{4.25}$$

where

$$S(k) = \int d^d r g(r) e^{-\mathbf{i} k \cdot r} \tag{4.26}$$

is the static structure factor!

That's something that can be measured by neutron scattering. It's just a property of the groundstate, in terms of which we've found an expression for the excitation spectrum (an upper bound at each k, actually). On general grounds, $S(k)$ has a peak at about $k \sim \frac{2\pi}{r_0}$. This is just because the particles are approximately equally spaced at a distance r_0, so $g(r)$ has a peak at r_0 (and a smaller one at nr_0, for $n = 2, 3 \cdots$; the form of $g(r)$ is similar to our free-boson calculation, except that it vanishes for $r < a$) as in the figure above. This means that $\epsilon(k)$ has a minimum there! That's the roton minimum.



Notice further that the wavefunction we've ended up with

$$\psi(k) = \sum_i e^{\mathbf{i} r_i \cdot k} \Phi_0$$

is perfectly good at any k, not just at large k, $k \sim \frac{2\pi}{a}$. In fact for small k it is a phonon state! To see this, note that the fourier transform of the density operator $\rho(r) = \sum_i \delta^d(r - r_i)$ is

$$\rho_k = \int d^d r e^{\mathbf{i} k \cdot r} \rho(r) = \sum_i e^{\mathbf{i} k \cdot r_i}$$

so that our trial state (4.16) is actually

$$\psi_k = \rho_k \Phi_0$$

– the creation of a perturbation of the density at wavenumber k, which at small k is a phonon.

This realization also makes it clearer that

$$\epsilon(k) = \frac{\langle \psi_k | (\mathbf{H} - E_0) | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle} = \frac{\langle \Phi_0 | \rho_k^\dagger [\mathbf{H}, \rho_k] | \Phi_0 \rangle}{\langle \Phi_0 | \rho_k^\dagger \rho_k | \Phi_0 \rangle} \tag{4.27}$$

in particular, that the denominator is $NS(k) = \langle \Phi_0 | \rho_k^\dagger \rho_k | \Phi_0 \rangle$. And in fact $S(k) \sim k$ at small k for a good reason, as we'll see below.

The energy spectrum can be measured by *inelastic* neutron scattering (where one keeps track of how much energy the neutrons lose) and it looks a lot like this function $\frac{\hbar^2 k^2}{2mS(k)}$ (which gives a rigorous upper bound on the right answer). Landau had earlier predicted a spectrum like this based on phenomenological considerations. It is roton excitations which make up the 'normal fluid fraction' that leads to dissipation in the

experiments described above. They are responsible for the fact that the critical velocity is smaller than v_s. And they can be seen to change the specific heat from the T^3 contribution of phonons once the temperature is big enough that they are not Boltzmann suppressed, *i.e.* $k_B T \sim \epsilon(k_{\rm roton})$. (This was the origin of Landau's suggestion.)

The roton minimum is a signature of incipient solidification. As we saw, the maximum in $S(k)$ arises because of a peak in the probability of finding the atoms equally-spaced. If it indeed formed a solid with spacing a, there would be a pole in $S(k)$ at $k = \frac{2\pi}{a}$, and hence a zero of the dispersion. This is just the image of $k = 0$ under an inverse lattice vector – the momentum space becomes periodic.

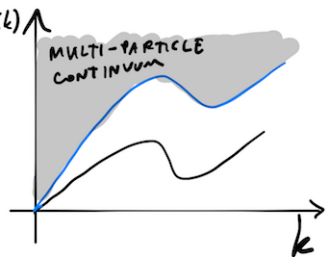
Here is some poetry motivating the ansatz (4.16). Consider again the configuration A where ψ is most positive, and B where ψ is most negative. To keep the energy small, we want these configurations to be maximally different. But we saw above that it is no use moving the atoms far away. Really the best we can do is move each of them by about half their separation – the atoms in configuration B should be in between those in configuration A. So we want to choose $f(r) = 1$ if r is occupied by an atom in configuration A, and $f(r) = -1$ if r is occupied by an atom in configuration B, and smoothly interpolate in between.

[Pines and Nozieres, *The Theory of Quantum Liquids*] What is the origin of the name *Single-Mode Approximation* (SMA)? Actually one can arrive at the same conclusion about the spectrum (though without learning about the wavefunction) by assuming a particular form of the spectrum, and hence of the *dynamical* structure factor (which we discussed earlier in the context of the TFIM) for the density:

$$S(k,\omega) = \sum_j \delta(\omega - \omega_j) |\langle \Phi_j | \rho_k | \Phi_0 \rangle|^2 \tag{4.28}$$

where $|\Phi_j\rangle$ is an eigenstate of $\mathbf{H}$ with energy $\hbar\omega_j + E_0$.
Suppose that the structure factor were dominated by a single mode with dispersion $\omega = \epsilon_k$:

$$S(k,\omega) = S_{\rm SMA}(k,\omega) = Z_k \delta(\omega - \epsilon_k) + \cdots . \tag{4.29}$$



This is an approximation which ignores all of the inevitable multiparticle states at larger ω (indicated by the $\cdots$ and depicted at right). First notice that the static structure factor is

$$S(k) = \frac{1}{N} \int d\omega S(k,\omega), \tag{4.30}$$

which in (4.28) determines $Z_k = S(k)$.

We can combine this information with various Inviolable Facts about the structure

factor called sum rules. Later we will see why they are true. The two that we'll need are

$$f\text{-sum rule}: \qquad \int d\omega \omega S(k,\omega) = \frac{N\hbar^2 k^2}{2m} \tag{4.31}$$

$$\text{compressibility sum rule}: \qquad \lim_{k\to 0} \int d\omega \frac{S(k,\omega)}{\omega} = \frac{N}{2mv_s^2} \tag{4.32}$$

where v_s is the speed of sound. To see why these might be useful here, observe that the variational energy above is exactly

$$\epsilon_k = \frac{\int d\omega \omega S(k,\omega)}{\int d\omega S(k,\omega)} \overset{(4.31),(4.30)}{=} \frac{\frac{N\hbar^2 k^2}{2m}}{NS(k)}.$$

But forget for a moment the variational calculation, and just plug in the SMA expression to the two sum rules. They give

$$\frac{k^2}{2m} = S(k)\epsilon_k, \qquad \frac{1}{2mv_s^2} = \lim_{k\to 0} \frac{S(k)}{\epsilon_k}. \tag{4.33}$$

The first equation reproduces our dispersion relation $\epsilon_k = \frac{\hbar^2 k^2}{2mS(k)}$. Plugging this into the second relation then says

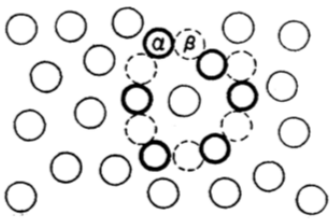
$$S(k) \overset{k\to 0}{\to} \frac{|k|}{2mv_s}.$$

So indeed we can guarantee that $S(k)$ is linear at small k as promised. Notice the consistency check that for small k this implies

$$\epsilon_k \overset{k\to 0}{\to} v_s|k|$$

so that indeed v_s is the speed of the sound mode. The moral reason for the f sum rule is the conservation of particle number, which is also the symmetry that's broken to produce the phonon as a Goldstone mode.

Finally, what is the origin of the name 'roton'? I believe it was introduced by Landau. Is it a good name? $f(r) = e^{\mathbf{i}k\cdot r}$ is a wave moving from an A site to a B site. In Feynman's paper linked above, he describes A and B as differing by the motion of a small group of particles around a ring, as in the figure at right (from his paper).



Feynman says this is like a small vortex ring. I'm not sure if this is a correct picture. An attempt to make it more correct is the following. Imagine making a wavepacket centered on the value of k at the minimum of the dispersion, so that the excitation is localized in space. The fact that it is a minimum means $\partial_K \epsilon = 0$ – the group velocity vanishes, so the excitation doesn't move. On the other hand, the particle current in

the region of the excitation is nonzero. This means that our ansatz cannot actually solve the Schrödinger problem, which implies current conservation. All of this is some words to motivate an improvement of the ansatz, something like:

$$\psi = \sum_i e^{\mathbf{i}k\cdot r_i + \sum_j h(r_{ij})} \Phi_0 \tag{4.34}$$

which can be chosen to conserve current. This is called a *backflow* improvement, since it describes the particles circulating back around from B to A. Obviously, we can find a better state if we generalize the trial wavefunction. This class of wavefunctions does seem to give a good improvement. I'm not sure about the words that go with it.

If you want to read more about this, a nice resource is this interesting article by Pines.

Part of the reason to devote some effort to this line of thought is that it plays an important role in our understanding of the excitation spectra of quantum Hall states. That is a subject for another time.

5 Interacting fermions

[We ran out of time to talk about the topics that follow.]

5.1 Where do spin interactions come from?

[Feynman §7.1] We've seen several examples of interacting spin systems, where I just wrote down a Hamiltonian in terms of (tensor products of) Pauli matrices. I explained a bit what might have happened to the position degrees of freedom of the electrons. But where does such a spin interaction come from? One might think it has something to do with magnetic dipole-dipole interactions, but actually in condensed matter there is a larger contribution.

Consider for a moment two *distinguishable* particles with Hamiltonian

$$\mathbf{H} = \mathbf{h}_0(1) + \mathbf{h}_0(2) + V(r_1, r_2),$$

with $V(r_1, r_2) = V(r_2, r_1)$. Suppose that ψ_α and ψ_β are eigenstates of $\mathbf{h}_0$ with energies ϵ_α and ϵ_β. The hamiltonian $\mathbf{H}$ has a symmetry under interchange of the two particles, so the groundstate must be an eigenstate of this operation, either symmetric or antisymmetric. With an eye towards considering identical fermions, consider the symmetric and antisymmetric states

$$\Psi_{S/A} \equiv (\Psi_{\alpha\beta} \pm \Psi_{\beta\alpha})/\sqrt{2}, \quad \Psi_{\alpha\beta}(r_1, r_2) \equiv \psi_\alpha(r_1)\psi_\beta(r_2).$$

Let's use these as trial wavefunctions for $\mathbf{H}$. Their expected energies are

$$E_{S/A} \equiv \left\langle \Psi_{S/A} \right| \mathbf{H} \left| \Psi_{S/A} \right\rangle = \epsilon_\alpha + \epsilon_\beta + \int d^d r_1 \int d^d r_2 \Psi^\star_{S/A}(r_1, r_2) V(r_1, r_2) \Psi_{S/A}(r_1, r_2) \tag{5.1}$$

$$\begin{aligned} &= \epsilon_\alpha + \epsilon_\beta + \frac{1}{2}\left(\int_{1,2} \Psi^\star_{\alpha\beta} V \Psi_{\alpha\beta} + \int_{1,2} \Psi^\star_{\beta\alpha} V \Psi_{\beta\alpha} \pm \int_{1,2} \Psi^\star_{\alpha\beta} V \Psi_{\beta\alpha} \pm \int_{1,2} \Psi^\star_{\beta\alpha} V \Psi_{\alpha\beta} \right) \\ &= \epsilon_\alpha + \epsilon_\beta + \int_{1,2} \Psi^\star_{\alpha\beta} V \Psi_{\alpha\beta} \pm \int_{1,2} \Psi^\star_{\beta\alpha} V \Psi_{\alpha\beta} \\ &\equiv \epsilon_\alpha + \epsilon_\beta + I \mp J \ . \end{aligned} \tag{5.2}$$

Now consider the same Hamiltonian for spinful fermions:

$$\mathbf{H} = \sum_{\alpha} \mathbf{a}^\dagger_{\alpha\sigma}\mathbf{a}_{\alpha\sigma}\epsilon_\alpha + \int d^d r_1 \int d^d r_2 V(r_1, r_2)\psi^\dagger_{r_1,\sigma}\psi^\dagger_{r_2,\sigma'}\psi_{r_2,\sigma'}\psi_{r_1,\sigma}.$$

Notice that the interactions are completely spin-independent. Again we'll focus on two orbitals α, β. The states of two fermions are completely antisymmetric (AS) under interchange of the two particles:

$$\mathbf{a}^\dagger_{\alpha\sigma}\mathbf{a}^\dagger_{\beta\sigma'}\left|0\right\rangle = -\mathbf{a}^\dagger_{\beta\sigma'}\mathbf{a}^\dagger_{\alpha\sigma}\left|0\right\rangle.$$

But there are four such states. The total antisymmetry can be accomplished in two ways: symmetric in space, and AS in spin, or AS in space, symmetric in spin. The symmetric combination of two spin-half particles is a triplet, spin $s = 1$ (three states), while the AS combination is the singlet, spin $s = 0$ (one state). We can write these states as

$$\left|S\right\rangle = \frac{1}{\sqrt{2}}\mathbf{a}^\dagger_{\alpha\sigma}\mathbf{a}^\dagger_{\beta\sigma'}\varepsilon_{\sigma\sigma'}\left|0\right\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} - \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)\left|0\right\rangle$$

$$\left|A,1\right\rangle = \mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\uparrow}\left|0\right\rangle, \qquad \left|A,0\right\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} + \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)\left|0\right\rangle, \qquad \left|A,-1\right\rangle = \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\downarrow}\left|0\right\rangle.$$

Their wavefunctions are, for example (using (1.34): $\mathbf{a}^\dagger_{\alpha\sigma} = \sum_r \mathbf{a}^\dagger_{r\sigma}\psi_\alpha(r)$)

$$\left\langle r_1\sigma, r_2\sigma'|S\right\rangle \equiv \frac{1}{\sqrt{2}}\left\langle 0\right|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}\left|S\right\rangle = \Psi_S(r_1, r_2)\left(\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} - \delta_{\sigma\downarrow}\delta_{\sigma'\uparrow}\right)/\sqrt{2}.$$

$$\left\langle r_1\sigma, r_2\sigma'|A,0\right\rangle \equiv \frac{1}{\sqrt{2}}\left\langle 0\right|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}\left|A,0\right\rangle = \Psi_A(r_1, r_2)\left(\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} + \delta_{\sigma\downarrow}\delta_{\sigma'\uparrow}\right)/\sqrt{2}.$$

Since the Hamiltonian is spin-independent, the variational energies of these states only depend on the orbital (position) part. But the symmetry of the states is precisely correlated with the total spin: the spatially-symmetric state has total spin Casimir $S^2 = \vec{S}\cdot\vec{S} = s(s+1) = 0$, while the spatially-AS state has $S^2 = 2$. Here $\vec{S} = \vec{S}_1 + \vec{S}_2$ is the total spin. Therefore the effective hamiltonian on the spin degrees of freedom is

$$H_{\text{eff}} = \epsilon_\alpha + \epsilon_\beta + I \mp J = E_S + (E_A - E_S)\frac{s(s+1)}{2} = E_S + 2J\frac{\vec{S}\cdot\vec{S}}{2} = 2J\vec{S}_1\cdot\vec{S}_2 + \text{const}$$

where in the last step we used

$$\vec{S}\cdot\vec{S} = (\vec{S}_1 + \vec{S}_2)^2 = 2\vec{S}_1\cdot\vec{S}_2 + S_1^2 + S_2^2 = 2\vec{S}_1\cdot\vec{S}_2 + \frac{3}{2}.$$

Thus a spin-symmetric interaction combines with the Pauli principle to produce a spin-spin interaction. Notice that the "exchange energy" J is so called because of its origin in (5.2). It depends on the overlaps of the single-particle states. In a solid, it turns out to be much bigger than the direct dipole-dipole interaction between the magnetic moments.

