Notes for Physics 217B

Leon Balents

Leon Balents[*]

UCSB

January 16th, 2018 – March 15th, 2018

Contents

[*]balents@kitp.ucsb.edu

List of Figures

1 What this course is about

Lecture 1 (1h 15mins)
January 16th, 2018

This is the second quarter of a course on quantum many body physics. The focus is on *fermions*, and matter built up from them. This is a pretty important subject since electrons are fermions, and the most quantum objects in ordinary matter are electrons. We will cover phenomena that occur uniquely with fermions, as well as methodology for studying fermionic systems.

2 Second quantization

We will heavily rely on the use of second quantization for fermions, as we did for bosons in the previous quarter. I assume you have seen this before in some previous class. Many good reviews are available. A compact discussion is given for example in Negele and Orland's book on *Quantum Many Body Physics*. Here we will just review the subject and make a few conceptual points.

2.1 *Bosons*

First let us remind ourselves how it all works for bosons (see also Sec.6.1 of my notes for 217a). We define boson annihilation operators a_i and creation

operators $a_i^\dagger$, which obey commutation relations

(1) $\quad [a_j, a_k^\dagger] = \delta_{jk},$

and

(2) $\quad [a_j, a_k] = 0, \qquad [a_j^\dagger, a_k^\dagger] = 0.$

These relations define the algebra of these operators. It does not immediately tell us the space of states these operators act on. Formally I guess this corresponds to choosing a representation of this algebra. The minimal one is the standard one we now describe. We can define number operators

(3) $\quad \hat{n}_j = a_j^\dagger a_j.$

and a good basis for the "Fock space" is the set of eigenstates of these operators:

(4) $\quad \hat{n}_j |n_1 n_2 \cdot n_N\rangle = n_j |n_1 n_2 \cdot n_N\rangle,$

where we define these number eigenstates to be normalized. We can explicitly construct these states by action on the vacuum, using the recursion relations

(5) $\quad a_j^\dagger |n_1 \cdots n_j \cdots n_N\rangle = \sqrt{n_j + 1} |n_1 \cdots n_j + 1 \cdots n_N\rangle.$

From this we can obtain

(6) $\quad |n_1 \cdots n_j \cdots n_N\rangle = \dfrac{1}{\sqrt{n_1! \cdots n_N!}} (a_1^\dagger)^{n_1} \cdots (a_N^\dagger)^{n_N} |0\rangle.$

Where $|0\rangle$ is the "vacuum" state of no particles, which is annihilated by all annihilation operators:

(7) $\quad a_j |0\rangle = 0.$

Eqs. (6,7) might be regarded as the definition of the basis states. We also have

(8) $\quad a_j |n_1 \cdots n_j \cdots n_N\rangle = \sqrt{n_j - 1} |n_1 \cdots n_j - 1 \cdots n_N\rangle.$

These relations are proved by using the fact that $[a_j^\dagger, \hat{n}_j] = a_j^\dagger$ and $[a_j, \hat{n}_j] = -a_j$, and normalization.

With the definition above of the basis states, we can verify that the Fock space so defined has a tensor product structure. So more formally

(9) $\quad |n_1 \cdots n_N\rangle = |n_1\rangle \otimes \cdots \otimes |n_N\rangle,$

and the bosonic operators are also tensor products

(10) $\quad a_j^\dagger = \mathbb{1} \otimes \mathbb{1} \cdots \otimes a^\dagger \otimes \cdots \mathbb{1},$

where the $a^\dagger$ operator appears in the j^{th} place on the right hand side above. The same form holds, *mutatis mutandis*, for the annihilation operator a_j. Instead of Eq. (5), we could have used the tensor product of states and operators, Eqs. (9,10) as a definition for bosons. The tensor product form is very natural, and indicates that boson states and operators at different "sites" $j \neq j'$ are independent. In the above discussion the labels need not be sites, but could be any other label for single particle states, e.g. momentum. But the site label is particularly natural and important because the direct product nature reflects the locality of physical space.

2.2 *Fermions*

We approach fermions by just replacing the bosonic commutation relations by anti-commutators:

$$\{c_j, c_k^\dagger\} = \delta_{jk}, \tag{11}$$

and

$$\{c_j, c_k\} = \{c_j^\dagger, c_k^\dagger\} = 0. \tag{12}$$

Here $\{A, B\} = AB + BA$ defines the anti-commutator. I will try to be consistent and mostly use the letter "c" for fermions and "a" for bosons.

These relations look innocuous. But they drastically change the physics. Note that Eq. (12) implies by taking $k = j$ that $c_j^2 = (c_j^\dagger)^2 = 0$. Moreover we see that the number operator $\hat{n}_j = c_j^\dagger c_j$ obeys

$$\hat{n}_j^2 = c_j^\dagger c_j c_j^\dagger c_j = c_j^\dagger (1 - c_j^\dagger c_j) c_j = c_j^\dagger c_j = \hat{n}_j. \tag{13}$$

This implies that the eigenvalues of $\hat{n}_j$ must obey $n_j^2 = n_j$, hence $n_j = 0, 1$ only. This is the famous Pauli exclusion principle. Consider first the case where we just have a single "site" $j = 1$ only (and drop the label). Then we can consider two normalized basis states $|0\rangle$ and $|1\rangle$, with the two possible eigenvalues. Since $\langle 0|\hat{n}|0\rangle = 0 = \langle 0|c^\dagger c|0\rangle$ is the norm of the state $c|0\rangle$ we must have

$$c|0\rangle = 0. \tag{14}$$

Similarly, using the anti-commutator, $\langle 1|cc^\dagger|1\rangle = \langle 1|(1 - \hat{n})|1\rangle = 0$ which implies

$$c^\dagger|1\rangle = 0. \tag{15}$$

Now

$$\hat{n}c^\dagger|0\rangle = c^\dagger c c^\dagger|0\rangle = c^\dagger(1 - c^\dagger c)|0\rangle = c^\dagger|0\rangle, \tag{16}$$

which implies that $c^\dagger|0\rangle = \lambda|1\rangle$ with some constant λ. Then normalization of the two basis states implies that $|\lambda|^2 = 1$. We can actually choose the relative

phase of the two basis states to make $\lambda = 1$. So

(17) $c^\dagger|0\rangle = |1\rangle$.

Now we act with c on this, $cc^\dagger|0\rangle = (1 - c^\dagger c)|0\rangle = |0\rangle$, which implies that

(18) $c|1\rangle = |0\rangle$.

That's all simple and consistent. Things get more complicated when we introduce multiple single-particle states, because of Eq. (12). Let us define the occupation number states according to

(19) $|n_1 n_2 \cdots n_N\rangle = (c_1^\dagger)^{n_1}(c_2^\dagger)^{n_2}\cdots(c_N^\dagger)^{n_N}|0\rangle$,

which is analogous to Eq. (6), but actually simpler because $n_j = 0, 1$ only so no non-trivial normalization factors arise. What is important though is that the *order* of the operators in Eq. (19) matters. The order is a convention. But we need to pick one and stick with it. Having done it, one can verify that

(20)
$$\begin{aligned} c_j^\dagger|n_1 n_2 \cdots 0_j \cdots n_N\rangle &= (-1)^{\sum_{k<j} n_k}|n_1 n_2 \cdots 1_j \cdots n_N\rangle, \\ c_j^\dagger|n_1 n_2 \cdots 1_j \cdots n_N\rangle &= 0, \end{aligned}$$

and

(21)
$$\begin{aligned} c_j|n_1 n_2 \cdots 1_j \cdots n_N\rangle &= (-1)^{\sum_{k<j} n_k}|n_1 n_2 \cdots 0_j \cdots n_N\rangle, \\ c_j|n_1 n_2 \cdots 0_j \cdots n_N\rangle &= 0. \end{aligned}$$

One can readily check that these relations, Eqs.(20,21) imply the anti-commutation relations of all the operators.

Comparing this to the boson case, we can see that the Hilbert space of fermions can be considered as a tensor product, but the fermionic operators are not simple in this sense: unlike in Eq. (10), a single fermion operator does not correspond to a tensor product of identity operators with a single non-trivial entry. In this sense, the fermion operators are not local. A more explicit way to think about this is the famous **Jordan-Wigner transformation**. We can identify the two occupation number states $n_i = 0, 1$ with two eigenstates of a Pauli matrix, $\sigma_i^z = +1, -1$, respectively, i.e. $n_i = (1 - \sigma_i^z)/2$, or $\sigma_i^z = (-1)^{n_i}$. Then we define the usual Pauli operators as direct products:

(22) $\sigma_j^\mu = \mathbb{1}_1 \otimes \cdots \otimes (\sigma^\mu)_j \otimes \mathbb{1} \cdots \otimes \mathbb{1}_N$,

with $\mu = x, y, z$. Then Eqs. (20)(21) imply that

(23) $c_j^\dagger = \sigma^z \otimes \sigma^z \otimes \cdots \otimes (\sigma^-)_i \otimes \mathbb{1} \cdots \otimes \mathbb{1}_N = \left(\prod_{k<j} \sigma_k^z\right) \sigma_j^-$,

where $\sigma_j^\pm = (\sigma_j^x \pm i\sigma_j^y)/2$ are the usual raising and lowering operators. Simi-

larly for the annihilation operator,

$$c_j = \sigma^z \otimes \sigma^z \otimes \cdots \otimes \left(\sigma^+\right)_i \otimes \mathbb{1} \cdots \otimes \mathbb{1}_N = \left(\prod_{k<j} \sigma_k^z\right) \sigma_j^+. \tag{24}$$

The representation of single fermion operators in terms of local Pauli operators is highly non-local. The product over σ_k^z in parenthesis in these equations is often called the Jordan-Wigner string.

It is useful to consider "bosonic" operators, by which I mean those involving an even number of fermi operators (these are called "physical" by Bravyi and Kitaev). For example $A_{jk} = c_j^\dagger c_k$, with $j < k$ for concreteness. We can see using the Jordan-Wigner transformation that

$$A_{jk} = -\left(\prod_{l=j}^{k-1} \sigma_l^z\right) \sigma_j^- \sigma_k^+. \tag{25}$$

In general, we see that a two-fermion operator like A_{jk}, which appears to act only on sites j and k, actually in the spin representation (where the tensor product is defined) acts on more sites, whose number depends on the separation of j and k. These formulae are general. We can consider the "site" label to be anything. In a one dimensional system, it would be natural to order the labels according to the actual spatial coordinate. In that case, we would see that when j and k are neighboring sites, the extra non-locality does not appear for bosonic operators. This means, roughly speaking, that for one dimensional systems, the spectrum and eigenstates of fermionic and bosonic systems with local Hamiltonians are similar.

However, in two or more dimensions, we must choose some artificial ordering of all the sites to define the strings (or equivalently, the signs in the basis in Eq. (19)). Then A_{jk} for many pairs of nearby sites in real space inevitably becomes highly non-local in the spin representation. So in dimensions greater than or equal to two, we can expect extremely different physics in fermionic systems from what we find in bosonic ones.

The major physical difference between fermions and bosons is that free fermions are still interesting! Slightly less facetiously, fermions are interesting because they can be stable at non-zero density without interactions, and can be generically gapless.

2.3 *Diagonalization and three classes of free fermion systems*

A generic free fermion Hamiltonian takes the form

$$H = \sum_{ij} h_{ij} c_i^\dagger c_j, \tag{26}$$

where h (the matrix whose entries are h_{ij}) is a hermitian matrix, $\mathsf{h} = \mathsf{h}^\dagger$. This is solved by transforming to the basis of eigenvectors of h:

$$\mathsf{h}\boldsymbol{\phi}^{(a)} = \epsilon_a \boldsymbol{\phi}^{(a)} \Leftrightarrow \sum_j h_{ij}\phi_j^{(a)} = \epsilon_a \phi_i^{(a)}. \tag{27}$$

The fermion operators can be traded for new ones using the basis change formula,

$$c_j = \sum_a \phi_j^{(a)} c_a, \tag{28}$$

which is a canonical transformation (preserving Eqs. (11,12)) for any $\boldsymbol{\phi}^{(a)}$ that form an orthonormal set. Then we have

$$H = \sum_a \epsilon_a c_a^\dagger c_a = \sum_a \epsilon_a \hat{n}_a. \tag{29}$$

This is now diagonal in the Fock basis, and the full spectrum is know. Specifically, the ground state is, up to a phase, just the one in which all negative energy eigenstates are occupied:

$$|\Psi_0\rangle = \prod_{a|\epsilon_a<0} c_a^\dagger |0\rangle. \tag{30}$$

Here we are absorbing the chemical potential/Fermi energy into the definition of the ϵ_a.

We will mainly be interested in systems with translational symmetry. In this case it may be advantageous to trade the site label i for a pair of labels: a coordinate $\boldsymbol{x}$ which belongs to the Bravais lattice, and indexes the unit cell containing the site, and a sublattice number $s = 1 \cdots n_\mathrm{b}$, where n_b is the number of sites/orbitals/single-particle states within a unit cell (it could include spin states etc.). The general translationally invariant Hamiltonian of this form can be written as

$$H = \sum_{\boldsymbol{x},\boldsymbol{x}'} \sum_{s,s'} h_{ss'}(\boldsymbol{x} - \boldsymbol{x}') c_{s\boldsymbol{x}}^\dagger c_{s'\boldsymbol{x}'}. \tag{31}$$

For this form, either with periodic boundary conditions or infinite volume, (quasi-)momentum $\boldsymbol{k}$ is a good quantum number. We can then go to a plane wave (Bloch) basis, which partly diagonalizes the Hamiltonian

$$c_{s\boldsymbol{x}} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} c_{s\boldsymbol{k}}, \tag{32}$$

where N is the number of unit cells. This is another use of the change of basis formula, for which we have taken an orthonormal basis which does not fully diagonalize the Hamiltonian (it instead breaks it into blocks of different

momentum). The Hamiltonian becomes

$$H = \sum_{\boldsymbol{k}} \sum_{ss'} \hat{h}_{ss'}(\boldsymbol{k}) c^\dagger_{s\boldsymbol{k}} c_{s'\boldsymbol{k}}. \tag{33}$$

Here $\hat{h}(\boldsymbol{k})$ is the *Bloch Hamiltonian*. By construction it is an $n_\mathrm{b} \times n_\mathrm{b}$ Hermitian matrix which has the periodicity of the reciprocal lattice:

$$\hat{h}(\boldsymbol{k} + \boldsymbol{Q}) = \hat{h}(\boldsymbol{k}), \tag{34}$$

if $\boldsymbol{Q}$ is in the reciprocal lattice, i.e. $\boldsymbol{Q} \cdot \boldsymbol{x}_j \in 2\pi\mathbb{Z}$ for all Bravais lattice vectors $\boldsymbol{x}_j$.