5.2 Ordering in Fermi systems.

[Leggett, §2.4] So the spins in an insulating magnet are the electron spins. This means that the spin operator is really

$$\vec{S}_r = \frac{1}{2}\psi^\dagger_{r\sigma}\vec{\sigma}_{\sigma\sigma'}\psi_{r\sigma'}$$

– it is really a fermion bilinear operator. When the magnetization is nonzero $m = \langle S^a \rangle \neq 0$, it means that there is an expectation value for a fermion bilinear, which is a bosonic operator. It is not quite a pair of fermions which condenses, since one of the operators is an annihilation operator, but this is an example of a fermionic system where there is long-range order (in this case diagonal long-range order).

Another example is helium. Above I said a collection of helium atoms was a good example to keep in mind in our discussion of bosons with short-range repulsion. But a helium atom is only approximately a bosonic particle; more microscopically it is made up of electrons and a helium nucleus, at least some of which are fermions. There is a more microscopic density matrix for these particles, which cannot have ODLRO of ρ_1. On the other hand, clearly the BEC phenomenon happens.

What is the analog of ρ_1, by which we gave a non-weak-coupling definition of BEC? Well, the idea is simply that reduced density matrices for a larger collection of particles can have a macroscopic eigenvalue. The next case beyond ρ_1 is the 2-particle density matrix:

$$\begin{aligned}\rho_2(r_1\sigma_1, r_2\sigma_2; r_1'\sigma_1', r_2'\sigma_2') &\equiv \sum_s p_s \sum_{\sigma_3\cdots\sigma_N} \sum_{r_3\cdots r_N} \Psi_s^\star(r_1\sigma_1, r_2\sigma_2, r_3\sigma_3\cdots r_N, \sigma_N)\Psi_s(r_1'\sigma_1', r_2'\sigma_2', r_3\sigma_3\cdots r_N, \sigma_N) \\ &= \zeta\rho_2(r_2\sigma_2, r_1\sigma_1; r_1'\sigma_1', r_2'\sigma_2').\end{aligned} \tag{5.3}$$

A few properties of ρ_2:

- ρ_2 is useful. It already made an appearance in our discussion of the single-mode approximation. Its diagonal entries give the pair correlator. And, for example, the expectation of the interaction energy can be written

$$\langle \mathbf{V} \rangle = \sum_{\sigma_1\sigma_2} \sum_{r_1 r_2} V(r_1 - r_2)\rho_2(12; 12).$$

- ρ_2 has all the information of ρ_1:

$$\rho_1(r\sigma, r'\sigma') = (N-1)\sum_{r_2\sigma_2} \rho_2(r\sigma, r_2\sigma_2; r'\sigma', r_2\sigma_2).$$

- Not every matrix with these properties actually arises as the reduced density matrix of some state.
- Like ρ_1, it is also related to a correlation function:
$$\rho_2(r_1\sigma_1, r_2\sigma_2; r_1'\sigma_1', r_2'\sigma_2') = \frac{1}{N(N-1)} \left\langle \psi^\dagger_{\sigma_1 r_1} \psi^\dagger_{\sigma_2 r_2} \psi_{\sigma_1' r_1'} \psi_{\sigma_2' r_2'} \right\rangle .$$
- As a good density matrix, $\mathrm{tr}\rho_2 = 1$.
- Finally, ρ_2 is hermitian as a $(2V)^2 \times (2V)^2$ matrix with $r_1\sigma_1 r_2\sigma_2$ regarded as one index.

This last property means that it can be diagonalized
$$\rho_2(r_1\sigma_1, r_2\sigma_2; r_1'\sigma_1', r_2'\sigma_2') = \sum_i \frac{n_i}{N(N-1)} \chi_i^\star(r_1\sigma_1 r_2\sigma_2) \chi_i(r_1'\sigma_1' r_2'\sigma_2')$$
and has real eigenvalues $\frac{n_i}{N(N-1)}$ and ON eigenvectors χ_i. These χ_i are 2-particle wavefunctions with the appropriate symmetry properties: $\chi_i(r_1\sigma_1 r_2\sigma_2) = \zeta\chi_i(r_2\sigma_2 r_1\sigma_1)$. $\mathrm{tr}\rho_2 = 1$ implies that $\sum_i n_i = N(N-1)$. Positivity of ρ_2 implies $n_i > 0$.

Now we encounter the question: how big are the n_i? The sum rule says that one could be as big as $N(N-1)$. A fact due to Yang (in the classic paper cited above) is that if there are s orbitals into which we are putting our fermions,
$$n_i \leq \frac{N(s-N+2)}{s} = \mathcal{O}(N).$$
(s must be bigger than N in order to have any fermionic states at all; if $s \gg N$ then this is just N. Often we care about $s = N/f$, *i.e.* filling fraction $f = N/s$ which is order-one in the thermodynamic limit, $N \to \infty$. In this case $n_i \leq (1-f)N$ in the thermodynamic limit.) CN Yang's proof of this (in the appendix of the paper linked above) is amusing: he uses trial wavefunctions (*i.e.* the variational principle) to bound the spectrum of ρ_2, it is a true physicist's proof, albeit a rigorous one. Now we can define the analog of BEC for fermions: If no n_i is order-N, the state is *normal*. If one eigenvalue $n_i \sim \mathcal{O}(N)$, we state the state exhibits *Cooper pairing*.

Unlike in the case of bosons, the free theory of fermions is in the normal state. Recall that for free fermions in free space,
$$\mathbf{n}_k \left|\Psi_0\right\rangle = n_k \left|\Psi_0\right\rangle , \quad n_k = \begin{cases} 0, & k > k_F \\ 1, & k < k_F \end{cases} .$$
I claim that the eigenvalues of ρ_2 for this state are also all 0 or 1. There is a huge degeneracy in the spectrum, and hence a big ambiguity in the form of the eigenvectors.

So to find examples of Cooper pairing or magnetic ordering starting from fermions, we'll have to include interactions.

5.3 Instabilities of a Fermi surface to repulsive interactions

Consider

$$\mathbf{H} = -t \sum_{\langle xy \rangle, \sigma} \mathbf{c}^\dagger_{x\sigma} \mathbf{c}_{y\sigma} + h.c. + U \sum_x (\mathbf{n}_x - 1)^2 = \mathbf{H}_t + \mathbf{H}_U \tag{5.4}$$

with $\mathbf{n}_x \equiv \sum_\sigma \mathbf{c}^\dagger_{x\sigma} \mathbf{c}_{x\sigma}$ is the total density operator at a site.

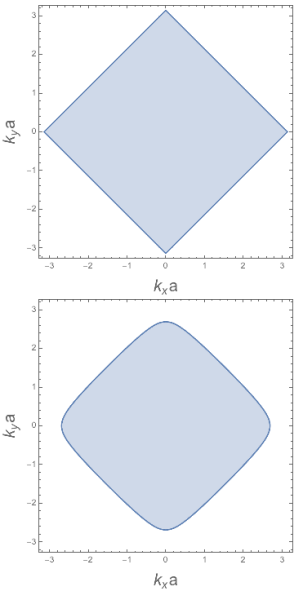
$$\mathbf{H}_t = \sum_{k,\sigma} \epsilon_k \mathbf{c}^\dagger_{k\sigma} \mathbf{c}_{k\sigma}$$

is diagonal in momentum space. ϵ_k is determined by the shape of the lattice; for example for the square lattice in 2d,

$$\epsilon_k = -2t(\cos k_x + \cos k_y);$$

I am working in units where the lattice spacing $a = 1$.

The *filling fraction* – the number of particles per orbital – plays a big role in the physics. We can think about setting this either by specifying the number of particles, or by adding a chemical potential and working in the grand canonical ensemble. The largest possible filling here is two particles per site, since the spin takes two values. Perhaps most interesting is the case of *half-filling*, where there is one particle per site on average. The Fermi sea at half-filling, and slightly-less-than half-filling are shown at right. We see that for any filling (other than 0 and 2 particles per site), the groundstate of $\mathbf{H}_t$ has a Fermi surface, and so we see that at $U = 0$, the system is metallic at low energies.



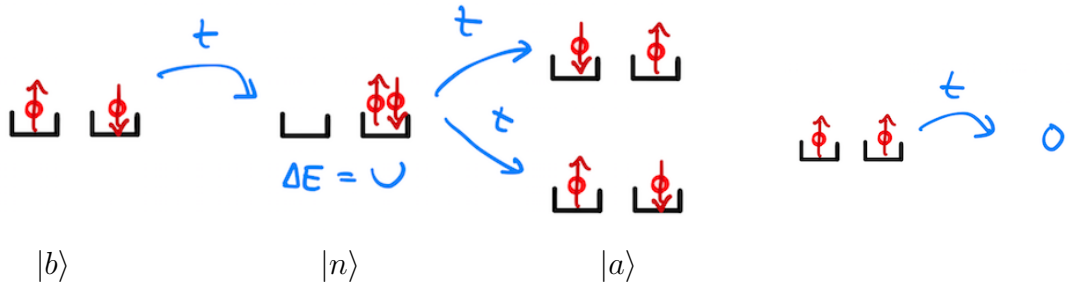
What happens if we turn on $U > 0$, repulsive interactions? Let's focus on half-filling. This is easy to answer if we set $U = \infty$. Then $\mathbf{H}_U$ demands that $\mathbf{n}_x = 1, \forall x$, exactly one particle per site. And there is a big energy gap above the groundstate space, proportional to U, to states where there are two particles at some site and zero particles at another. So this is a Mott insulator again. Unlike in the case of spinless bosons however, this groundstate space is hugely degenerate, because the spin of each particle is not specified. (The same would have happened for spinful bosons.) It becomes a spin system.

At $U/t \gg 1$, this degeneracy is split by the hopping term. We can figure out the effective hamiltonian for the spin system using degenerate perturbation theory. In this

case, we have to go to second order, because the perturbing hamiltonian always takes us out of the degenerate subspace. Second-order degenerate perturbation theory says that the matrix elements of the effective hamiltonian (for $|a\rangle, |b\rangle \in X$, the degenerate subspace) are

$$\langle a| \mathbf{H}_{\text{eff}} |b\rangle = -\sum_{n \notin X} \frac{\langle a| \Delta\mathbf{H} |n\rangle\langle n| \Delta\mathbf{H} |b\rangle}{E_n - E_X}.$$

The crucial ingredient can be seen by considering just two sites. A sketch of the processes involved are:



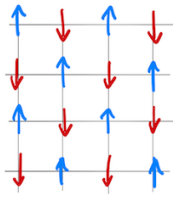
$|b\rangle$ $|n\rangle$ $|a\rangle$

Notice that the whole calculation is $\mathsf{SU}(2)$-spin-rotation symmetric. The result, as you will find on the homework, is

$$\mathbf{H}_{\text{eff}} = +\frac{4t^2}{U} \sum_{\langle xy \rangle} \vec{\mathbf{S}}_x \cdot \vec{\mathbf{S}}_y.$$

This mechanism for producing an antiferromagnetic Heisenberg interaction is called *superexchange*. On a bipartite lattice, the groundstate will be the *Neel state*, where

$$\left\langle \vec{\mathbf{S}}_{\vec{x}=(x,y)} \right\rangle = (-1)^{x+y} \hat{z}$$



or its images under $\mathsf{SU}(2)$ spin rotations. (Note that if the lattice is *frustrated*, it is much more difficult to determine the groundstate of the AFM Hamiltonian, and the result can be a much more interesting quantum state, such as a *spin liquid*. In this terminology, the idea is that a magnetic state such as the Neel state involves ordering of the spins, and is therefore like a spin *solid*. So solid is to liquid as magnet is to spin liquid.)

Now, what about when U/t is not infinite but t is not zero? To learn something about what happens there, we can do mean field theory.

Mean field theory of square-lattice Hubbard model at half-filling. To get a hint of what is a good mean-field ansatz, observe that at each site

$$(\mathbf{n}-1)^2 = 1 - \left(\mathbf{c}^\dagger \sigma^z \mathbf{c}\right)^2 = 1 - (\mathbf{n}_\uparrow - \mathbf{n}_\downarrow)^2.$$

The easiest way to see this is to observe that the BHS is diagonal in the number basis, and simply evaluate both sides in all four possible states of a single site:

$n_\uparrow n_\downarrow$	00	01	10	11
LHS	1	0	0	1
RHS	1	0	0	1

Notice that both are smaller when there is a single electron at the site, $n = n_\uparrow + n_\downarrow = 1$. So we can interpret large U as favoring $1 = \left(\mathbf{c}^\dagger \sigma^z \mathbf{c}\right)^2$, which can happen for either value of $\mathbf{S}^z = \mathbf{c}^\dagger \sigma^z \mathbf{c} = \pm 1$.

To develop a mean field theory, we can make the following replacement in the Hamiltonian:

$$\left(\mathbf{c}^\dagger \sigma^z \mathbf{c}\right)^2 \rightsquigarrow 2\left\langle \mathbf{c}^\dagger \sigma^z \mathbf{c}\right\rangle \mathbf{c}^\dagger \sigma^z \mathbf{c} - \left\langle \mathbf{c}^\dagger \sigma^z \mathbf{c}\right\rangle^2.$$

Why do we need to subtract the constant $\langle \mathbf{S}^z\rangle^2$? It matters if we want to treat $\langle \mathbf{S}^z\rangle$ as the variational parameter, and determine it by minimizing $\langle \mathbf{H}\rangle$. You can check that in the case of the TFIM it is required in order to reproduce the result of our product state variational calculation. Another very useful way to think about this is that we are using the Hubbard-Stratonovich trick: replace $U(\mathbf{S}^z)^2$ by $-\mathbf{S}^z\sigma + \frac{\sigma^2}{2U}$ where σ is an auxiliary bosonic variable. The equations of motion for σ are $\sigma = U\mathbf{S}^z$, and plugging back into the Hamiltonian gives back our previous Hamiltonian. If instead we ignore the fluctuations of σ, we arrive at the mean-field hamiltonian.

For our trial state, we choose one with

$$\left\langle \mathbf{c}^\dagger_{\vec{x}} \sigma^z \mathbf{c}_{\vec{x}}\right\rangle = \langle \mathbf{S}^z(\vec{x})\rangle = M(-1)^{x+y}, \quad \vec{x} = (x,y),$$

since we had such luck with the AFM solution at large U. We'll choose M to produce the best energy expectation. To do so we must find the groundstate energy of

$$\mathbf{H}_{\mathrm{MF}} = \sum_{k\sigma} \mathbf{c}^\dagger_{k\sigma}\mathbf{c}_{k\sigma}\epsilon_k - 2UM\sum_x (-1)^{x+y}\mathbf{c}^\dagger_x \sigma^x \mathbf{c}_x + UM^2V$$

where V is the number of sites of the lattice. Fortunately (not an accident), this is an Easy Problem, *i.e.* $\mathbf{H}_{\mathrm{MF}}$ is quadratic in canonical fermion operators. The idea here is that we will choose as our variational state the groundstate of a gaussian problem (the fermionic analog of a product state).