We can finish the diagonalization by finding eigenvectors of $\hat{h}(\boldsymbol{k})$

$$\hat{h}(\boldsymbol{k}) \boldsymbol{\phi}^{(n)}_{\boldsymbol{k}} = \epsilon_n \boldsymbol{\phi}^{(n)}_{\boldsymbol{k}}, \tag{35}$$

and writing

$$c_{s\boldsymbol{k}} = \sum_n \phi^{(n)}_{s\boldsymbol{k}} c_{a\boldsymbol{k}}. \tag{36}$$

Then and we can trade the abstract eigenstate label a for the pair $(\boldsymbol{k}, n)$, where n is a discrete "band" index. Then the diagonal Hamiltonian is

$$H = \sum_n \sum_{\boldsymbol{k}} \epsilon_{n\boldsymbol{k}} c^\dagger_{n\boldsymbol{k}} c_{n\boldsymbol{k}}, \tag{37}$$

where $\epsilon_{n\boldsymbol{k}}$ describes the dispersion of the n^{th} band. Several distinct situations can be envisioned:

1. **Insulators**: All bands have entirely negative or entirely positive energies, i.e.

$$\begin{aligned} &\epsilon_{n\boldsymbol{k}} < 0 && n \leq n_1, \\ &\epsilon_{n\boldsymbol{k}} > 0 && n > n_1, \end{aligned} \tag{38}$$

   for all $\boldsymbol{k}$. The ground state has the first n_1 bands occupied and the others empty, and there is an excitation gap $\Delta = \min_{n>n_1} \epsilon_{n\boldsymbol{k}} - \max_{n\leq n_1} \epsilon_{n\boldsymbol{k}}$.

2. **Zero gap semiconductor** or **semi-metal**: Here some bands reach zero energy at their maxima or minima:

$$\begin{aligned} &\epsilon_{n\boldsymbol{k}} \leq 0 && n \leq n_1, \\ &\epsilon_{n\boldsymbol{k}} \geq 0 && n > n_1, \end{aligned} \tag{39}$$

   and the equalities are satisfied for some non-zero locus in momentum space. Examples are Dirac and Weyl systems, where bands touch at a single point in two or three-dimensional momentum space, quadratic band touching systems like bulk HgTe, and nodal line semi-metals where bands touch over curves in momentum space.

3. **Metals**: Here some bands have both positive and negative energies, i.e. $\epsilon_{n\boldsymbol{k}} = 0$ is satisfied for a surface (set of co-dimension one) in momentum space for at least one n. This is called the Fermi surface. The Fermi surface divides momentum space into regions of occupied and unoccupied states.

Notably, in cases two and three above there is no energy gap above the ground state: an excitation with arbitrarily low energy can be made by adding or removing one or more fermion whose energy is as close to zero as we wish. This occurs extremely simply, even without interactions. By contrast, for bosons to be gapless, we need either to perform some fine-tuning to make the minimum energy boson state approach zero energy, or we need the mechanism of spontaneous symmetry breaking (like the superfluidity discussed in the previous quarter's notes), or some more exotic mechanism is required.

3 Free fermion phases

Lecture 2 (1h 15mins)
January 18th, 2018

3.1 *Metals at the free fermion level*

Many of the properties of metals are captured by the simple free fermion theory. We'll return to why this is the case – what is called Fermi liquid theory – later in the class. For now I want to go over some of the amazing properties of free fermion metals, which arise due to the presence of a Fermi surface. The Fermi surface means that there are a huge number of low energy excitations, from all the possible electron and hole states near the surface.

One of things we will do repeatedly is to try to focus on the low energy degrees of freedom in a problem. In the context of free fermions, this means to consider only the single particle states close to the chemical potential or Fermi energy. For a metal, this is exactly the vicinity of the Fermi surface. Instead of writing the full Hamiltonian including all the bands, Eq. (37), we can instead assume all the single particle states more than some energy E_0 below the chemical potential are always occupied, while all states more than E_0 above the chemical potential are always empty, and simply retain those states within the band $\epsilon_F - E_0 < \epsilon_{n\boldsymbol{k}} < \epsilon_F + E_0$. The energy E_0 we choose should be larger than some energies we are interested in probing, like the thermal energy $k_B T$, or frequency $\hbar\omega$ of a probe, but still small compared to microscopic energies (which thankfully are of the order of $10^4 K$ in metals). When the the latter smallness is sufficient, we can expand the dispersion $\epsilon_{n\boldsymbol{k}}$ around the Fermi energy, i.e. Taylor expand in $\boldsymbol{k} - \boldsymbol{K}$, where $\boldsymbol{K}$ is a point on the Fermi surface. We re-express the momenta in the cut-off range as

$$\boldsymbol{k}(\boldsymbol{K}, q) = \boldsymbol{K} + \hat{\boldsymbol{v}}_F(\boldsymbol{K}) q, \tag{40}$$

where $\boldsymbol{v}_F(\boldsymbol{K}) = \boldsymbol{\nabla}\epsilon_n(\boldsymbol{k})|_{k=\boldsymbol{K}}$ is the Fermi velocity at the point $\boldsymbol{K}$, which is normal to the Fermi surface, and q measures the distance to the Fermi surface. The result is

$$H = \sum_{\boldsymbol{K}\in \mathrm{FS}} \sum_{|q|<\Lambda} v_F(\boldsymbol{K}) q \, c^\dagger_{\boldsymbol{K}+\hat{\boldsymbol{v}}_F(\boldsymbol{K})q} c_{\boldsymbol{K}+\hat{\boldsymbol{v}}_F(\boldsymbol{K})q}, \tag{41}$$

with $\Lambda \sim E_0/v_F$ (it could be taken constant or varying along the Fermi surface). Here we have suppressed band indices, but one may keep in mind that the Fermi surface may arise from several bands, and may contain multiple disjoint pieces. The parameters in the low energy theory are the Fermi surface itself and the collection of Fermi velocities. Notably, the energy dispersion is linear around the Fermi surface, and the form of Eq. (41) strongly resembles a collection of many one-dimensional Hamiltonians, since the dispersion depends locally only on the single component (q) of the momentum, with $\boldsymbol{K}$ appearing more like an "index" to count different "patches" of the Fermi surface.

This form has a very strong contrast to a typical relativistic field theory, where the minimum energy states lie all near the origin in momentum space. Most importantly, it has far more low energy states. Indeed, it is hard to find examples with *more* low energy states than in a free electron metal. This has a lot of consequences:

1. **Power law correlations:** Just about any correlation function in a free fermion system has slowly-decaying power-law components. This includes the electron Green's function, the density-density and spin-spin correlation functions, the pair field correlation function, etc.