The AFM ordering doubles the unit cell and therefore halves the Brillouin zone (we're using $(-1)^{x+y} = e^{\mathbf{i}(\pi,\pi)\cdot(x,y)}$):

$$\sum_x (-1)^{x+y} \mathbf{c}_x^\dagger \sigma^z \mathbf{c}_x = \sum_k{}' \mathbf{c}_k^\dagger \sigma^z \mathbf{c}_{k+Q} + h.c., \quad \vec{Q} \equiv (\pi,\pi)$$

in units with lattice spacing $a = 1$. Let's use $\sum_k'$ to denote a sum over half the previous Brillouin zone (BZ). This folding of the BZ means that where previously we had two bands (one for each spin), we now have four states at each value of k, a 4×4 matrix. Fortunately it is a very simple 4×4 matrix:

$$\mathbf{H}_{\rm MF} = \sum_k{}' \begin{pmatrix} \mathbf{c}_k^\dagger, \mathbf{c}_{k+Q}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_k & -2UM\sigma^z \\ -2UM\sigma^z & \epsilon_{k+Q} \end{pmatrix} \begin{pmatrix} \mathbf{c}_k \\ \mathbf{c}_{k+Q} \end{pmatrix} + UM^2V.$$

Now here's where there's something special about half-filling: at half-filling

$$\epsilon_{k+Q} = -\epsilon_k \tag{5.5}$$

(this property is called *nesting*). The eigenvalues of the matrix

$$h(k) \equiv \begin{pmatrix} \epsilon_k & -2UM\sigma^z \\ -2UM\sigma^z & -\epsilon_k \end{pmatrix} = \epsilon_k Z - 2UM\sigma^z X$$

are

$$\pm\sqrt{\epsilon_k^2 + (2UM)^2} \equiv \pm E_k$$

independent of the sign of σ^z. (Recall that the eigenvalues of the 2×2 matrix $h = h_0 \mathbb{1} + h_x X + h_y Y + h_z Z$ are $h_0 \pm \sqrt{h_x^2 + h_y^2 + h_z^2}$.)

In terms of the creation and annihilation operators for the normal modes, $\mathrm{d}_{\pm\sigma}(k)$[27],

$$\mathbf{H}_{\rm MF} = \sum_{k,\sigma}{}' \Big(E_k \mathrm{d}_{+\sigma}^\dagger(k) \mathrm{d}_{+\sigma}(k) - E_k \mathrm{d}_{-\sigma}^\dagger(k) \mathrm{d}_{-\sigma}(k) \Big) + VUM^2.$$

[27] We actually don't need the form of these normal modes for our purposes here, but for completeness, they are

$$\mathrm{d}_{+\sigma}(k) = -v(k)\sigma^z_{\sigma\sigma'} \mathbf{c}_{\sigma'}(k) + u(k)\mathbf{c}_\sigma(k+Q) \tag{5.6}$$
$$\mathrm{d}_{-\sigma}(k) = u(k)\mathbf{c}_\sigma(k) + v(k)\sigma^z_{\sigma\sigma'} \mathbf{c}_{\sigma'}(k+Q) \tag{5.7}$$

where $\begin{pmatrix} -v\sigma^z & u \\ u & v\sigma^z \end{pmatrix}$ is the matrix which diagonalizes $h(k)$ above, and

$$u_k = \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\epsilon_k}{E_k}}, \quad v_k = \sqrt{1 - u_k^2}.$$

The groundstate at half-filling is

$$|\text{MF gs}\rangle = \prod_k \mathrm{d}^\dagger_{-\sigma}(k)\left|\tilde{0}\right\rangle$$

where $\left|\tilde{0}\right\rangle$ is the vacuum with $\mathrm{d}_{\pm\sigma}\left|\tilde{0}\right\rangle = 0$ – it is *not* the state with no **c**-electrons, which instead satisfies $\mathbf{c}(k)\,|0\rangle = 0$!! This state involves completely filling the bottom band – it is a band insulator – and has energy

$$E_0(M) = -2{\sum_k}' E(k) + M^2 UV. \tag{5.8}$$

Notice that $|E_k|$ grows with M, so it is favorable to increase M if $U > 0$. To minimize over M requires

$$0 = UV - {\sum_k}' \frac{4U^2}{E_k} \quad \Leftrightarrow \quad \boxed{\frac{4U}{V}{\sum_k}' \frac{1}{E_k} \stackrel{!}{=} 1}. \tag{5.9}$$

We would like to solve this condition for the variational parameter M, the amount of AFM order. In the thermodynamic limit, the condition is

$$1 = 4U \int_{\mathrm{BZ}'} \frac{\text{đ}^d k}{\sqrt{4U^2M^2 + \epsilon_k^2}} = 4U \int \frac{d\epsilon g(\epsilon)}{4U^2M^2 + \epsilon^2}$$

where

$$g(\epsilon) = \int_{\mathrm{BZ}'} \text{đ}^d k \delta(\epsilon - \epsilon_k)$$

is the density of states at energy ϵ. The dominant contribution comes from near the Fermi surface (where the denominator is smallest), where we can treat $g(\epsilon) \simeq g(\epsilon_F)$ as a constant. So we can approximate the integral as

$$1 \simeq 4Ug(\epsilon_F) \int_{-t}^{t} \frac{d\epsilon}{\sqrt{\epsilon^2 + 4U^2M^2}} = 8Ug(\epsilon_F) \log \frac{t}{2|UM|} \tag{5.10}$$

whose solution is

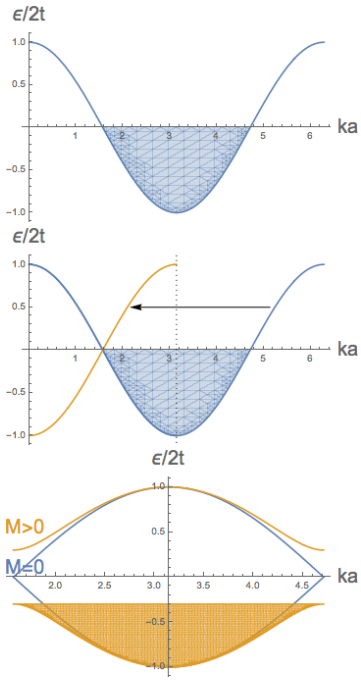
$$|M| \simeq \frac{t}{U} e^{-\frac{1}{8g(\epsilon_F)U}}. \tag{5.11}$$

Notice that as $U \to 0^+$, M vanishes (along with all of its U-derivatives). (5.11) is not a formula we could ever get in perturbation theory in U.

The next figure is a cartoon of what happened. We started with a Fermi surface (top); the spin density wave $\langle S^z \rangle = Me^{\mathbf{i}\pi(x+y)}$ broke translation invariance and folded the BZ in half (middle); this allows the two parts of the Fermi surface to hybridize, leading to a new bandstructure (bottom) which has a lower groundstate energy. (By

'hybridize' I just mean the usual thing that happens when two levels with the same quantum numbers try to cross – there is an avoided crossing[28].)

A simpler, lower-dimensional example where the cartoon is a precise description is in the 1d case, where this is called the spin-Peierls instability of 1d metals. The ordinary Peierls instability of 1d metals involves instead of spin-ordering, a condensation of phonons which enlarges the unit cell, and produces an energy gap in the electronic spectrum, which lowers the energy of the filled bands. (See the homework and notes from discussion section.)



The role of half-filling here is to make it so the integrals behave as in the 1d case. The crucial phenomenon is that different patches of the Fermi surface are separated by the ordering wavevector Q ($\epsilon_k = -\epsilon_{k+Q}$), as we used in (5.5). If not for this property, there would have been an extra term in $h = h_0 \mathbb{1} + h_x X + h_z Z$ proportional to the identity, and we would have had $E(k) = h_0 \pm \sqrt{h_x^2 + h_z^2}$, which would remove the log from (5.10).

Away from half-filling, the Fermi surface is no longer perfectly nested, and the wave-vector at which the ordering wants to happen generalizes from $\vec{Q} = \pm(\pi, \pi)$ to $\vec{Q} = \pm 2\vec{k}_F$, so that again $\vec{Q}$ connects antipodal points on the Fermi surface, but they are not nested.

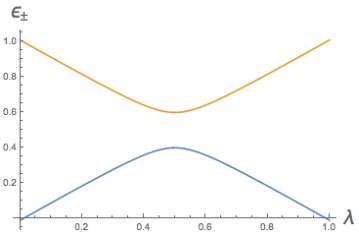
So with repulsive interactions, the would-be-metallic state at half-filling on the square lattice is unstable to spin-ordering. One reason to care about electrons on the square lattice at half-filling is that it is a pretty good model of an undoped cuprate

[28] Maybe I should be more explicit about this. Consider a hamiltonian which depends on one parameter λ, which has two levels which approach each other near say $\lambda = \frac{1}{2}$. The other eigenvalues are all far away and far from each other, so we can just think about these two:

$$h_0 = \begin{pmatrix} \lambda & 0 \\ 0 & 1-\lambda \end{pmatrix} = \frac{1}{2}\lambda \mathbb{1} + \left(\lambda - \frac{1}{2}\right) Z.$$

But this is not the most generic 2×2 hermitian matrix with this property. The most generic such matrix is instead

$$h = \frac{1}{2}\lambda \mathbb{1} + \left(\lambda - \frac{1}{2}\right) Z + h_x X + h_y Y = h_0 \mathbb{1} + \vec{h} \cdot \vec{\sigma}.$$



(If there is time-reversal symmetry, we must have $h_y = 0$, but that won't change the conclusion.) The eigenvalues of h are $h_0 \pm \sqrt{|h|^2}$, which do not collide. Having a collision requires fine-tuning of some kind.

superconductor, such as La_2CuO_4. The copper and oxygen atoms form planes of square lattices on which the electrons can hop. The undoped material is indeed an antiferromagnet. Increasing the doping leads eventually to the destruction of the AFM order and the formation of a superconducting state.

Next we'll see what happens with attractive interactions. I claim that the result is superconductivity – BEC of electron pairs $\mathbf{b}^\dagger(x) = \mathbf{c}^\dagger_\uparrow \mathbf{c}^\dagger_\downarrow$.

5.4 Attractive interactions between electrons and Cooper pairs

But aren't the Coulomb interactions between electrons repulsive, since they have like charge? Electrons in a solid also interact with each other through the phonon modes. The idea is familiar to anyone who has sat on a squishy mattress at the same time as someone else: each person makes an indentation in the mattress – some excitation of (many!) phonons. That indentation is then a potential well into which the other person is attracted.

To give a slightly more quantitative account of this phonon-mediated attraction between electrons, consider

$$\mathbf{H}_{\text{e-ph}} = -t \sum_{\langle ij \rangle} \mathbf{c}^\dagger_i \mathbf{c}_j + h.c. + g \sum_{\langle ij \rangle} \mathbf{c}^\dagger_i \mathbf{c}_j u_{ij} + \mathbf{H}(u).$$

Here we can think of $u_{ij} \equiv \mathbf{q}_i - \mathbf{q}_j$ as representing the phonon modes, and we can take $\mathbf{H}(u)$ as the balls-and-springs model with which we began the course. We will regard g as a small parameter. The groundstate at $g = 0$ is just

$$|\text{gs of FS}\rangle \otimes |\text{gs of lattice}\rangle .$$

We treat g as a perturbation:

$$\Delta\mathbf{H} = g \sum_{ij} \mathbf{c}^\dagger_i \mathbf{c}_j u_{ij} = \sum_{p,q} g(q) \mathbf{c}^\dagger_{p-q} \mathbf{c}_p \mathbf{a}^\dagger_q + h.c.$$

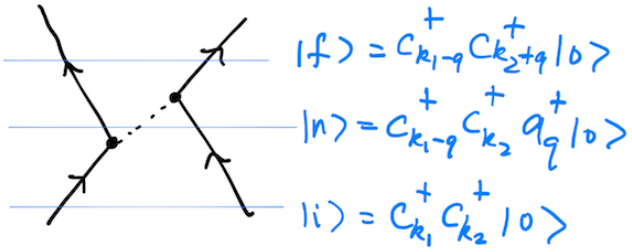
where $g(q)$ is some function (which actually vanishes at $q = 0$ by translation symmetry). At right is a visualization of an associated process, where a single electron emits a phonon; the associated amplitude is g. (The complex conjugate process where an electron absorbs a phonon is also mediated by this term.)

In perturbation theory a transition amplitude takes the form

$$(2\pi)^d \delta^d(p_F - p_I) \mathcal{M}_{fi} = \langle f | \Delta\mathbf{H} | i \rangle - \sum_n \frac{\langle f | \Delta\mathbf{H} | n \rangle \langle n | \Delta\mathbf{H} | i \rangle}{E_n - E_i - \mathbf{i}\epsilon} + \mathcal{O}(\Delta\mathbf{H}^3).$$

Consider an initial and final state with two electrons and no phonons

$$|i\rangle \equiv \mathbf{c}^\dagger_{k_1}\mathbf{c}^\dagger_{k_2}\,|\mathrm{FS}\rangle\otimes|0\rangle\,, \quad |f\rangle \equiv \mathbf{c}^\dagger_{k_1-q}\mathbf{c}^\dagger_{k_2+q}\,|\mathrm{FS}\rangle\otimes|0\rangle\,.$$



Our interaction term makes or destroys phonons, and so the first order term for this choice of i, f vanishes. In the second-order term, the intermediate state is

$$|n\rangle = \mathbf{c}^\dagger_{k_1-q}\mathbf{c}^\dagger_{k_2}\mathbf{a}^\dagger_q\,|\mathrm{FS}\rangle\otimes|0\rangle$$

with energy $E_n - E_i = \epsilon_{k_1-q} + \epsilon_{k_2} + \omega_q - (\epsilon_{k_1} + \epsilon_{k_2})$.
At right is a visualization of this process, a Feynman diagram. The end result of this second order term is to produce a transition between 2-electron states

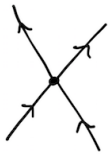
$$|k_1, k_2\rangle \mapsto |k_1 - q, k_1 + q\rangle$$

with transition amplitude

$$V_{q,k_1,k_2} = -\frac{g^2(q)}{\epsilon_{k_1-q} + \omega_q - \epsilon_{k_1}} < 0.$$

It is negative as a general consequence of 2d-order perturbation theory: the 2d-order contribution is always negative if the intermediate state has higher energy than the initial state. If our interest is only in the electronic states, this is just the same result as if we had an *attractive* two-body electron interaction of the form

$$\Delta\mathbf{H}_{\mathrm{eff}} = \sum_{k_1,k_2,q} V_{q,k_1,k_2}\mathbf{c}^\dagger_{k_1-q}\mathbf{c}^\dagger_{k_2+q}\mathbf{c}_{k_1}\mathbf{c}_{k_2}\ .$$



There are many other points of view from which to reach this conclusion. Perhaps the easiest is using path integrals. Very sketchily, the basic idea is

$$\int [Dq] e^{\mathbf{i}S[c]+\mathbf{i}\int\left((\dot{q})^2-(\vec{\nabla}q)^2-gqc^\dagger c\right)} = e^{\mathbf{i}S[c]+\int\int c^\dagger cDc^\dagger c}$$

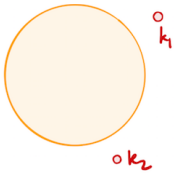
where $D = \langle qq\rangle$.

So the conclusion is that in some metals, there is a net attraction between electrons. For a more complete discussion of the competition between the screened Coulomb force and the phonon-mediated attraction, I recommend §5.2 of Leggett's book.

Cooper problem. [Baym, chapter 8] Now we will examine a simple model which demonstrates that in the presence of attractive interactions, electrons near a Fermi

surface will pair up. The model, due to Cooper, is a brutal simplification of the actual situation. We consider two opposite-spin electrons above an inert Fermi sea:

$$|\psi\rangle \equiv \sum_{k_1,k_2} a_{k_1,k_2}\psi^\dagger_{k_1\uparrow}\psi^\dagger_{k_2\downarrow}|\mathrm{FS}\rangle \equiv \sum_{k_1k_2} a_{k_1k_2}\,|k_1k_2\rangle\,.$$



We only include (attractive) interactions between these two electrons, and ignore their interactions with the electrons filling the Fermi sea, and the interactions between the electrons filling the Fermi sea. The result will be a boundstate even for arbitrarily weak interactions. Later we'll come back and discuss the shortcomings of this model and its conclusions.

The Schrodinger problem $\mathbf{H}\,|\psi\rangle = E\,|\psi\rangle$ is

$$Ea_{k_1k_2} = (\epsilon_{k_1}+\epsilon_{k_2})a_{k_1k_2} + \sum_{k_1'k_2'}\langle k_1k_2|\,\mathbf{V}\,|k_1'k_2'\rangle\,a_{k_1'k_2'}. \tag{5.12}$$

We will assume the interaction is translation invariant, so that

$$\langle k_1k_2|\,\mathbf{V}\,|k_1'k_2'\rangle = \delta_{K,K'}V_{k,k'}(K), \quad K\equiv k_1{+}k_2, K'\equiv k_1'{+}k_2', \;\; k\equiv(k_1{-}k_2)/2, k'\equiv(k_1'{-}k_2')/2,$$

so that K denotes the center of mass momentum, and k denotes the relative momentum between the two particles. As a very crude model of the inter-electron attraction resulting from phonon exchange described above, we take

$$V_{k,k'}(K) = \begin{cases} -\frac{v_0}{V}, & k_F < k_1,k_2,k_1',k_2' < k_a \\ 0, & \text{else} \end{cases}, \quad v_0>0.$$

Here k_a is a wavenumber larger than k_F beyond which the phonons no longer mediate the attractive force. Then, writing $a_{k_1k_2}\equiv a_k(K)$, the eigenvalue problem becomes

$$(E-\epsilon_{k_1}-\epsilon_{k_2})a_k(K) = -\frac{v_0}{V}{\sum_{k'}}' a_{k'}(K). \tag{5.13}$$

The $'$ on the sum restricts the integration region to $k_F < |K/2 \pm k'| < k_a$. Dividing the BHS by $E-\epsilon_{k_1}-\epsilon_{k_2}$ and summing $\sum_k'$ gives

$${\sum_k}' a_k(K) = -\frac{v_0}{V}{\sum_k}'\frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}{\sum_{k'}}' a_{k'}(K)$$

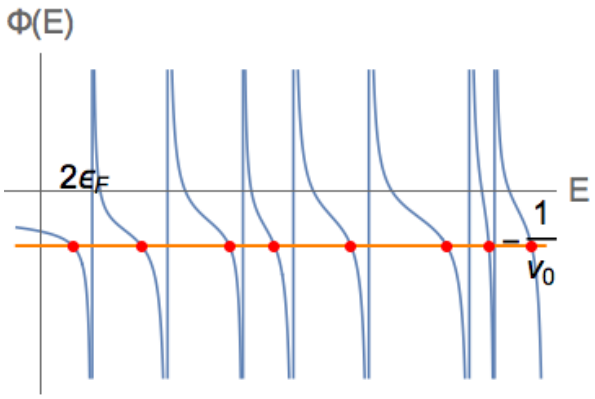
but now $\sum_k' a_k(K) = \sum_{k'}' a_{k'}(K)$ is a nonzero constant and therefore

$$\boxed{1 = -\frac{v_0}{V}{\sum_k}'\frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}}. \tag{5.14}$$

Following Baym, we can solve this equation graphically. Let

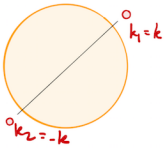
$$\Phi(E) \equiv \frac{1}{V}\sum_k{}' \frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}.$$

This function, for a simple choice of ϵ_k, is plotted at right. In terms of Φ, the eigenvalue problem is $\Phi(E) = -\frac{1}{v_0}$ (the orange line).



The function $\Phi(E)$ has poles at every possible energy of a two-particle state in the free problem, $\epsilon(k_1)+\epsilon(k_2)$ (for $k_{1,2}$ in the range where the interaction is nonzero). The crossings of $\Phi(E) = -\frac{1}{v_0}$ that occur at $E > 2\epsilon_F$ are just like the corresponding states of the unperturbed system. These states become a continuum as $V \to \infty$. But you can see that there is one crossing that occurs for $E < 2\epsilon_F$, at $E = E_b \equiv 2\epsilon_F - 2\Delta$. This is a boundstate, below the 2-particle continuum, which wouldn't exist if not for the attractive interaction.

Let's focus on $K = 0$, which will give the largest binding energy. Then $k_1 = k, k_2 = -k$ are on opposite sides of the Fermi surface.



$$\Phi_{K=0}(E) = \int_{k_F}^{k_a} \frac{\mathrm{d}^d k}{E-2\epsilon_k} = \int_{\epsilon_F}^{\epsilon_a} \frac{d\epsilon g(\epsilon)}{E-2\epsilon}$$

where $g(\epsilon) \equiv \int \mathrm{d}^d k \delta(\epsilon_k - \epsilon)$ is our friend the density of states at single-particle energy ϵ, and $\epsilon_a \equiv \epsilon_{k_a}$. Near the Fermi surface again we can approximate $g(\epsilon) \simeq g(\epsilon_F)$ as a constant, and we find

$$\Phi_{K=0}(E) \simeq g(\epsilon_F)\int_{\epsilon_F}^{\epsilon_a} \frac{d\epsilon}{E-2\epsilon} \overset{E<2\epsilon_F}{=} -\frac{g(\epsilon_F)}{2}\log\left|\frac{2\epsilon_a - E}{2\epsilon_F - E}\right| \overset{!}{=} -\frac{1}{v_0}.$$

The solution for the binding energy is

$$\Delta = \frac{\epsilon_a - \epsilon_F}{e^{\frac{2}{v_0 g(\epsilon_F)}} - 1} \simeq \epsilon_D e^{-\frac{2}{v_0 g(\epsilon_F)}}$$

where ϵ_D is the Debye energy, roughly the maximum energy of a phonon excitation, and we used the fact that $v_0 g(\epsilon_F)$ is small because the coupling is weak. Again this is non-perturbative in the coupling v_0.

The momentum-space wavefunction of the boundstate is $a_k(K) \propto \frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}$, so in position space it is

$$\psi(r_1, r_2) \sim e^{\mathbf{i}K\cdot\frac{r_1+r_2}{2}} \frac{1}{V}\sum_k{}' \frac{e^{\mathbf{i}k\cdot(r_1-r_2)}}{E-\epsilon_{k_1}-\epsilon_{k_2}}.$$

In the thermodynamic limit, the relative wavefunction is

$$\int' \mathrm{d}^d k \frac{e^{\mathbf{i}k\cdot r_{12}}}{E-\epsilon_{k_1}-\epsilon_{k_2}} \overset{K=0}{\simeq} \frac{\sin k_F|r_{12}|}{|r_{12}|} \sin\left(\frac{|r_{12}|}{\xi}\right),$$

where $\xi = \frac{2k_F}{m\Delta}$ is the size of the pair. Notice that the state is a relative s-wave, *i.e.* it is spherically symmetric. This is made possible by the fact that the two electrons have opposite spin.

In an actual metal, the role of our two special electrons is played by every electron near the Fermi surface. They all want to form pairs with their antipodal partners (and less so with other electrons), and condense. If we apply an electric field, the Fermi surface shifts and they'll want instead to form pairs with definite nonzero K. This is a supercurrent.

This actually happens to electrons in metals, in the fermionic isotope of helium ^{3}He at $T < 0.0026^\circ K$, and to nucleons in the core of a neutron star.

What role is played by the Fermi surface? If we redo the analysis with $k_F = 0$, the conclusion is very different. Instead $\Phi(E) = \frac{m}{\pi^2}\left(-k_a + 2\sqrt{m\Delta}\arctan\frac{k_a}{2\sqrt{m\Delta}}\right)$. In order for this to hit $-1/v_0$, we need

$$\frac{1}{v_0} < \frac{k_a m}{\pi^2}$$

– an interaction strength above a nonzero threshold value is required in order to create a boundstate. In the case with a Fermi surface, an arbitrarily weak interaction suffices.

A warning: in a real metal, the Fermi sea electrons are not inert! This leads to an important modification of the outcome. Instead of a boundstate at negative $E - 2\epsilon_F$, instead one finds an *instability* – a mode whose energy has a positive imaginary part. The instability is to the formation of a condensate of Cooper pairs. More on this next.

5.5 Instabilities of a Fermi surface to attractive interactions

So consider again a Hamiltonian of the form (5.4)

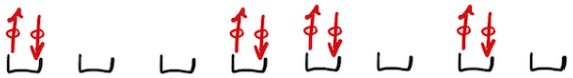
$$\mathbf{H} = -t \sum_{\langle xy \rangle, \sigma} \mathbf{c}^\dagger_{x\sigma} \mathbf{c}_{y\sigma} + h.c. + U \sum_x (\mathbf{n}_x - 1)^2 \tag{5.15}$$

with $\mathbf{n}_x \equiv \sum_\sigma \mathbf{c}^\dagger_{x\sigma} \mathbf{c}_{x\sigma}$. Let's focus again on the square lattice, so

$$\mathbf{H}_t = \sum_k \epsilon_k \mathbf{c}^\dagger_{k\sigma} \mathbf{c}_{k\sigma}, \quad \epsilon_k = -2t \left(\cos(k_x a) + \cos(k_y a)\right) - \mu.$$

$\mu = 0$ is half-filling. For $U > 0$ we found an instability to antiferromagnetic ordering, both at large U/t and at any U/t for half-filling.

$\boxed{U < 0}$ Now we'll consider what happens if the interactions are attractive. First consider $U \to -\infty$. The term $U(n_x - 1)^2 = -|U|(n_x - 1)^2$ then insists that $n_x = 0$ or 2 at each site. Again there is a degeneracy of 2^V states, where V is the number of lattice sites.



This looks very much like our picture of a condensate of the bosons created by

$$\mathbf{b}^\dagger_x \equiv \mathbf{c}^\dagger_{x\uparrow} \mathbf{c}^\dagger_{x\downarrow},$$

Cooper pairs. (This is not quite a canonical boson, but it can still condense.) Notice that we've made no assumptions about the filling, μ is arbitrary.

To make progress away from $U = -\infty$ let's rewrite the interaction to develop a mean field theory that incorporates this bose condensation of pairs.

$$U(n_x - 1)^2 = U n_x^2 - 2U n_x + U,$$

the second term is a shift of the chemical potential which we absorb into μ, and the third term is a constant which we ignore. The remaining actual interaction is

$$U n_x^2 = U \left(\mathbf{c}^\dagger_{x\uparrow} \mathbf{c}_{x\uparrow} + \mathbf{c}^\dagger_{x\downarrow} \mathbf{c}_{x\downarrow} \right)^2 \tag{5.16}$$

$$= 2U \mathbf{c}^\dagger_{x\uparrow} \mathbf{c}_{x\downarrow} \mathbf{c}^\dagger_{x\downarrow} \mathbf{c}_{x\downarrow} = -2U \mathbf{c}^\dagger_{x\uparrow} \mathbf{c}^\dagger_{x\downarrow} \mathbf{c}_{x\downarrow} \mathbf{c}_{x\downarrow} \tag{5.17}$$

since $\mathbf{c}^2 = 0$. Now we approximate the hamiltonian by

$$\mathbf{H}_{\rm MF} = \sum_k \mathbf{c}^\dagger_{k\sigma}\mathbf{c}_{k\sigma}(\epsilon_k - \mu) - 2U\sum_x \left(\underbrace{\left\langle \mathbf{c}^\dagger_{x\uparrow}\mathbf{c}^\dagger_{x\downarrow}\right\rangle}_{\equiv\Delta}\mathbf{c}_{x\uparrow}\mathbf{c}_{x\downarrow} + \mathbf{c}^\dagger_{x\uparrow}\mathbf{c}^\dagger_{x\downarrow}\underbrace{\left\langle \mathbf{c}_{x\uparrow}\mathbf{c}_{x\downarrow}\right\rangle}_{=-\Delta^\star} - \left\langle \mathbf{c}^\dagger_{x\uparrow}\mathbf{c}^\dagger_{x\downarrow}\right\rangle\left\langle \mathbf{c}_{x\uparrow}\mathbf{c}_{x\downarrow}\right\rangle \right) \tag{5.18}$$

$$= \sum_k \mathbf{c}^\dagger_{k\sigma}\mathbf{c}_{k\sigma}(\epsilon_k - \mu) - 2U\sum_x \left(\Delta\mathbf{c}_{x\uparrow}\mathbf{c}_{x\downarrow} + \Delta^\star\mathbf{c}^\dagger_{x\downarrow}\mathbf{c}^\dagger_{x\uparrow}\right) - 2VU|\Delta|^2 \tag{5.19}$$

$$= \sum_k \left(\mathbf{c}^\dagger_{k\sigma}\mathbf{c}_{k\sigma}(\epsilon_k - \mu) + 2U\left(\Delta^\star\mathbf{c}^\dagger_{k\uparrow}\mathbf{c}^\dagger_{-k\downarrow} + \Delta\mathbf{c}_{k\uparrow}\mathbf{c}_{-k\downarrow}\right)\right) - 2U|\Delta|^2V. \tag{5.20}$$

In the last step we made the ansatz that Δ is uniform in space, figuring that this will minimize the energy. Notice the weird sign in front of the $|\Delta|^2$ term; this is a consequence of fermi statistics $\left\langle \mathbf{c}_{x\uparrow}\mathbf{c}_{x\downarrow}\right\rangle = -\left\langle \mathbf{c}^\dagger_{x\uparrow}\mathbf{c}^\dagger_{x\downarrow}\right\rangle^\star = -\Delta^\star$. Notice that $\mathbf{H}$ had a symmetry under $\mathbf{c} \to e^{\mathbf{i}\theta}\mathbf{c}$, associated with particle number conservation. $\mathbf{H}_{\rm MF}$ does not have this symmetry, only a $\mathbb{Z}_2$ subgroup $\mathbf{c} \to -\mathbf{c}$. The way to think about this is: we are using $\mathbf{H}_{\rm MF}$ as a way to construct a trial wavefunction for $\mathbf{H}$ (in particular its groundstate). Based on the above discussion, we expect the groundstate of $\mathbf{H}$ to spontaneously break this $\mathsf{U}(1)$ symmetry, so we are building this into $\mathbf{H}_{\rm MF}$.