2. $2k_F$ **oscillations**: The size of the Fermi surface itself, e.g. its diameter $2k_F$ in the simplest spherical case, appears via characteristic oscillations in physical quantities like the density near a boundary, or the interactions between dilute magnetic moments in a metal. These are called "Friedel oscillations".

3. **Thermodynamics:** The large number of low energy states means that the entropy of a free electron metal is large even at low temperature, in fact it is linear in temperature T. Accordingly, the specific heat behaves like $c \sim \gamma T$, where γ is known as the Sommerfeld constant. The thermodynamic spin and orbital susceptibilities are also large and become constant at low temperature.

4. **Response and conductivity:** Having so many low energy excitations means that the metal responds strongly to small perturbations. Within linear response theory, this is related to the behavior of retarded correlation functions at low frequency. Metals respond strongly to magnetic and electric fields, for example they have large conductivity, large imaginary spin susceptibilities (this has consequences for NMR for example). Metals also have large thermal conductivity. Transport of charge and heat are complicated subjects we will return to later in the class.

As an example, let's look in some detail at a simple correlation function, the density-density one. For this purpose we can consider the simplest model of a free electron gas, or more generally a single band, so $\epsilon_{n\boldsymbol{k}} \to \epsilon_{\boldsymbol{k}}$. Then the band wavefunctions

$$\phi_j^{\boldsymbol{k}} \to \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j}. \tag{42}$$

where V is the volume in units of lattice sites. This means the density operator becomes

$$\hat{n}(\boldsymbol{x}) = \frac{1}{V}\sum_{k,q} c^\dagger_{k+q} c_k e^{iq\cdot x}. \tag{43}$$

Now consider the density-density correlation function

$$\langle \hat{n}(\boldsymbol{x})\hat{n}(\boldsymbol{x}')\rangle = \frac{1}{V^2}\sum_{k,q}\sum_{k',q'} \langle \Psi_0 | c^\dagger_{k+q} c_k c^\dagger_{k'+q'} c_{k'} | \Psi_0\rangle e^{i(q\cdot x + q'\cdot x)}. \tag{44}$$

Recognizing that the ground state has occupied states within the Fermi surface and empty without, we see that there are two contributions. If $\boldsymbol{q} = \boldsymbol{q}' = 0$, then the quantity inside the expectation value reduces to the product of two number operators, and the result of the sums over $\boldsymbol{k}$ and $\boldsymbol{k}'$ just gives the total number of particles squared. If this is not true, then the electron removed at momentum $\boldsymbol{k}'$ by the last annihilation operator should be put back by the first one at $\boldsymbol{k}+\boldsymbol{q}$, which forces $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$. Similarly $\boldsymbol{q'} = \boldsymbol{k} - \boldsymbol{k}' = -\boldsymbol{q}$. In this case, we require $\boldsymbol{k}'$ inside the Fermi surface and $\boldsymbol{k}$ outside it. So the result is

$$\langle \hat{n}(\boldsymbol{x})\hat{n}(\boldsymbol{x}')\rangle = \bar{n}^2 + \frac{1}{V^2}\sum_{|\boldsymbol{k}|>k_F}\sum_{|\boldsymbol{k}'|<k_F} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{x}-\boldsymbol{x}')}. \tag{45}$$

Taking the continuum limit, we obtain

$$\begin{aligned}\langle \hat{n}(\boldsymbol{x})\hat{n}(\boldsymbol{x}')\rangle &= \bar{n}^2 + \int_{\boldsymbol{k}}\int_{|\boldsymbol{k}'|<k_F} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{x}-\boldsymbol{x}')} - \int_{|\boldsymbol{k}|<k_F}\int_{|\boldsymbol{k}'|<k_F} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{x}-\boldsymbol{x}')} \\ &= \bar{n}^2 - \bar{n}\delta(\boldsymbol{x}-\boldsymbol{x}') - \left|\int_{|\boldsymbol{k}|<k_F} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}\right|^2, \end{aligned} \tag{46}$$

where we introduce the notation $\int_{\boldsymbol{k}} = \int \frac{d^d\boldsymbol{q}}{(2\pi)^d}$ in d dimensions. In three dimensions, we can evaluate the final integral explicitly

$$\begin{aligned}\int_{|\boldsymbol{k}|<k_F} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} &= \int_0^\infty dk\, k^2 \int_{-1}^{1} d\cos\theta\, \frac{2\pi}{(2\pi)^3} e^{ik|\boldsymbol{x}-\boldsymbol{x}'|}, \\ &= \frac{-k_F}{2\pi^2|\boldsymbol{x}-\boldsymbol{x}'|^2}\left(\cos k_F|\boldsymbol{x}-\boldsymbol{x}'| - \frac{\sin k_F|\boldsymbol{x}-\boldsymbol{x}'|}{k_F|\boldsymbol{x}-\boldsymbol{x}'|}\right). \end{aligned} \tag{47}$$

Using the fact that for a spinless electron gas, the density is related to the Fermi energy by $\bar{n} = k_F^3/6\pi^2$, we can write this as

$$\frac{\langle \hat{n}(\boldsymbol{x})\hat{n}(\boldsymbol{x}')\rangle}{\bar{n}^2} = 1 - \left|\frac{3}{(k_F|\boldsymbol{x}-\boldsymbol{x}'|)^2}\left(\frac{\sin k_F|\boldsymbol{x}-\boldsymbol{x}'|}{k_F|\boldsymbol{x}-\boldsymbol{x}'|} - \cos k_F|\boldsymbol{x}-\boldsymbol{x}'|\right)\right|^2, \tag{48}$$

neglecting the delta-function part. A Taylor expansion shows that this function

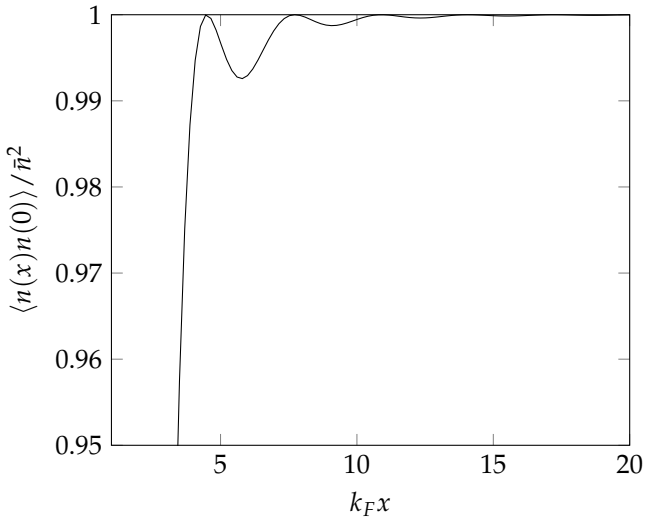


Figure 1: Tail of the density density correlations of a 3d electron gas.

vanishes as $|\boldsymbol{x} - \boldsymbol{x}'| \to 0$. This is called a "correlation hole", and reflects the fact that two fermions cannot occupy the same position, as a consequence of the Pauli principle. For larger $|\boldsymbol{x} - \boldsymbol{x}'|$, it oscillates and approaches unity, as shown in Fig. 1. These $2k_F$ oscillations are a Hallmark of the Fermi surface.