Solution of $\mathbf{H}_{\rm MF}$. $\mathbf{H}_{\rm MF}$ is quadratic in canonical fermion operators, so we should be able to solve it. It has an unfamiliar ingredient, namely $\mathbf{c}^\dagger\mathbf{c}^\dagger$ terms. The name for the general strategy for getting rid of such terms is called a Bogoliubov transformation. The idea, as you saw on the homework, is to introduce new creation and annihilation operators which mix the $\mathbf{c}$s and $\mathbf{c}^\dagger$s in terms of which the Hamiltonian does not have such terms. Here a particle-hole transformation on just the down spins does the job:

$$\mathrm{d}_{k\downarrow} \equiv \mathbf{c}^\dagger_{-k\downarrow} \qquad \implies \mathrm{d}^\dagger_{k\downarrow} = \mathbf{c}_{-k\downarrow} \tag{5.21}$$

$$\mathrm{d}_{k\uparrow} \equiv \mathbf{c}_{+k\uparrow} \qquad \implies \mathrm{d}^\dagger_{k\uparrow} = \mathbf{c}^\dagger_{k\uparrow}. \tag{5.22}$$

You can check these are also canonical fermion operators. In terms of them,

$$\mathbf{H}_{\rm MF} = \sum_k (\epsilon_k - \mu)\,\mathrm{d}^\dagger_{k\uparrow}\mathrm{d}_{k\uparrow} - \sum_k (\epsilon_k - \mu)\,\mathrm{d}^\dagger_{k\uparrow}\mathrm{d}_{k\uparrow} + \sum_k (\epsilon_k - \mu) + 2U\sum_k \left(\mathrm{d}^\dagger_{k\uparrow}\mathrm{d}_{k\downarrow}\Delta^\star + h.c.\right) - 2UV|\Delta|^2$$

$$= \left(\mathrm{d}^\dagger_{k\uparrow}, \mathrm{d}^\dagger_{k\downarrow}\right)\begin{pmatrix}\epsilon_k - \mu & 2\Delta^\star U \\ 2\Delta U & -(\epsilon_k - \mu)\end{pmatrix}\begin{pmatrix}\mathrm{d}_{k\uparrow} \\ \mathrm{d}_{k\downarrow}\end{pmatrix} - U|\Delta|^2V + \text{const} \tag{5.23}$$

(where by constant, I mean independent of Δ). The matrix is $\sigma^z(\epsilon-\mu)+\sigma^x(-2U\mathrm{Re}\,\Delta)+\sigma^y(-2U\mathrm{Im}\,\Delta)$ whose eigenvalues are $\pm\sqrt{(\epsilon_k-\mu)^2+4U^2|\Delta|^2}$. Therefore (suppose we're at less than half-filling, so we partially fill the bottom band)

$$E_0^{\rm MF} = +|U||\Delta|^2V - \sum_k^{k_F}\sqrt{(\epsilon_k-\mu)^2+4U^2|\Delta|^2}.$$

In the thermodynamic limit, the energy density is

$$E_0^{\rm MF}/V = |U||\Delta|^2 - \int^{k_F} \text{đ}^d k \sqrt{(\epsilon_k - \mu)^2 + 4U^2|\Delta|^2} = |U||\Delta|^2 - \int^{\mu} d\epsilon g(\epsilon) \sqrt{(\epsilon - \mu)^2 + 4U^2|\Delta|^2}.$$

Minimizing the energy requires

$$1 = |U| \int^0 \frac{d\epsilon g(\mu + \epsilon)}{\sqrt{\epsilon^2 + 4U^2|\Delta|^2}} \simeq |U| g(\epsilon_F) \int_{-t}^0 \frac{d\epsilon}{\sqrt{\epsilon^2 + 4U^2|\Delta|^2}} \tag{5.24}$$

$$= |U| g(\epsilon_F) \log \frac{t + \sqrt{t^2 + 4U^2|\Delta|^2}}{2|\Delta||U|} \simeq |U| g(\epsilon_F) \log \frac{t}{2|\Delta||U|}. \tag{5.25}$$

The solution for Δ is

$$|\Delta| \simeq \frac{t}{2|U|} e^{-\frac{1}{4g(\epsilon_F)|U|}}.$$

Thus, attractive interactions between fermions produce condensation of fermion pairs. If the fermions carry electric charge (as electrons do), this is superconductivity.

You may have noticed some close parallels between this discussion and that of the AFM. At half-filling there is a precise map which takes $U \to -U$, $(-1)^x \mathbf{c}_x^\dagger \vec{\sigma} \mathbf{c}_x \to \mathbf{c}_{x\uparrow}^\dagger \mathbf{c}_{x\downarrow}^\dagger$. It is basically the particle-hole transformation on just the down spins that we did to solve $\mathbf{H}_{\rm MF}$.

5.6 An addendum on mean field theory for interacting fermions

[de Gennes, *Superconductivity of Metals and Alloys*, chapter 5] Consider an interacting Hamiltonian of the form

$$\mathbf{H} = -t \sum_{\langle ij \rangle} \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{j\sigma} + hc + V \sum_i \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\downarrow} \mathbf{c}_{i\uparrow} \equiv \mathbf{T} + \mathbf{V}.$$

We would like to find the gaussian state $|\text{MF}\rangle$ which minimizes the expectation value $\langle \text{MF}| \mathbf{H} |\text{MF}\rangle$ (at fixed average particle number $N = \sum_i \left\langle \mathbf{c}_i^\dagger \mathbf{c}_i \right\rangle$. By gaussian state, I mean a Slater determinant $\prod_\alpha \text{d}_\alpha^\dagger \left|\tilde{0}\right\rangle$, where the d_α are some collection of modes, to be determined.

A useful device for accomplishing this is to define an auxiliary quadratic Hamiltonian whose groundstate is $|\text{MF}\rangle$. In this case, we can consider

$$\mathbf{H}_{\rm MF} = \mathbf{T} - \sum_i \mu_i \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{i\sigma} + \sum_i \left(\Delta_i \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger + hc - |\Delta_i|^2 \right).$$

So the thing we want to extremize over the choice of ds and occupation numbers is

$$F \equiv \langle \text{MF}| \mathbf{H} |\text{MF}\rangle - \lambda \left(\sum_i \left\langle \mathbf{c}_i^\dagger \mathbf{c}_i \right\rangle - N \right) - TS. \tag{5.26}$$

I include the TS term in the free energy to emphasize that the same strategy works at finite temperature; let's set $T = 0$ from now on. Because $|\mathrm{MF}\rangle$ is a gaussian state, we can compute (5.26) using Wick's theorem (all expectation values below are in the state $|\mathrm{MF}\rangle$):

$$F = \langle \mathbf{T} \rangle - \lambda \left(\sum_i \left\langle \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{i\sigma} \right\rangle - N \right) + V \sum_i \left(\left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \right\rangle \left\langle \mathbf{c}_{i\downarrow} \mathbf{c}_{i\uparrow} \right\rangle + \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\uparrow} \right\rangle \left\langle \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\downarrow} \right\rangle - \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow} \right\rangle \left\langle \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\uparrow} \right\rangle \right). \tag{5.27}$$

In this expression I actually haven't assumed that $|\mathrm{MF}\rangle$ is translation invariant. But let's assume time-reversal invariance, so that $\left\langle \mathbf{c}_\uparrow^\dagger \mathbf{c}_\downarrow \right\rangle = 0$ and we can drop the last term.

Now consider varying (5.27) with respect to the choice of modes and filling:

$$\delta F = \delta \langle \mathbf{T} \rangle - \lambda \delta \left\langle \mathbf{c}_\sigma^\dagger \mathbf{c}_\sigma \right\rangle + V \sum_i \left(\left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \right\rangle \delta \left\langle \mathbf{c}_{i\downarrow} \mathbf{c}_{i\uparrow} \right\rangle + \delta \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \right\rangle \left\langle \mathbf{c}_{i\downarrow} \mathbf{c}_{i\uparrow} \right\rangle \tag{5.28}$$

$$+ \delta \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\uparrow} \right\rangle \left\langle \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\downarrow} \right\rangle + \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\uparrow} \right\rangle \delta \left\langle \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\downarrow} \right\rangle \Big). \tag{5.29}$$

But now consider the free energy associated with the mean field hamiltonian:

$$F_{\mathrm{MF}} = \langle \mathrm{MF} | \, \mathbf{H}_{\mathrm{MF}} \, | \mathrm{MF} \rangle - \lambda \left(\sum_i \left\langle \mathbf{c}_i^\dagger \mathbf{c}_i \right\rangle - N \right) - TS.$$

Since $|\mathrm{MF}\rangle$ is the groundstate of $\mathbf{H}_{\mathrm{MF}}$ with the right particle number, the variation is zero:

$$\delta F_{\mathrm{MF}} = \delta \langle \mathbf{T} \rangle - \sum_i (\mu_i + \lambda) \delta \left\langle \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{i\sigma} \right\rangle + \sum_i \left(\Delta_i \delta \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \right\rangle + hc \right). \tag{5.30}$$

Using (5.30) to eliminate the common terms in (5.28) and independently equating the coefficients of $\delta \left\langle \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{i\sigma} \right\rangle$ and $\delta \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \right\rangle$, we find

$$-\mu_i = V \left\langle \mathbf{c}_{i\downarrow}^\dagger \mathbf{c}_{i\downarrow} \right\rangle \tag{5.31}$$

$$-\mu_i = V \left\langle \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\uparrow} \right\rangle \tag{5.32}$$

$$\Delta_i = V \left\langle \mathbf{c}_{i\downarrow} \mathbf{c}_{i\uparrow} \right\rangle \ . \tag{5.33}$$

These are the self-consistency conditions we should impose. Notice that the terms (5.29) lead to a renormalization of the chemical potential due to the interactions.

6 Linear response

[Pines and Nozieres, chapter 2] What happens in an experiment? Pretty inevitably, what happens involves two steps (1) the experimenter pokes at the system somehow. This means changing the hamiltonian by $\mathbf{H} = \mathbf{H}_0 + V(t)$ for some perturbation $V(t)$. (2) the experimenter measures the response of the system.

Here we make two further assumptions. First, that the system starts in equilibrium before the experimenter shows up. This means either the groundstate or the canonical ensemble at temperature T.

Second, we assume that the poking is weak enough that the response is *linear* in the perturbation. This means that the response is entirely a property of the unperturbed system. In particular, it will be determined by equilibrium correlation functions, which as we've seen and will see in more detail below are related to the low-lying spectrum of the system.

A good simple example to keep in mind (during the more abstract bits below) is the response of an RLC circuit to an applied voltage. As in that example, the response can come in two varieties: dissipative and reactive (or reversible).

So suppose we kick the system by an operator $\mathcal{O}_B$. What this means is that the source is a time dependent perturbation to the Hamiltonian, $H = H_0 + V(t)$:

$$V(t) = \int \mathrm{d}^{D-1}x \phi_B(t,x)\mathcal{O}_B(x) \ .$$

Here $\phi_B(t,x)$ is a function the experimenter gets to pick.

The response is

$$\begin{aligned} \langle \mathcal{O}_A \rangle(t,x) &\equiv \mathrm{Tr}\ \rho(t)\, \mathcal{O}_A(x) \\ &= \mathrm{Tr}\ \rho_0\, U^{-1}(t)\mathcal{O}_A(t,x)U(t) \end{aligned}$$

The initial state is $\rho_0 = e^{-\beta H_0}/Z$ or $\rho_0 = |\Phi_0\rangle\langle\Phi_0|$, the projector onto the groundstate. In the last step we are using interaction picture, where $U(t) = \mathcal{T} e^{-\mathbf{i}\int^t V(t')\mathrm{d}t'}$, and $\mathcal{O}_A(t,x) = e^{\mathbf{i}\mathbf{H}_0 t}\mathcal{O}_A(x)e^{-\mathbf{i}\mathbf{H}_0 t}$ is the unperturbed evolution.

I think I should explain this step a bit more. First, in the Schrödinger picture, only the states evolve: $\mathbf{i}\partial_t\rho(t) = [\mathbf{H}, \rho(t)]$ so that $\rho(t) = U_H(t)\rho_0 U_H^{-1}(t)$, with $U_H = e^{-\mathbf{i}\mathbf{H}t}$. The expectation value we want is

$$\mathrm{tr}\rho(t)\mathcal{O}_A(x) = \mathrm{tr}\rho_0 U_H^{-1}(t)\mathcal{O}_A(x)U_H(t) = \mathrm{tr}\rho_0 U^{-1}(t)\mathcal{O}_A(x,t)U(t)$$

where at the last step we wrote

$$U_H(t) = U_0(t)U(t), \quad U_0(t) \equiv e^{-\mathbf{i}\mathbf{H}_0 t} \quad \mathcal{O}_A(x,t) \equiv U_0^{-1}\mathcal{O}_A(x)U_0. \tag{6.1}$$

This last expression is the *interaction picture* evolution of the operators – they evolve by the unperturbed Hamiltonian. The first expression in (6.1) defines the interaction picture evolution operator $U = U_H U_0^{-1}$. Using $\mathbf{i}\partial_t U_H = U_H \mathbf{H}, \mathbf{i}\partial_t U_0 = \mathbf{H}_0 U_0$, we have

$$\mathbf{i}\partial_t U(t) = U_0^{-1}\left(-\mathbf{H}_0 + \mathbf{H}\right)U = U_0^{-1}VU = U_0^{-1}VU_0U_0^{-1}U = V(t)\mathbf{U}$$

where $V(t)$ is the evolution of V by the unperturbed hamiltonian. What is the solution of $\mathbf{i}\partial_t U = V(t)U$? I claim, by the Fundamental Theorem of Calculus, that

$$\begin{aligned}
U(t) &= U(0) - \mathbf{i}\int_0^t dt_1 V(t_1)U(t_1) && (6.2)\\
&\overset{(6.2)}{=} U(0) - \mathbf{i}\int_0^t dt_1 V(t_1)\left(U(0) - \mathbf{i}\int_0^{t_1} dt_2 V(t_2)U(t_2)\right) && (6.3)\\
&= \cdots && (6.4)\\
&= \sum_{n=0}^{\infty}(-\mathbf{i})^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n V(t_1)V(t_2)\cdots V(t_n)U(0). && (6.5)
\end{aligned}$$

The initial time is arbitrary. Suppose we are evolving from time t_i, so $U(t = t_i) = \mathbb{1}$. Then

$$\begin{aligned}
U(t,t_i) &= \sum_{n=0}^{\infty}(-\mathbf{i})^n \int_{t_i}^t dt_1 \int_{t_i}^{t_1} dt_2 \cdots \int_{t_i}^{t_{n-1}} dt_n V(t_1)V(t_2)\cdots V(t_n)\\
&= \sum_{n=0}^{\infty}(-\mathbf{i})^n \int_{t_i}^t dt_1 \int_{t_i}^{t_1} dt_2 \cdots \int_{t_i}^{t_{n-1}} dt_n \mathcal{T}\left(V(t_1)V(t_2)\cdots V(t_n)\right)\\
&= \sum_{n=0}^{\infty}(-\mathbf{i})^n \frac{1}{n!} \int_{t_i}^t dt_1 \int_{t_i}^t dt_2 \cdots \int_{t_i}^t dt_n \mathcal{T}\left(V(t_1)V(t_2)\cdots V(t_n)\right) && (6.6)
\end{aligned}$$

In the first step I used the fact that the operators are already time ordered (this followed from the differential equation we are solving, since the V always acts from the left). In the second step we used the fact that the time-ordered integrand doesn't change if we permute the labels on the times. So we can just average over the $n!$ possible orderings of n times. If we pull out the time-ordering symbol, this is an exponential series:

$$U(t,t_i) = \mathcal{T}\left(e^{-\mathbf{i}\int_{t_i}^t dt' V(t')}\right).$$

The time-ordered exponential is defined by its Taylor expansion.

Now linearize in the small perturbation:

$$\begin{aligned}\delta\langle\mathcal{O}_A\rangle(t,x) &= -\mathbf{i}\mathrm{Tr}\ \rho_0\int^t \mathrm{d}t'[\mathcal{O}_A(t,x),\delta H(t')]\\ &= -\mathbf{i}\int \mathrm{d}^{D-1}x'\int^t \mathrm{d}t'\langle[\mathcal{O}_A(t,x),\mathcal{O}_B(t',x')]\rangle\phi_B(t',x')\\ &= \int \mathrm{d}^D x' G^R_{\mathcal{O}_A\mathcal{O}_B}(x,x')\phi_B(x')\end{aligned}$$

The *retarded Green's function* (or *response function*) for two observables $\mathcal{O}_A$ and $\mathcal{O}_B$ is

$$G^R_{\mathcal{O}_A\mathcal{O}_B}(t,x) \equiv -\mathbf{i}\theta(t)\langle[\mathcal{O}_A(t,x),\mathcal{O}_B(0,0)]\rangle \tag{6.7}$$

where $\theta(t) = 1$ for $t > 0$, else zero, is the usual Heaviside function. The time evolution of the operators here is by the unperturbed Hamiltonian $\mathcal{O}(t,x) = e^{\mathbf{i}\mathbf{H}_0 t}\mathcal{O}(x)e^{-\mathbf{i}\mathbf{H}_0 t}$, as above. So we care about the retarded Green's function because it determines what $\langle\mathcal{O}_A\rangle$ does if we kick the system via $\mathcal{O}_B$.