The envelope of the oscillations depends upon the dimensionality, decaying in three dimensions like $1/x^4$ as seen from Eq. (48). In lower dimensions the decay is slower, so the oscillations are more pronounced. The result looks qualitatively similar to the density-density correlation function in a classical liquid: the oscillations indicate the tendency to local crystallinity, and their decay reflects the liquidity. The free fermi gas is therefore a kind of liquid of fermions, whose crystallinity is stronger in lower dimensions as the decay is slower there.

This is just one example. Many other correlation functions behave similarly. For example, if we restore spin, the spin-spin correlation function has the same form as the density-density one (*show it!*!).

3.2 *Two dimension Dirac fermions and graphene*

Now we will move from metals to nodal semi-metals. They arise in many contexts, and are an important topic in current research (2018). We will discuss a few examples in two and three dimensions. By far the longest studied example is two-dimensional graphene. Working out the band structure of graphene is by now a standard classroom problem, starting from a tight-binding model of a single π orbital for electrons on each site of a honeycomb lattice. You can find it discussed in many many places, for example this Reviews of Modern Physics article.

For completeness, we include a brief exposition here. The geometry is shown in Fig. 2. The lattice sites are divided into A and B sublattices, con-

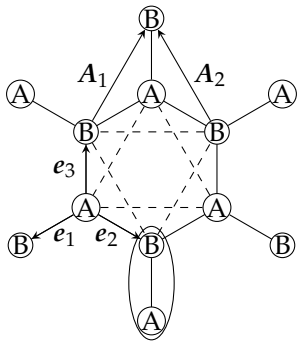


Figure 2: A hexagon of the honeycomb lattice. Nearest-neighbor bonds are obvious, and representative second neighbor bonds are shown with dashed lines. Two linearly independent Bravais lattice (translation) vectors $\boldsymbol{A}_1$, $\boldsymbol{A}_2$ are shown, as are the three nearest-neighbor vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$. A unit cell consists of a pair of A and B sites, one of which is enclosed by an ellipse.

nected by nearest-neighbor bonds shown as solid lines. We define a unit cell containing two sites on a vertical bond, for example the pair in the ellipse drawn in the figure. A site is indexed by the coordinate of its unit cell, which we take to be the coordinate of the A site within that cell, and the sublattice $s = 1, 2 = A, B$. The A sites are then located at the sites of the triangular Bravais lattice, for which we may take $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ shown in the figure as primitive lattice vectors. We define also the three nearest-neighbor vectors $\boldsymbol{e}_i$, $i = 1, 2, 3$ as shown. One can see that $\boldsymbol{A}_1 = \boldsymbol{e}_3 - \boldsymbol{e}_1 = -2\boldsymbol{e}_1 - \boldsymbol{e}_2$ and $\boldsymbol{A}_2 = \boldsymbol{e}_3 - \boldsymbol{e}_2 = -2\boldsymbol{e}_2 - \boldsymbol{e}_1$. The basis vectors $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$ of the reciprocal lattice are defined by $\boldsymbol{B}_i \cdot \boldsymbol{A}_j = 2\pi\delta_{ij}$ as usual. If we define vectors $\boldsymbol{b}_i$ such that $\boldsymbol{b}_i \cdot \boldsymbol{e}_j = 2\pi\delta_{ij}$ for $i, j = 1, 2$, then we can find that $\boldsymbol{B}_1 = (-2\boldsymbol{b}_1 + \boldsymbol{b}_2)/3$, and $\boldsymbol{B}_2 = (-2\boldsymbol{b}_2 + \boldsymbol{b}_1)/3$.

With all these definitions, it is straightforward to write down the Bloch Hamiltonian for the nearest-neighbor model. We obtain

(49)
$$\hat{h}(\boldsymbol{k}) = -t \begin{pmatrix} 0 & 1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{A}_2} + e^{-i\boldsymbol{k}\cdot\boldsymbol{A}_1} \\ 1 + e^{i\boldsymbol{k}\cdot\boldsymbol{A}_2} + e^{i\boldsymbol{k}\cdot\boldsymbol{A}_1} & 0 \end{pmatrix} = \begin{pmatrix} 0 & f(\boldsymbol{k}) \\ f^*(\boldsymbol{k}) & 0 \end{pmatrix},$$

with

(50) $$f(\boldsymbol{k}) = -t\left(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{A}_2} + e^{-i\boldsymbol{k}\cdot\boldsymbol{A}_1}\right).$$

We see that $\hat{h}(\boldsymbol{k})$ is indeed periodic and smooth, as expected. Band touching occurs when $f(\boldsymbol{k})$ vanishes identically, i.e. both real and imaginary parts. This occurs at the two inequivalent corners of the Brillouin zone, denoted $\boldsymbol{K}$ and $\boldsymbol{K}'$. If we take the length of the nearest-neighbor bond to be unity, then $\boldsymbol{A}_1 = (\sqrt{3}/2, 3/2)$, $\boldsymbol{A}_2 = (-\sqrt{3}/2, 3/2)$, and it is easily verified that f vanishes at

the points $\boldsymbol{K} = (4\pi/(3\sqrt{3}), 0)$, $\boldsymbol{K}' = -\boldsymbol{K}$. Taylor expanding, we have

$$f(\pm\boldsymbol{K} + \boldsymbol{k}) \sim \frac{3}{2} t(\pm k_x - i k_y). \tag{51}$$

Since the eigenvalues of the matrix in Eq. (49) are $\pm|f(\boldsymbol{k})|$, this implies that the bands touch linearly.

The Bloch Hamiltonian already appears as a 2×2 matrix whose index we denote a, b etc. and which lies in the sublattice space. To include spin, we would also require a spin-1/2 index $\sigma = \uparrow, \downarrow$. In a low energy description, which linearizes the dispersion around the Dirac points, there is an additional "valley" index $A = 1, 2$, which labels the two Brillouin zone corners. The continuum fields are defined simply by separating the momentum components which are in a small neighborhood of the Dirac points:

$$c_{a\alpha,\boldsymbol{K}_A+\boldsymbol{k}} = \psi_{Aa\alpha,\boldsymbol{k}}, \qquad \text{for } |\boldsymbol{k}| \ll 1. \tag{52}$$

Putting this all together, the low energy Hamiltonian is

$$H = \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} v(\mu^z \tau^x k_x + \tau^y k_y)\psi_{\boldsymbol{k}}. \tag{53}$$

Here $\boldsymbol{k}$ measures the deviation of the momentum from the Dirac point. The fermions are described by a spinor $\psi = \psi_{Aa\alpha}$, where $\boldsymbol{\tau}$ Pauli matrices act on the sublattice a space, $\boldsymbol{\mu}$ act on the valley space (you can see Eq. (53) is diagonal in the valley space because it only involves μ^z), and $\boldsymbol{\sigma}$ act on the spin space (these are not present because spin-orbit coupling is weak and can be neglected). We keep the indices implicit for compactness as much as possible.

The Hamiltonian in Eq. (53) is easy to diagonalize. It is already diagonal in the valley and spin subspaces, so we can treat μ^z in the Hamiltonian as a constant = ±1 (its eigenvalues). We are left with a 2×2 matrix in the $\boldsymbol{\tau}$ space. The eigenvalues of this matrix are easy to find by for example rotating it by an SU(2) rotation to the τ^z direction. One has

$$\epsilon_\pm = \pm v\sqrt{k_x^2 + k_y^2} = \pm v|k|. \tag{54}$$

We see the dispersion is just a relativistic "light-cone" of conduction and valence bands intersecting at $\boldsymbol{k} = 0$.

Stability of the Dirac point

A key question is whether this behavior is generic. That is, we may have made a small mistake in our Hamiltonian by neglecting some term, and would correcting this lead to the removal of this intersection point and fundamental modification of the spectrum? This certainly appears possible, since the 2d Dirac equation allows a mass term. Even if we "freeze" the valley and spin degrees of freedom, i.e. just consider the two component Dirac equation for fixed spin and valley quantum numbers, one can add a term of the form $m\psi^\dagger\tau^z\psi$ to the Hamiltonian above which is known as a Dirac mass, and will indeed

remove the intersection point. Maybe some principle (symmetry?) prohibits adding this term? Perhaps there are other allowed perturbations?

Let us start with the simple-minded answer, which is just based on the Dirac Hamiltonian, Eq. (53) and symmetries. We ask what might prevent adding a term proportional to $\psi^\dagger M \tau^z \psi$ to the Hamiltonian? Here M could be a matrix in the spin and valley spaces. So long as this anti-commuted with the two matrices inside Eq. (53), it will serve as a mass. First, it is natural to assume spin rotation symmetry, $SU(2)_\sigma$, because spin-orbit coupling is weak in graphene so this is a good approximation microscopically. This requires M to not contain any of the spin Pauli matrices. Second, we impose translational symmetry, which means that quasi-momentum is conserved up to a reciprocal lattice vector, and so there is no scattering between valleys. This requires M to not contain μ^x or μ^y. These two constraints allow matrices of the form $M \sim \mathbb{1}, \mu^z$, i.e. mass terms τ^z and $\mu^z\tau^z$. Now consider time-reversal symmetry. This changes the sign of momentum, and hence interchanges the two Dirac points, which means $\mu^z \to -\mu^z$. The matrix τ^z simply labels the sublattices, so it is time-reversal invariant. Thus of the two remaining options, only the $M \sim 1$ or pure τ^z mass is time-reversal invariant. If we assume time-reversal symmetry, we still need one more symmetry to prevent the addition of τ^z. For this, we need to require some symmetry which interchanges the two sublattices, for example inversion around the center of a bond. Under this operation, $\tau^z \to -\tau^z$, and so inversion symmetry removes the finally remaining mass term. We conclude that the Dirac points remain intact if we maintain four conditions: 1. spin rotation symmetry $SU(2)_\sigma$, 2. inversion symmetry, 3. the translation symmetry of the honeycomb lattice, and 4. time-reversal symmetry.

This analysis is acceptable but uninspiring, and leaves open other possible questions. Later, we will return to reconsider the stability in topological terms, and see that a more elegant explanation is possible.

3.3 *Three dimensional Weyl fermions*

Lecture 3 (1h 15mins)
January 23rd, 2018

The 2d Dirac fermion requires some symmetry to protect it. In three dimensions, there are "nodes" or band intersections that do not require any symmetry other than the translational symmetry required to define bands themselves. These are known as Weyl points.

We assume the "generic" situation that bands in a three dimensional system, including the effects of spin-orbit coupling, are non-degenerate. This is true *unless* band degeneracy is enforced by the combination of inversion and time-reversal symmetry. Assuming non-degenerate bands, we consider the possibility that two bands approach one another in energy near some point $\boldsymbol{K}$. To study the putative band crossing, we can focus only on those two bands, which restricts the Bloch hamiltonian, $\hat{h}(\boldsymbol{k})$ to a two dimensional matrix, which, by assumption, has degenerate eigenvalues at $\boldsymbol{q} = 0$. Writing $\boldsymbol{k} = \boldsymbol{K} + \boldsymbol{q}$, one may expand this matrix to leading linear order in $\boldsymbol{q}$ as

$$\hat{h}(\boldsymbol{K} + \boldsymbol{q}) = A_\mu q_\mu \mathbb{I} + B_{\mu\nu} q_\mu \boldsymbol{\tau}_\nu, \tag{55}$$

where $\mathbb{I}$ is the identity matrix and $\boldsymbol{\tau}_\nu$ are the Pauli matrices. By design, this Hamiltonian has degenerate eigenvalues at $\boldsymbol{q} = 0$. Now suppose we make a small perturbation of the system, shifting $\hat{h} \to \hat{h} + \hat{g}$, where $\hat{g}$ is a small constant Hermitian matrix. We can always express $\hat{g} = g_0\mathbb{I} + g_\nu\boldsymbol{\tau}_\nu$. Thus the perturbed Bloch Hamiltonian becomes

$$\hat{h} \to (A_\mu q_\mu + g_0)\mathbb{I} + (B_{\mu\nu}q_\mu + g_\nu)\boldsymbol{\tau}_\nu. \tag{56}$$

The perturbed Hamiltonian has degenerate bands when the coefficients of all the Pauli matrices vanish. This occurs when $B^T\boldsymbol{q} + \boldsymbol{g} = 0$, or $\boldsymbol{q} = -(B^T)^{-1}\boldsymbol{g}$, which is simply a point slightly shifted from the original band crossing. We see that a small generic perturbation of the system does not remove the band crossing, but only shifts it. We conclude from this simple analysis that the band crossing is protected, although its location is not. We will understand the protection more deeply later in Sec. 4.2.

Such a band crossing is "accidental" in the sense that it is unconnected to any symmetry. We can understand the occurrence of the accidental crossing by a counting argument. To obtain two degenerate eigenvalues of a generic two dimensional matrix requires tuning three parameters to zero: the coefficients of the three Pauli matrices, or equivalently the naïve energy level difference (τ^z) and the matrix elements between the two levels (τ^x, τ^y). In three dimensions, the three components of momentum provide three such parameters. Thus accidental band crossings occur generically in three dimensions, but not in two.