Now Fourier transform:

$$\delta\langle\mathcal{O}_A\rangle(\omega,k) = G^R_{\mathcal{O}_A\mathcal{O}_B}(\omega,k)\delta\phi_B(\omega,k) \tag{6.8}$$

where

$$G^R_{\mathcal{O}_A\mathcal{O}_B}(\omega,k) = -\mathbf{i}\int \mathrm{d}^{D-1}x\mathrm{d}t\ e^{\mathbf{i}\omega t-\mathbf{i}k\cdot x}\theta(t)\langle[\mathcal{O}_A(t,x),\mathcal{O}_B(0,0)]\rangle\ .$$

Note that if we want to think about the perturbations in Fourier space, *e.g.* for a single mode

$$V = \int d^d x\ e^{\mathbf{i}q\cdot x-\mathbf{i}\omega t}\varphi(q,\omega)\mathcal{O}_B(q,\omega)$$

then we must add a small imaginary part to the frequency,

$$-\mathbf{i}\omega t \to (-\mathbf{i}\omega+\eta)t \tag{6.9}$$

so that the perturbation goes away at early times. This is required so that we are actually describing a system that begins in its groundstate.

Linear response, an example.

perturbation: an external electric field, $E_x = i\omega A_x$
couples via $\delta H = \int d^d x A_x J^x$ where J is the electric current. That is, $\mathcal{O}_B = J_x$.

response: also the electric current, $\mathcal{O}_A = J_x$. Then let's look at (6.8) in this case. It's safe to assume $\langle J\rangle_{E=0} = 0$. (Actually this can be rigorously proved in some circumstances and goes by the name of Bloch's (other) theorem.) So (6.8) takes the form

$$\langle J(\omega,k)\rangle = G^R_{JJ}(\omega,k)A_x(\omega,k) = G^R_{JJ}(\omega,k)\frac{E_x}{i\omega}$$

Compare this expression to Ohm's law: $J = \sigma E$, which defines the conductivity σ. (Really it is a tensor since J and E are both vectors.)

$$\implies \text{Kubo formula:} \qquad \boxed{\sigma(\omega, k) = \frac{G^R_{JJ}(\omega, k)}{\mathbf{i}\omega}}$$

As a second example about which we'll say a bit more, consider the case where $\mathcal{O}_A = \mathcal{O}_B = \rho$, the density. Then

$$V = \sum_q \int đ\omega \rho_q^\dagger \varphi(q, \omega) e^{-\mathbf{i}\omega t} + h.c.$$

where $\varphi(q, \omega)$ is the fourier transform of some scalar potential. For example, if we shoot at the system a heavy probe particle with velocity V and position R; then $\varphi(q, \omega) = 2\pi V_q e^{-\mathbf{i}q\cdot R}\delta(\omega - q \cdot V)$. If we assume that the perturbation is small enough, then everything is linear and each q, ω is independent of all the others, and the response is

$$\delta \langle \rho(q, \omega) \rangle = G^R_{\rho\rho}(q, \omega)\varphi(q, \omega).$$

By inserting into (6.7) a representation of the identity in the energy eigenbasis $\mathbb{1} = \sum_n |n\rangle\langle n|$, (with $\mathbf{H}|n\rangle = (E_0 + \omega_n)|n\rangle$) we can develop a spectral representation of G^R. A key ingredient is the fourier representation of the theta function:

$$\theta(t) = -\mathbf{i} \int đ\epsilon \frac{e^{\mathbf{i}\epsilon t}}{\epsilon - \mathbf{i}\eta}$$

where $\eta > 0$ is infinitesimal. Its point in life is to push the pole into the UHP ϵ plane; when $t > 0$ we can close the contour in the UHP and we pick up the residue of the pole, but when $t < 0$ we must close the contour in the LHP and we do not. The result is

$$G^R_{\rho\rho}(q, \omega) = \sum_n |\langle n|\rho_q^\dagger|0\rangle|^2 \left(\frac{1}{\omega - \omega_n + \mathbf{i}\eta} - \frac{1}{\omega + \omega_n + \mathbf{i}\eta} \right) \tag{6.10}$$

$$= \int_0^\infty d\omega' S(q, \omega') \left(\frac{1}{\omega - \omega' + \mathbf{i}\eta} - \frac{1}{\omega + \omega' + \mathbf{i}\eta} \right) \tag{6.11}$$

where in the second step we used the spectral representation of the dynamical structure factor from (3.10)[29]. So G^R and S contain equivalent information. Using the f-sum

[29] In (3.10), we wrote it (the spectral representation of the dynamical structure factor) for the operator Z_q in a spin system. The general expression is

$$S_{\mathcal{O}\mathcal{O}}(q, \omega) = \sum_n |\langle n|\mathcal{O}_q|0\rangle|^2 2\pi\delta(\omega - \omega_n).$$

rule (proved on the homework) we learn that at high energy the response function is fixed

$$G^R_{\rho\rho}(q,\omega) \overset{\omega\to\infty}{\to} \frac{2}{\omega^2}\int_0^\infty \omega' d\omega' S(q,\omega') = \frac{Nq^2}{m\omega^2},$$

independent of any dynamics.

A common response to a perturbation localized in time is exponential decay: $e^{-\gamma t}, \gamma > 0$. What does this mean for $G^R(q,\omega)$? A pole in the LHP at $\omega = \omega_R - \mathbf{i}\gamma t$. Because of (6.9) our definition of G^R actually defines it directly only in the UHP, but the expression (6.10) allows us to analytically continue to the whole complex plane (minus the singularities, which determine the spectrum). The locations of the poles in the integrand of (6.10) determine the response. It has poles at $\omega = \pm\omega_n - \mathbf{i}\eta$. As we've seen, the spectrum often is described by some low-lying single-particle states below a multi-particle continuum. The continuum happens when the poles bunch up together and produce a branch cut in G^R.

The fact that G^R is analytic (no singularities) in the UHP is equivalent to *causality*: $G^R(q,t) = 0$ if $t < 0$ – the response comes after the cause. If one computes G^R somehow and finds a pole in the UHP frequency plane, it means an assumption was violated. The thing it usually means is that the putative groundstate is unstable, and the pole in the UHP represents the instability which (initially) grows exponentially in time.

Just as for the response of a linear circuit to an external voltage source, the real and imaginary parts of G^R have very different interpretations. The real part is the reactive, reversible part, while the imaginary part describes dissipation (like resistors, which come with a single time derivative, and are therefore $\pi/2$ out of phase with the source). Using the fact that

$$\lim_{\eta\to 0}\frac{1}{x-a+\mathbf{i}\eta} = P\frac{1}{x-a} - \mathbf{i}\pi\delta(x-a)$$

where P means principal part, (6.11) implies

$$\mathrm{Re}\, G^R_{\rho\rho}(q,\omega) = \int_0^\infty d\omega' S(q,\omega') P\left(\frac{2\omega'}{\omega^2-(\omega')^2}\right) \tag{6.12}$$

$$\mathrm{Im}\, G^R_{\rho\rho}(q,\omega) = -\pi\left(S(q,\omega) - S(q,-\omega)\right). \tag{6.13}$$

You can see that $\mathrm{Re}\, G^R$ is even in ω, while $\mathrm{Im}\, G^R$ is odd. The imaginary part of G^R is basically just $S(q,\omega)$, but arranged in such a way that $-\omega \mathrm{Im}\, G^R(q,\omega) > 0$. This positivity is a powerful thing. For one thing, it follows from this that the average work done on the system is positive – in equilibrium, there is only damping, never anti-damping.

Because of the analyticity in the UHP, the real and imaginary parts of G^R are related by Kramers-Kronig dispersion relations.

Compressibility and the associated sum rule. Consider now $\omega = 0$ and q small (compared to the inverse separation of particles). This is a perturbation by a static force field which is smoothly varying in space. The force felt by each particle is $-\vec{\nabla}\varphi$ which is

$$\mathcal{F}(r) = -\mathbf{i}q\varphi(q,0)e^{\mathbf{i}q\cdot r} + h.c..$$

Now think about the problem macroscopically. Such a (small) force leads to a change in the density $\delta\rho$, which in turn leads to a change in the pressure of the fluid

$$\delta P(r) = \frac{\delta\rho(r)}{\kappa N}. \tag{6.14}$$

This last expression is the definition of the *compressibility* κ of the material. In equilibrium, the force associated with the induced pressure gradients cancel out the external force, and therefore

$$0 = -\vec{\nabla}\delta P + N\mathcal{F}$$

from which we conclude

$$\langle\delta\rho(r)\rangle = -N^2\kappa\varphi(q,0)e^{\mathbf{i}q\cdot r} + h.c..$$

Comparing with our expression for $\delta\rho$ in terms of G^R, we learn that in the regime where this hydrodynamic description is valid

$$G^R_{\rho\rho}(q,0) \overset{q\to 0}{\to} -N^2\kappa = -\frac{N}{mv_s^2}. \tag{6.15}$$

In the last step we used the fact that the macroscopic description knows about sound waves[30].

[30]Here's a reminder about how this happens. It involves only two ingredients: (1) the continuity equation for the number density, which says particles do not disappear

$$0 = \dot{\rho} + \vec{\nabla}\cdot\vec{J} = \dot{\rho} + \vec{\nabla}\cdot(\rho\vec{u})\,. \tag{6.16}$$

(2) Newton's law in the form

$$-\vec{\nabla}p = m\rho\frac{D\vec{u}}{Dt} = m\rho\left(\partial_t\vec{u} + (\vec{u}\cdot\vec{\nabla})\vec{u}\right) \tag{6.17}$$

(which is called Euler's equation). The second term in the convective derivative we will ignore because we are going to expand to linear order about the static configuration where $\rho = \rho_0$ and $\vec{u} = 0$. Let $\rho = \rho_0(1+s)$ where s is small. Let's focus on one dimension for simplicity. The continuity equation then says to linear order that $\partial_x u = -\partial_t s$. Euler's equation (6.17) says

$$\partial_t u = -\frac{\partial_x p}{m\rho} = -\frac{1}{m\kappa N}\partial_x s.$$

In the second step, we used the definition (6.14) of the compressibility κ and the chain rule. Taking

Combining (6.15) with the relation between G^R and S (6.11) we learn the long-heralded compressibility sum rule

$$\frac{N}{2mv_s^2} = -\frac{1}{2}\lim_{q\to 0} G^R_{\rho\rho}(q,0) = -\frac{1}{2}\lim_{q\to 0}\left(\mathrm{Re}G^R_{\rho\rho}(q,0) + \mathbf{i}\mathrm{Im}G^R_{\rho\rho}(q,0)\right) \tag{6.18}$$

$$= -\frac{1}{2}\lim_{q\to 0}\int_0^\infty d\omega' S(q,\omega')P\left(\frac{2\omega'}{0-\omega'^2}\right) \tag{6.19}$$

$$= \lim_{q\to 0}\int_0^\infty d\omega \frac{S(q,\omega)}{\omega} \tag{6.20}$$

(the third step uses (6.12), and (6.13) to see that for static perturbations, $\mathrm{Im}\, G^R$ vanishes).

$\partial_x(BHS)$ then gives

$$\ddot{s} = \frac{1}{m\kappa N}\partial_x^2 s$$

so $v_s^2 = \frac{1}{m\kappa N}$. Note that this is the isothermal sound speed, since this whole discussion happened at fixed temperature ($T = 0$ in fact).

7 Atoms, Molecules, Solids

[Commins, Tong]

Atoms. There are three kinds of atoms.

- Hydrogen is exactly solvable and we understand everything about it.
- Helium is just barely solvable.
- Then there is Everything Else.

The key to our understanding of Everything Else is the Central Force Approximation (CFA). It is just like mean field theory: the idea is to approximate the force on a given electron (from the nucleus *and* all of the other electrons) by some average force, which is also spherically-symmetric about the nucleus. There are several methods to figure out what we should use for this effective potential, which are the subject of §7.1.

A piece of physics which immediately falls out of this approximation is *screening*. The presence of the $N-1$ other electrons of charge $-e$ will screen the electric field of the charge $+Ze$ nucleus. The form of the resulting potential must look like $\frac{Ze}{r}$ for very small r (when no other electrons are enclosed in the sphere of radius r), and like $\frac{(Z-(N-1))e}{r}$ for very large r (when all the others are enclosed). It can be written in the form

$$V_{\text{eff}} = -\frac{Z(r)e^2}{r},$$

where $Z(r)$ starts at Z at $r=0$ and decays to $Z-N+1$ at large r. We'll see that screening is a key ingredient in the structure of the periodic table.

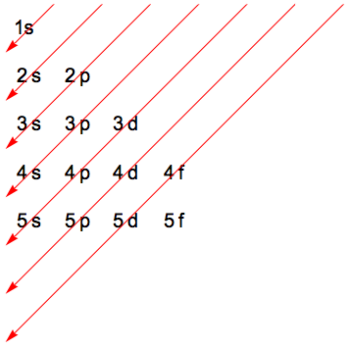
Hydrogen reminder. Since we're going to work with spherically-symmetric potentials which often fall off like $1/r$, hydrogen wavefunctions will be useful. Recall that the eigenstates of $\mathbf{H} = \frac{p^2}{2m} - \frac{Ze^2}{r}$ are labelled by three quantum numbers (n,l,m) where $n = 1,2,3...$, $l = 0 \ldots n$, $m = -l, -l+1 \ldots l-1, l$. l, m are orbital angular momentum quantum numbers. And we use this dumb spectroscopic notation that $l=0$ is called s, $l=1$ is called p, $l=2$ is called d, $l=3$ is called f. The energy spectrum only depends on n, $E_n = -\frac{Z^2}{2n^2}$ (in atomic units $m_e = 1 = e^2$) – it is completely independent of the angular momentum, so there is a huge degeneracy (broken by small effects such as relativity and coupling to nuclear spin). The groundstate energy (of the (1,0,0) state) in the right units is $-\frac{Z^2}{2}$.

$Z > 1$ atoms. A good approximation to the hamiltonian of all atoms is

$$\mathbf{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_i V_{\text{nucl}}(r_i) - \sum_{i<j} V_{\text{int}}(r_{ij}), \quad V_{\text{nucl}}(r) = \frac{-Z}{|r|}, \quad V_{\text{int}}(r) = \frac{1}{|r|}.$$

(It ignores relativistic corrections, nuclear spin, spin-orbit couplings, all of which we understand well, in the case of hydrogen at least, but which give small effects.) There is no dependence on the electron spin.

To get started, we will treat the interactions between electrons as a perturbation. Then at zeroth order, we just fill orbitals of hydrogen (with $e^2 \to Ze^2$ as above). There is a big degeneracy because of the weird accidental fact that $E_{\text{hydrogen}}(n,l)$ only depends on n. In fact there is a specific order in which these orbitals are filled (which is called aufbau), shown at right. What picks this order?



Helium ground state. To begin let's think about helium, $Z = 2$. The ground-state, to zeroth order in the interactions, is

$$\Psi(r_1, r_2) = \psi_{100}(r_1)\psi_{100}(r_2), \quad \text{with} \quad \psi_{100}(r) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0}. \tag{7.1}$$

Can I put the two electrons in the same orbital? Yes because they carry spin: I can do this as long as the spin wavefunction is antisymmetric. So the actual wavefunction is what I wrote above times the spin singlet. This has $E_0^{(0)} = 2\,(-Z^2/2)\,|_{Z=2} = -4$ in atomic units. The experimental result is -2.903 in these units.

We can improve the result by a little perturbation theory in the ee interaction term:

$$\Delta E_0^{(1)} = \langle 100|\,\langle 100|\,\frac{1}{r_{12}}\,|100\rangle\,|100\rangle = \frac{5}{8}Z = \frac{5}{4}.$$

I do not want to spend time talking about this integral, but you can do it using the partial-wave expansion

$$\frac{1}{|r_{12}|} = \frac{1}{r_>} \sum_{\ell=0}^{\infty} P_\ell(\cos\theta) \left(\frac{r_<}{r_>}\right)^\ell$$

where θ is the angle between $\vec{r}_1$ and $\vec{r}_2$, and $r_> = \max(|r_1|, |r_2|)$.

We can do even better using the variational method. A good idea is to let Z vary. This is a way to allow for screening. Instead of (7.1), we'll try $\psi(r) \propto e^{-\lambda r/a_0}$, and treat λ as a variational parameter. We find (by exactly the same calculation which I just skipped over)

$$\langle \mathbf{H} \rangle_\lambda = Z^2 - 2Z\lambda + \frac{5}{8}\lambda$$

which is minimized by $\lambda_{\min} = Z - \frac{5}{16}$ with

$$\langle \mathbf{H} \rangle_{\lambda_{\min}} = -\left(Z - \frac{5}{16}\right)^2 = -2.85 \tag{7.2}$$

which is not bad at all. This method does even better for larger-Z ions with two electrons[31]. The lesson from this calculation is that the charge of the nucleus is screened by the other electrons.

Helium excited states. There are also some lessons to be learned from the excited states of helium. The orbital wavefunction must involve one electron in the (100) state (call it α) and one in one of the $(2lm)$ states, of which there are 4 (1 state with $l = 0$ and 3 with $l = 1$), which we'll call β. So, including spin, there are actually 16 degenerate states. Fortunately, they are organized by symmetries – the states with different l cannot be mixed with each other by the rotation-invariant hamiltonian. And **H** is completely independent of the spin.

As in our discussion of the exchange interaction, we can organize these states into symmetric and antisymmetric orbitals $\Psi_{S/A}(r_1 r_2) = \frac{1}{\sqrt{2}}(\psi_\alpha(r_1)\psi_\beta(r_2) \pm \psi_\beta(r_1)\psi_\alpha(r_2))$. To make a fermion state, the spin wavefunction must have the opposite symmetry property, so the allowed states are: $\Psi_A \otimes$ triplet , $\Psi_S \otimes$ singlet. Again the hamiltonian is spin-independent, so just as before the variational energies are just

$$E_{S/A} = \epsilon_\alpha + \epsilon_\beta + I \pm J$$

where the exchange integral is

$$J = \int\int \psi_\alpha(r_1)\psi_\beta(r_2)\frac{1}{|r_1 - r_2|}\psi_\beta(r_1)\psi_\alpha(r_2) = \int\int \psi_\alpha(r_1)\psi_\beta(r_1)\frac{1}{|r_1 - r_2|}\psi_\alpha(r_2)\psi_\beta(r_2)$$

where I used the fact that these wavefunctions are real. I claim that $J \geq 0$. Recall from E&M that $\vec{\nabla}^2\phi = -4\pi\rho$ is solved by $\phi(r) = \int \frac{\rho(r')d^3r'}{|r-r'|}$. If we let $4\pi\rho(r_1) = \psi_\alpha(r_1)\psi_\beta(r_1)$, then

$$J = \int d^3r\phi(r)4\pi\rho(r) = -\int \phi\vec{\nabla}^2\phi \stackrel{\text{IBP}}{=} \int \left(\vec{\nabla}\phi\right)^2 \geq 0.$$

The intuition is that the AS wavefunction has lower interaction energy, since $\Psi_A(r_1 = r_2) = 0$ so it avoids the region where $\frac{1}{|r_1-r_2|}$ is large. So the triplets have lower energy than the singlets.

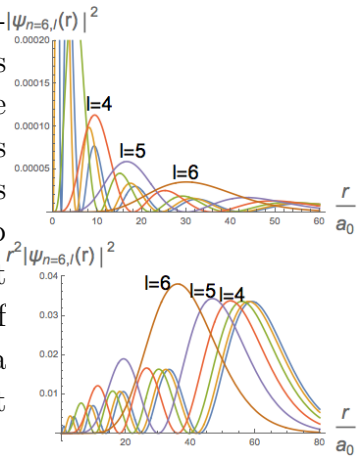
[31] What about the smaller-Z ion? That is, let's try to add a second electron to hydrogen, to get H^-. The calculation (7.2) predicts $\langle H\rangle = -.528$, which is larger than the groundstate energy of neutral H (E = -1/2) plus the electron at infinity (E=0), which gives $E = -.5$. However, there actually *is* a (weakly bound) boundstate of H^-, with $E = -.528$. A better variational ansatz, which incorporates the fact that only the inner electron does screening, is of the form

$$\psi(r_1, r_2) \propto e^{-\lambda(sr_> + r_<)}$$

where $r_> = \max(r_1, r_2)$, $r_< = \min(r_1, r_2)$, and both s and λ are variational parameters. For $Z = 1$, this gives $\langle H\rangle = -.506$. This calculation *proves* the existence of such a boundstate, since it gives an upper bound on the energy. Thanks to Jiashu Han for asking about this.

But what about $2s$ versus $2p$? Well it turns out that $(I \pm J)_{2s} < (I \pm J)_{2p}$. So the $2s$ is lower energy than $2p$ (just like in the periodic table).

I will not dwell on why this is true because the correct explanation for aufbau is not here. The correct explanation is that the larger-l hydrogen orbitals have less weight near the origin. This means that the effective potential they see is more highly screened, and therefore they are less bound. As you can see at right, this statement is a little subtle. The top figure shows the squares of the $n = 6$ functions. But what really matters is the measure, which has an extra factor of r^2; this is plotted in the bottom figure, and there the maxima actually move in as l increases. However, it is still true that the support near the origin *decreases* as l increases.



7.1 Self-consistent mean-field theories

This is a subject which seems fancy and which involves lots of names of people, but the names really each refer to a very simple, sometimes quite dumb, variational ansatz for the wavefunction.

Hartree. The Hartree ansatz is just a product state: $\Psi = \psi_{\alpha_1}(r_1) \cdots \psi_{\alpha_N}(r_N)$. This is often a ridiculous thing to do. It ignores Fermi statistics! We could at least pacify Pauli by taking $\alpha_i \neq \alpha_j$. But often it's not so bad (as we saw above) because we can tensor it with an appropriate spin wavefunction. Using the CFA, we could label these orbitals by hydrogen quantum numbers (n, m, l), but I'll continue to use the composite index α (which includes spin).

The idea is that we treat the ψs themselves (the whole single-particle wavefunction) as variational parameters. The variational energy is

$$\langle \mathbf{H} \rangle = \sum_{i=1}^{N} \int d^3r \left(\frac{\hbar^2}{2m} |\vec{\nabla} \psi_{\alpha_i}|^2 - \frac{Z}{r} |\psi_{\alpha_i}(r)|^2 \right) + \sum_{i<j} \int d^3r \int d^3r' \frac{\psi^\star_{\alpha_i}(r) \psi^\star_{\alpha_j}(r') \psi_{\alpha_j}(r') \psi_{\alpha_i}(r)}{|r - r'|}.$$

To keep the states normalized, the thing we can vary freely should have Lagrange multipliers:

$$F[\psi] = \langle \mathbf{H} \rangle - \sum_i \epsilon_i \left(\int |\psi_i|^2 - 1 \right).$$

Its variation is

$$0 \stackrel{!}{=} \frac{\delta F}{\delta \psi^\star_{\alpha_i}} \tag{7.3}$$

$$= \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{Z}{r} + \sum_{j\neq i} \int d^3r' \frac{|\psi_{\alpha_j}(r)|^2}{|r-r'|} \right) \psi_{\alpha_i}(r) - \epsilon_i \psi_{\alpha_i}(r). \tag{7.4}$$

This looks just like the Schrödinger equation, with energy eigenvalue $\epsilon = \epsilon_i$, and

$$V_{\text{eff}}(r) = -\frac{Z}{r} + U_{\alpha_i}(r)$$

with

$$U_{\alpha_i} = \sum_{j\neq i} \int d^3r' \frac{|\psi_{\alpha_j}(r)|^2}{|r-r'|} \tag{7.5}$$

representing the electrostatic repulsion of the $N-1$ other electrons. Notice that it depends on the ψ_{α_j}s! It's hard to know where to start to solve these horrible coupled equations. But actually there's a strategy that works pretty well.

1. Make a guess for some spherically-symmetric function $U_{\alpha_i}(r)$.
2. Solve (7.4) and find the ψ_{α_i}.
3. Determine the U_{α_i} from (7.5).
4. Construct a spherically-symmetric version of it by averaging: $U_{\text{round}}(|r|) \equiv \frac{1}{4\pi}\int d\Omega U(r)$.
5. Redo the previous steps, starting from U_{round}.

This procedure will actually converge, given a reasonable starting point. The output is a set of ϵ_i and a set of optimal occupied single particle states ψ_{α_i}. The variational estimate for the groundstate energy is not quite just $\sum_i \epsilon_i$, but rather

$$E_0 \leq \langle \mathbf{H} \rangle = \sum_i \epsilon_i - \sum_{j\neq i} \int\int \frac{|\psi_{\alpha_i}(r)|^2 |\psi_{\alpha_j}(r')|^2}{|r-r'|}.$$

Hartree-Fock. This improvement, due to Slater and Fock actually starts with an allowed electron wavefunction:

$$|\Psi\rangle = \mathbf{a}^\dagger_{\alpha_1} \cdots \mathbf{a}^\dagger_{\alpha_N} |0\rangle$$

where $\alpha = (n, l, m, \sigma)$ is a composite label for all the quantum numbers. That is, the ansatz for the wavefunction is a Slater determinant

$$\Psi(r_1\sigma_1 \cdots r_N\sigma_N) = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \psi_{\alpha_1}(r_1) & \cdots & \psi_{\alpha_1}(r_N) \\ \vdots & \ddots & \vdots \\ \psi_{\alpha_N}(r_1) & \cdots & \psi_{\alpha_N}(r_N) \end{pmatrix}.$$

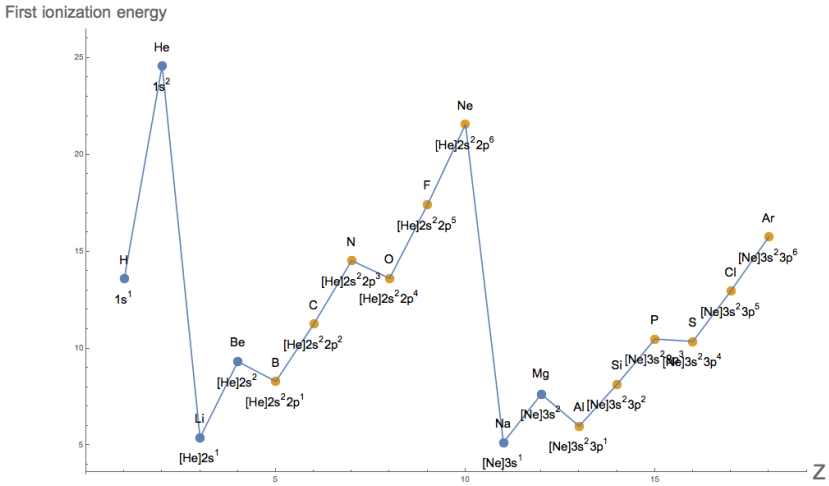
By just the kind of calculation we've been doing all quarter, the energy expectation is

$$\langle \mathbf{H} \rangle = \langle \mathbf{H} \rangle_{\text{Hartree}} - \sum_{i<j} \int d^3r \int d^3r' \frac{\psi_{\alpha_i}(r)\psi_{\alpha_j}(r')\psi_{\alpha_i}(r')\psi_{\alpha_j}(r)}{|r-r'|} \delta_{\sigma_i\sigma_j}.$$

This extra term $J_{ij} \geq 0$ is exactly the exchange integral we encountered above. It only appears when the electrons involved have the same spin, since otherwise they are distinguishable. Its physical origin is in the form of the pair correlator for free fermions (1.85) (again, only of the same spin)– because of Fermi statistics, the electrons avoid each other. This means that each electron is surrounded by an 'exchange hole,' which lowers its Coulomb energy. By the same argument as above $J_{ij} \geq 0$. So this term *lowers* the energy when the spins are aligned. In the context of materials, this leads to (Slater) ferromagnetism.

This rule in the context of chemistry is named after Hund. It makes predictions for the binding energies as a function of Z. In particular, when a shell is half-filled, all of the electrons in the valence shell can have the same spin, and benefit from the exchange energy term. Adding one more electron requires it to have the opposite spin, and there should therefore be a decrease in the binding energy.

This is borne out by the plot at right of the first ionization energies (the energy cost to remove one electron) as a function of Z, which shows *e.g.* a step between nitrogen and oxygen where the $2p$ orbital goes from half-filled (N is [Be]$2p^3$) to one-more-than-half-filled (O is [Be]$2p^4$). There is a similar step between phosphorus and sulfur during the filling of the 3p shell.



Incidentally, I made this plot with Mathematica, which knows all of this information through the command 'ElementData'.

Again we can treat the ψs as variational parameters. The Hartree-Fock equations

(obtained by varying the energy expectation value plus Lagrange multipliers) is

$$0 \stackrel{!}{=} \frac{\delta}{\delta\psi^\star_{\alpha_i}}\left(\langle \mathbf{H}\rangle - \sum_i \epsilon_i\left(\int |\psi_i|^2 - 1\right)\right) \tag{7.6}$$

$$= \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{Z}{r} + U_{\alpha_i}(r)\right)\psi_{\alpha_i}(r) - \sum_j \delta_{\sigma_i\sigma_j}\int d^3r' \frac{\psi^\star_{\alpha_j}(r')\psi_{\alpha_i}(r')}{|r-r'|}\psi_{\alpha_j}(r) - \epsilon_i\psi_{\alpha_i}(r). \tag{7.7}$$

The extra term relative to the Hartree equations (7.4) (associated with the exchange term in the energy) is like a nonlocal potential. It represents an attractive charge density of electrons with the same spin.

To emphasize the unity of methods between atomic physics and all of our previous discussion of many-body systems, let's re-derive the Hartree-Fock(-Slater) equations (7.7) using an auxiliary (quadratic) mean-field Hamiltonian, as explained more systematically in §5.6. The actual hamiltonian is

$$\mathbf{H} = \sum_r \mathbf{a}^\dagger_r\left(-\frac{\vec{\nabla}^2}{2m} + V_{\text{ext}}(r)\right)\mathbf{a}_r + \sum_{r<r'} V(r,r')\mathbf{a}^\dagger_r\mathbf{a}^\dagger_{r'}\mathbf{a}_{r'}\mathbf{a}_r \equiv \mathbf{T} + \mathbf{V}_{\text{ext}} + \mathbf{V},$$

where here V_{ext} is the potential from the nucleus, and $V(r,r')$ is the electron-electron interaction. We want to find the *gaussian* state $\prod_\alpha \mathrm{d}^\dagger_\alpha\left|\tilde{0}\right\rangle$ with the lowest expected energy. Such a state is the groundstate of some quadratic hamiltonian. So let

$$\mathbf{H}_{\text{MF}} = \sum_r \mathbf{a}^\dagger_r\left(-\frac{\vec{\nabla}^2}{2m} + V_{\text{ext}}(r) + U(r)\right)\mathbf{a}_r + \sum_{r,r'}\mathbf{a}^\dagger_r\Gamma_{rr'}\mathbf{a}_{r'}.$$

This contains an in-general non-local hopping term Γ, which we will see is required by the exchange term. The potentails $U_r, \Gamma_{rr'}$ are to be determined.