The band crossing is called a "Weyl point", because the Hamiltonian in Eq. (55) can be cast in the form of the Weyl equation. By a suitable coordinate change, we can make $B_{\mu\nu}$ diagonal. Then the Hamiltonian is written as

$$\hat{h}(\boldsymbol{q}) = \boldsymbol{A}\cdot\boldsymbol{q}\mathbb{I} + \sum_\mu v_\mu q_\mu \boldsymbol{\tau}_\mu. \tag{57}$$

Here we expressed the diagonalized coefficient of the Pauli operators as a velocity v_μ. The resulting energy levels are

$$\epsilon_\pm = \boldsymbol{A}\cdot\boldsymbol{q} \pm \sqrt{\sum v_\mu^2 q_\mu^2}. \tag{58}$$

This is an anisotropic Dirac-like dispersion in three dimensions, with a "tilt" given by the $\boldsymbol{A}\cdot\boldsymbol{q}$. In particle physics, the Weyl equation was devised as a kind of "square root" of the Dirac equation. Like $\hat{h}$ in Eq. (57), the Weyl equation is a 2×2 matrix one, instead of the 4×4 matrix form of the (probably) more familiar Dirac equation. The price paid for taking the square root is that Weyl fermions are necessarily massless: as we have seen, there is no perturbation which removes the band crossing. Eq. (58) generalizes the dispersion of Weyl fermions from particle physics (which are constrained by Lorenz invariance) to an anisotropic and tilted form. When the tilt $\boldsymbol{A}$ is small, it describes two tilted cones touching at a point, such that the only states at zero energy are those at the touching point $\boldsymbol{q} = 0$. However, it can and does happen that the tilt $\boldsymbol{A}$ is large enough that it overcomes the the band splitting terms in some

directions of momentum space. In this case the states at zero energy are not limited to $\boldsymbol{q} = 0$, and there is no energy at which the support of the states is limited to a single point. Rather, there is some complex evolution of a Fermi surface at all energies. This situation has come to be known as a "type II" Weyl point, and the simpler former case as a "type I" Weyl point.

3.4 *Three dimensional Dirac fermions*

Three dimensional Dirac fermions, whose low energy dynamics are described by the 4-component Dirac equation, also can occur in solids, though not accidentally. Dirac points occur in systems with *both* inversion and time-reversal symmetry (a priori it is possible also in an antiferromagnet which maintains invariance under simultaneous time-reversal and translation symmetry, but I am not aware of a known example). These constraints alone imply that all bands are two-fold degenerate at every quasi-momentum $\boldsymbol{k}$. The Dirac point corresponds to a crossing of two of these two-fold degenerate bands at some point. Returning to the "constraint counting" arguments earlier, to achieve degeneracy of these four levels requires tuning a large number of off-diagonal matrix elements to vanish, clearly more than the three components of momentum that are available. This is why Dirac points do not occur accidentally.

However, an additional ingredient of symmetry can be enough to allow Dirac points to occur. There are several ways they can happen. Let's describe one, which is how you might understand the material Cd_3As_2. We can understand this system by thinking of it as a tetragonal distortion of an underlying cubic material. Cubic semiconductors are quite common: all the big semiconductor materials like Si, Ge, and GaAs are cubic. In such a cubic system there are bands which are predominantly built from p orbitals, which at the atomic level have orbital angular momentum $\ell = 1$. Taking into account the spin $s = 1/2$ of the electron, spin-orbit coupling can build from these orbital total angular momentum states $j = 1/2$ and $j = 3/2$. With spherical symmetry and time-reversal symmetry, the four states of the $j = 3/2$ multiplet are degenerate. This gives us the building blocks for a Dirac system.

In a cubic semiconductor, the Bloch Hamiltonian describing the states built from the $j = 3/2$ orbitals is a 4×4 matrix, which is a function of momentum, and can be expressed in terms of sums and products of the $j = 3/2$ matrices $\boldsymbol{J}$. We can expand it near the origin in momentum space. Take $\boldsymbol{k} = 0$ first. It must be a polynomial in the spin matrices. Cubic symmetry acts on $\boldsymbol{J}$ like a vector, and $\boldsymbol{J}$ is odd under time-reversal symmetry. So the allowed terms are

$$\hat{h} = a\mathbb{I} + a|J|^2 + b|J|^4 + c(J_x^4 + J_y^4 + J_z^4). \tag{59}$$

Now for $j = 3/2$, all these terms are constants, proportional to the identity. This means the Bloch Hamiltonian at $\boldsymbol{k} = 0$ is a constant, which implies the 4 states remain unsplit due to these symmetries. Now we can add in terms which are linear or quadratic in momentum. Inversion symmetry is important because under it, $\boldsymbol{k} \to -\boldsymbol{k}$ but $\boldsymbol{J} \to \boldsymbol{J}$, because angular momentum is a pseudovector. This means linear terms in momentum are not allowed. The expansion for the Bloch Hamiltonian therefore starts at the quadratic level, and

there are just three terms:

$$\hat{h} = \alpha k^2 + \beta(\boldsymbol{k}\cdot\boldsymbol{J})^2 + \gamma(k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2). \quad (60)$$

We chose the energy at $k = 0$ to be zero. This equation describes two two-fold degenerate quadratically dispersing bands. Depending on the magnitude and signs of the constants α, β, γ, they either disperse both upward, both downward, or one upward and one downward. For simplicity, let us take $\gamma \approx 0$. Then the Hamiltoian is diagonalized by simply choosing the quantization axis of $\boldsymbol{J}$ along the momentum, and there are two sets of energies:

$$\epsilon_{\pm\frac{1}{2}} = (\alpha + \beta/4)k^2, \qquad \epsilon_{\pm\frac{3}{2}} = (\alpha + 9\beta/4)k^2. \quad (61)$$

We can choose $\beta < 0$ and $|\beta|/4 < \alpha < 9|\beta|/4$, in which case the $\boldsymbol{J}\cdot\hat{\boldsymbol{k}} = \pm 1/2$ band disperses upward and the $\boldsymbol{J}\cdot\hat{\boldsymbol{k}} = \pm 3/2$ band disperses downward. This is a "quadratic band touching" semi-metal. It is a semi-metal because since one band disperses in both directions, there is no place to put the Fermi level in a gap. This situation occurs in the famous material HgTe. In more conventional semiconductors like Si etc, both these bands disperse downward and are considered valence bands.

To get to a Dirac semi-metal, let us consider stretching or compressing the system along the z axis, to convert it to tetragonal symmetry. This process leaves inversion, time-reversal, and C_4 four-fold rotational symmetry around the z axis intact. It does however allow a non-trivial term at $\boldsymbol{k} = 0$: we can add to the Bloch Hamiltonian

$$\hat{h}'(\boldsymbol{k}) = \lambda J_z^2. \quad (62)$$

We assume the distortion is such that $\lambda > 0$. This has the effect of lifting the degeneracy between the $\boldsymbol{J}\cdot\hat{\boldsymbol{k}} = \pm 1/2$ and the $\boldsymbol{J}\cdot\hat{\boldsymbol{k}} = \pm 3/2$, with the latter being lifted up relative to the former. Consider the Bloch Hamiltonian then for the special line $k_x = k_y = 0$:

$$\hat{h}(0, 0, k_z) = \alpha k_z^2 - |\beta| k_z^2 J_z^2 + \lambda J_z^2. \quad (63)$$

This just describes two two-fold degenerate parabolas, one pointing up and one down, which cross at some momentum $k_z = \pm k_0$, with $k_0 = \sqrt{\lambda/|\beta|}$. This crossing is a potential Dirac point. Let us ask, along this line, how robust this crossing is? The bands which cross have $J_z = \pm 1/2$ and $J_z = \pm 3/2$. We know that, so long as inversion and time-reversal are maintained, the bands must remain two-fold degenerate. So we need to ask if these two bands continue to cross under an arbitrary but small (symmetry preserving) perturbation? Perturbations that shift each of the two bands separately will not remove the crossing point, only move it along the line. But can the crossing be removed? This requires off-diagonal matrix elements that mix different J_z states. However, under a C_4 rotation, each of the four states transforms differently, $|J_z\rangle \to e^{i\pi J_z/2}|J_z\rangle$, where the phase factor $e^{i\pi J_z/2}$ takes the four distinct values $e^{i3\pi/4}, e^{i\pi/4}, e^{-i\pi/4}, e^{-i3\pi/4}$. This is sufficient to prevent any term which

mixes these states. Importantly, C_4 symmetry leaves any momentum along the $k_x = k_y = 0$ line invariant, so remains a good symmetry for any k_z, including at the band crossing. This is enough to conclude the crossing is stable.