All expectation values below are evaluated in the groundstate of $\mathbf{H}_{\text{MF}}$, so we can use Wick's theorem:

$$\langle\mathbf{H}\rangle = \langle\mathbf{T}\rangle + \langle\mathbf{V}_{\text{ext}}\rangle + \sum_{r<r'} V(rr')\left(\left\langle\mathbf{a}^\dagger_r\mathbf{a}_r\right\rangle\left\langle\mathbf{a}^\dagger_{r'}\mathbf{a}_{r'}\right\rangle - \left\langle\mathbf{a}^\dagger_r\mathbf{a}^\dagger_{r'}\right\rangle\left\langle\mathbf{a}^\dagger_{r'}\mathbf{a}_r\right\rangle\right)$$

where I have assumed that $\left\langle\mathbf{a}^\dagger\mathbf{a}^\dagger\right\rangle = 0$ – no superconductivity. Its variation with respect to the choice of orbitals and filling of $|\text{MF}\rangle$ is

$$\delta\langle\mathbf{H}\rangle = \delta\langle\mathbf{T}\rangle + \delta\langle\mathbf{V}_{\text{ext}}\rangle + 2\sum_{r<r'} V(rr')\left(\left\langle\mathbf{a}^\dagger_r\mathbf{a}_r\right\rangle\delta\left\langle\mathbf{a}^\dagger_{r'}\mathbf{a}_{r'}\right\rangle - \left\langle\mathbf{a}^\dagger_r\mathbf{a}^\dagger_{r'}\right\rangle\delta\left\langle\mathbf{a}^\dagger_{r'}\mathbf{a}_r\right\rangle\right).$$

We want this to vanish in order to give the best trial wavefunction. On the other and, since $|\mathrm{MF}\rangle$ is its groundstate, the variation of $\langle \mathbf{H}_{\mathrm{MF}} \rangle$ is zero:

$$0 = \delta \langle \mathbf{H}_{\mathrm{MF}} \rangle = \delta \langle \mathbf{T} \rangle + \delta \langle \mathbf{V}_{\mathrm{ext}} \rangle + \sum_r U(r) \delta \left\langle \mathbf{a}_r^\dagger \mathbf{a}_r \right\rangle + \sum_{rr'} \Gamma_{rr'} \delta \left\langle \mathbf{a}_r^\dagger \mathbf{a}_{r'} \right\rangle .$$

Therefore

$$U(r) = \sum_{r'} V_{rr'} \left\langle \mathbf{a}_{r'}^\dagger \mathbf{a}_{r'} \right\rangle \tag{7.8}$$

$$\Gamma_{rr'} = V_{rr'} \left\langle \mathbf{a}_{r'}^\dagger \mathbf{a}_r \right\rangle . \tag{7.9}$$

The HFS equations (7.7) are just the eigenvalue equations for $\mathbf{H}_{\mathrm{MF}}$ with the potentials determined by these self-consistency conditions.

Thomas-Fermi. I would be remiss if I didn't mention one more, simpler approximation. It is useful when there are very many particles, such as in a large-Z atom (say $Z > 10$), or in a metal. It is useful also for electron stars and neutron stars and solids and nuclei and molecules and cold atoms. The idea is to treat the electrons as a fluid, whose density is determined locally by the potential.

To see how this might happen, recall the free electron gas, in free space, in equilibrium at temperature T. The number of electrons per unit volume with momentum near p is

$$dn = 2 \frac{\text{đ}^3 p}{e^{\frac{\epsilon_p - \mu}{T}} + 1} = 2 f(p) \, \text{đ}^3 p. \tag{7.10}$$

The 2 is for spin. As $T \to 0$, the Fermi function approaches a step function $f(p) = \begin{cases} 0, & |p| > p_F \\ 1, & |p| < p_F \end{cases}$. Thus the number density is

$$n = 2 \int \text{đ}^3 p f(p) \overset{T=0}{=} \frac{p_F^3}{3\pi^2}$$

and the kinetic energy density is

$$u = 2 \int \text{đ}^3 p \frac{p^2}{2m} f(p) \overset{T=0}{=} \frac{3^{5/3} \pi^{4/3}}{\pi} \frac{\hbar^2}{m_e} n^{5/3}.$$

Now subject this system to a *slowly-varying* potential, $V(r) = -e\Phi(r)$. In the hamiltonian, the potential and the chemical potential only appear in the combination

$\mu + V(r)$. So the idea is just to replace $\mu \to \mu + V(r)$ in the expression for the phase-space density (7.10). It is an assumption of *local equilibrium*, generally a synonym for *hydrodynamics*. Local equilibrium means that nearby patches of fluid are in equilibrium, including chemical equilibrium. But chemical equilibrium means the μ is the same. Therefore, μ is constant, and in our replacement

$$\mu = \epsilon_F = \frac{p_F^2}{2m} \quad \to \quad \mu \equiv \frac{p_F^2(r)}{2m} - e\Phi(r)$$

we see that we must let $p_F = p_F(r)$ the Fermi momentum vary with position. This gives (assuming spherical symmetry of the applied potential and everything else)

$$n(r) = \int_0^{p_F(r)=2m\sqrt{e\phi+\mu}} 2p^2 dp 4\pi = \frac{(2m)^{3/2}}{3\pi^2} \left(e\Phi(r) + \mu\right)^{3/2}.$$

So this is a relation between the density and the electrostatic potential. There is a second relation, namely Gauss' law. For example, in the case of the electron cloud around a nucleus

$$\vec{\nabla}^2 \Phi = en(r) - Ze\delta^3(r).$$

Defining $e\Phi_0 \equiv e\Phi + \mu$, we have

$$\vec{\nabla}^2 \Phi_0 = e\alpha \Phi_0^{3/2}$$

(here $\alpha \equiv \frac{(2m)^{3/2}}{3\pi^2}$) with the boundary conditions that near the nucleus, the only charge is the nuclear charge: $\Phi_0(r) \stackrel{r\to 0}{\to} \frac{Ze}{4\pi r}$. (The boundary condition at $r \to \infty$ specifies the number of electrons.) By non-dimensionalizing this equation, we can learn that the sizes of atoms go like $Z^{-1/3}$. To see how, look at Commins §12.4.

To slick up our understanding of the TF approximation, note that we can get the above equations by minimizing the functional

$$F[n] = E_0[n] - \mu \left(\int d^3 r n(r) - N \right).$$

Here the groundstate energy, in this approximation is

$$E_0[n] = c \int d^3 r n(r)^{5/3} + \int \frac{Ze^2 n(r)}{r} d^3 r + \frac{e^2}{2} \int\int \frac{n(r)n(r')}{|r-r'|} - \mu \left(\int n - N \right). \quad (7.11)$$

Its variation is

$$0 = \frac{\delta F[n]}{\delta n(r)} = \frac{5}{3} c n^{2/3}(r) - \mu - e\Phi(r), \quad \text{with} \quad \nabla^2 \Phi(r) = en(r) - Ze\delta^3(r).$$

Thomas-Fermi screening. As a tiny hint of the applications of this perspective, let us see what it says about screening. Let us imagine applying an *infinitesimal* extra electrostatic potential $\delta\phi$ to our system. It satisfies Gauss' law:

$$-\vec{\nabla}^2\delta\phi = -4\pi e\left(n_{\rm ind}(r)\right). \tag{7.12}$$

On the RHS here is some recognition that the charges will move around in response to the applied field. (And I am writing an equation for just the *additional* potential, so we do not include on the RHS the equilibrium distribution, or *e.g.* the nuclear charge, only the *induced* charge.) If $\delta\phi$ is small, we may use linear response:

$$n_{\rm ind}(q,\omega) = -\chi(q,\omega)e\delta\phi(q,\omega)$$

where χ is the compressibility (defined by this relation). Now use the TF approximation (with α as above):

$$n(r) = \alpha\left(\mu + e(\Phi(r)+\delta\phi(r))\right)^{3/2} \tag{7.13}$$

$$= n_0 + \frac{\partial n}{\partial\mu}e\delta\phi(r) + \mathcal{O}(\delta\phi^2)\ . \tag{7.14}$$

So in this approximation, $n_{\rm ind}(r) = -\chi_0 e\delta\phi(r)$ where $\chi_0 = -\partial_\mu\int^\mu d\epsilon g(\epsilon) = -g(\epsilon)$, where $g(\epsilon)$ is the density of states. But then we also have Gauss' law:

$$-\vec{\nabla}^2(\Phi+\delta\phi) = -4\pi e n_0 + 4\pi e^2\chi_0\delta\phi.$$

The solution of this equation goes like

$$\delta\phi(r) \sim \frac{e^{-q_{\rm TF}r}}{r}$$

with $q_{\rm TF}^2 = 4\pi e^2|\chi_0|$. It says that as a result of screening, in this approximation, the Coulomb law is replaced by an exponentially decaying potential, and hence force. The correct answer is not quite so extreme and more interesting. In particular, in a metal, it behaves like $\frac{\cos 2k_F r}{r^3}$.

Warnings. These methods are widely used and very successful. The Hartree-Fock approximation makes precise what people mean when they speak of filling hydrogen orbitals in an interacting system. However, the true groundstate need not be a single Slater determinant (the fermion analog of a product state): it will almost certainly be a complicated superposition of such states, meaning that the electrons will be entangled. But, approximating the effect of all the other electrons as a central potential is clearly a truncation. Also, we are ignoring spin-orbit coupling, which grows like Z^2 along columns of the periodic table.

7.2 Problems involving more than one nucleus

So far in this chapter we've been discussing ways to deal with the interactions between two or more electrons orbiting a single nucleus of charge Z. We've mostly focussed on neutral atoms, but the same methods apply if the number of electrons is not equal to Z. The periodic table is an important part of chemistry. Another important part is chemical bonding, whereby one atom sticks to another. We could understand something about this, too, if we had time.

Born-Oppenheimer approximation. Nuclei are much (at least 2000 times) heavier than electrons. This fact is what allows us to make progress on problems with more than one nucleus, such as molecules (a few nuclei) or solids (many many nuclei). The idea is: first treat the positions R of the nuclei as fixed. Solve for the groundstate energy of the electron system in the potential $V_{\rm ext}(r)$ created by the nuclei, $E_0(R)$. Now minimize this over R to find where the nuclei want to be.

We can check a posteriori that this was a good approximation using dimensional analysis and the uncertainty principle. The electronic coordinates satisfy $\Delta x \Delta p \sim 1$; an atom has size $\Delta x \sim a_0$, so $\Delta p \sim 1/a_0$, and the electronic energies go like $E_e \sim \frac{\Delta p^2}{2m_e} = \frac{\hbar^2}{2ma_0^2} = 1$ (in atomic units, naturally). How much energy does it cost to excite the nuclei? Near the minimum of $E_0(R)$ it is a harmonic oscillator, so $E_{\rm vib} \sim M\omega^2 x^2$. Dissociation happens when $x \sim 1$ and costs energy $\sim E_e \sim 1 \sim M\omega^2$. Therefore the splittings between (SHO) vibrational levels go like $\Delta E_{\rm vib} = \hbar\omega \sim \sqrt{\frac{m_e}{M}}$. What about rotational motion? $E_{\rm rot} = \frac{\hbar^2 \ell(\ell+1)}{MR_0^2}$ where R_0 is the optimal separation between nuclei, also of order $R_0 \sim a_0 = 1$. So the rotational splittings have $\Delta E_{\rm rot} \sim \frac{m_e}{M}$, which is of order 10^{-3} or smaller.

So, given $V_{\rm ext}(r)$, we want to find the groundstate of

$$\mathbf{H} = \mathbf{T} + \mathbf{V} + \int d^d r V_{\rm ext}(r) n(r)$$

where $\mathbf{T} = \sum_i \frac{\mathbf{p}_i^2}{2m}$ and $\mathbf{V} = \sum_{i<j} V_{\rm int}(r_{ij})$. Notice that the first two terms are the same for all of these problems, wherever the nuclei are. And the input external potential (by which all these problems differ) only enters multiplying the density $n(r)$. We usually think of doing this by finding the groundstate wavefunction Φ_0, and then determining the density through

$$n(r) = \sum_\sigma n_\sigma(r) = \langle \Phi_0 | \, \psi^\dagger_{r\sigma} \psi_{r\sigma} \, | \Phi_0 \rangle \, . \tag{7.15}$$

Weirdly, it is also true that the density determines the groundstate wavefunction, and hence the groundstate energy. That is, different $V_{\rm ext}$ necessarily give rise to different groundstate electron densities $n(r)$. The proof (due to Kohn) is sweet: Suppose otherwise, *i.e.* suppose $V_{\rm ext}$ and $V'_{\rm ext}$ (with groundstates Φ_0, Φ'_0) lead to the same $n(r)$.

Assuming the groundstate is nondegenerate, the variational theorem says

$$E_0 = \langle\Phi_0|\,\mathbf{H}\,|\Phi_0\rangle < \langle\Phi_0'|\,\mathbf{H}\,|\Phi_0'\rangle = \langle\Phi_0'|\,\mathbf{H}'\,|\Phi_0'\rangle + \langle\Phi_0'|\,(\mathbf{V}-\mathbf{V}')\,|\Phi_0'\rangle = E_0' + \int n'\,(V_{\text{ext}} - V_{\text{ext}}')\,.$$

But the same is true with the primes and unprimes switched:

$$E_0' < E_0 + \int n\,(V_{\text{ext}}' - V_{\text{ext}})\,.$$

Adding the previous two equations says, with strict inequality,

$$\int n\,(V_{\text{ext}}' - V_{\text{ext}}) < \int n'\,(V_{\text{ext}}' - V_{\text{ext}})$$

which forbids $n = n'$.

This means that the groundstate energy E_0 and the many-body wavefunction $\Phi_0(r_1 \cdots r_N)$ are purely functionals of $n(r)$, a single function of d variables. Appreciate for a moment how crazy this is. (A case where it is manifestly true is when there is only one particle: then $\psi(r) = \sqrt{n(r)}$, and we lose no information since $\psi(r)$ has no nodes.)

Moreover, the n which minimizes the energy expectation is the correct one. Here's why: suppose $n(r)$ arises from some state $\Psi[n]$ by (7.15). Then

$$E_0[n] = \langle\Psi[n]|\,(\mathbf{T}+\mathbf{V})\,|\Psi[n]\rangle + \int V_{\text{ext}} n \equiv E_{\text{int}}[n] + \int V_{\text{ext}} n. \tag{7.16}$$

But by the variational theorem

$$E_0[\text{any other } n \text{ which comes from a } |\Psi\rangle] > E_0[n_0],$$

where n_0 is the density in the true groundstate. Notice that the minimization of (7.16) then describes a Legendre transform of a *fixed, universal* functional $E_{\text{int}}[n]$, which is the same form any atom or molecule or solid (the information about which only enters through V_{ext}). It is like a philosopher's stone. This realization leads to the development called Density Functional Theory, which proceeds further by approximating the functional in various ways. The simplest is the Thomas-Fermi approximation, where $E_{\text{int}}[n] = c\int n^{5/3}(r)d^3r + \frac{e^2}{2}\int\int \frac{n(r)n(r')}{|r-r'|}$ as in (7.11). The next simplest possibility is called the *local density approximation*, developed by Kohn and Lu Sham, with spectacular success in determining electronic structure for many situations[32].

[32] For more, try Chapter 15 of the book by Girvin and Yang, *Modern Condensed Matter Physics*. I found this history of Kohn's path towards the discovery of DFT quite compelling. This paper by Banks also provides a well-encapsulated introduction.