To see that it is a Dirac point, we should linearize the Bloch Hamilonian in all three directions around the crossing point, $\boldsymbol{k} = (q_x, q_y, k_0 + q_z)$. Plugging this into the Bloch Hamiltonian and linearizing in $\boldsymbol{q}$ we obtain

$$\hat{h}(k_0\hat{\boldsymbol{z}} + \boldsymbol{q}) \sim 2(\alpha - |\beta|J_z^2)k_0 q_z - |\beta|k_0 \left[q_x\{J_x, J_z\} + q_y\{J_y, J_z\}\right]. \tag{64}$$

One can check that this satisfies all symmetries. For $j = 3/2$ matrices, the matrices $\{J_x, J_z\}$ and $\{J_y, J_z\}$ are non-trivial. Define the matrices:

$$\Gamma_3 = \frac{5}{4}\mathbb{I} - J_z^2 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{65}$$

$$\Gamma_1 = -\frac{1}{\sqrt{3}}\{J_x, J_z\} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{66}$$

$$\Gamma_2 = -\frac{1}{\sqrt{3}}\{J_y, J_z\} = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}. \tag{67}$$

One can readily check that these satisfy the Clifford algebra,

$$\Gamma_\mu\Gamma_\nu + \Gamma_\nu\Gamma_\mu = 2\delta_{\mu\nu}. \tag{68}$$

and the Hamiltonian can be rewritten as

$$\hat{h}(k_0\hat{\boldsymbol{z}} + \boldsymbol{q}) \sim uq_z + v_1(q_x\Gamma_1 + q_y\Gamma_2) + v_3 q_z\Gamma_3 \tag{69}$$

with $v_1 = \sqrt{3}|\beta|k_0$ and $v_3 = 2|\beta|k_0$ and $u = 2(\alpha - 5/4|\beta|)k_0$. This describes an anisotropic Dirac cone with a tilt u. In the second quantized representation, the Dirac point Hamiltonian becomes

$$H = \sum_{\boldsymbol{q}} \psi_{\boldsymbol{q}}^\dagger \left(\boldsymbol{u}\cdot\boldsymbol{q} + \sum_{\mu=1}^{3} v_\mu q_\mu \Gamma_\mu\right)\psi_{\boldsymbol{q}}, \tag{70}$$

with $v_2 = v_1$, and $\boldsymbol{u} = (0, 0, u)$.

For a more general discussion, I suggest you look at a recent review article by Peter Armitage and collaborators. We will not talk much more about 3d Dirac semimetals.

4 Berry curvature and topology

Lecture 4 (1h 15mins)
January 25th, 2018

4.1 *Dirac point*

Let us reconsider the stability of a 2d Dirac point from a bit more sophisticated point of view. The best way to address this question is to use a (mildly) non-trivial combination of symmetry and topology. It turns out the intersection is robust so long as we maintain: 1. spin rotation symmetry $SU(2)_\sigma$, 2. inversion symmetry, 3. the translation symmetry of the honeycomb lattice, and 4. time-reversal symmetry. The first is a good approximation for graphene because spin-orbit coupling is very weak for carbon. The second, third, and fourth conditions are true for ideal graphene without applied fields, but might be violated under some conditions.

How do we see the robustness? Well the first condition of $SU(2)_\sigma$ symmetry implies the Hamiltonian is spin independent. So we can just think of the two spin states separately. Then we have, away from the Dirac points, non-degenerate bands for each physical momentum (note: the valley index actually specifies the patch in momentum space, and so the condition (3) of translational symmetry implies that different valleys do not mix). The bands are defined from the eigenvalue problem of the Bloch Hamiltonian, Eq. (35), which we can rewrite in bra-ket notation as

$$\hat{h}(\boldsymbol{k})|\phi_{\boldsymbol{k}}^{(n)}\rangle = \epsilon_n|\phi_{\boldsymbol{k}}^{(n)}\rangle. \tag{71}$$

In this case, $n = 1, 2 = +, -$ for the conduction and valence bands, and $\hat{h}(\boldsymbol{k})$ can be taken as a 2×2 matrix. As $\boldsymbol{k}$ is varied smoothly, so long as the two bands do not touch, the eigenvalues vary smoothly, and likewise the phase of the eigenstates may chosen so that they too vary smoothly, at least for small (local) changes in $\boldsymbol{k}$. For such smoothly defined and normalized states, we can define a quantity to describe the variation,

$$\boldsymbol{\mathcal{A}}_n(\boldsymbol{k}) = \mathrm{Im}\left[\langle\phi_{\boldsymbol{k}}^{(n)}|\boldsymbol{\nabla}_{\boldsymbol{k}}|\phi_{\boldsymbol{k}}^{(n)}\rangle\right]. \tag{72}$$

This is known as the Berry gauge field or Berry connection (note that the overlap inside the square brackets is purely imaginary due to the normalization condition of the eigenstate). We call this a gauge field because there is an unphysical freedom to choose the phase of the Bloch eigenstate at every $\boldsymbol{k}$. Changes in this choice correspond to a transformation

$$|\phi_{\boldsymbol{k}}^{(n)}\rangle \to e^{i\chi_n(\boldsymbol{k})}|\phi_{\boldsymbol{k}}^{(n)}\rangle, \tag{73}$$

with an arbitrary smooth phase $\chi(\boldsymbol{k})$. Under this change, the Berry gauge field transforms as

$$\boldsymbol{\mathcal{A}}_n(\boldsymbol{k}) \to \boldsymbol{\mathcal{A}}_n(\boldsymbol{k}) + \boldsymbol{\nabla}\chi_n(\boldsymbol{k}). \tag{74}$$

The quantity which is invariant under this gauge transformation is mathematically the same as a magnetic flux. In two dimensions, there is just one

component

$$\mathcal{B}_n(\boldsymbol{k}) = \frac{\partial \mathcal{A}_{nx}}{\partial k_y} - \frac{\partial \mathcal{A}_{ny}}{\partial k_x}. \tag{75}$$

Now let us consider the properties of $\mathcal{B}_n$ under the inversion and time-reversal symmetries we have yet to use. Under inversion, $\boldsymbol{k} \to -\boldsymbol{k}$, which, because of the derivatives implies that $\mathcal{B}_n(-\boldsymbol{k}) = \mathcal{B}_n(\boldsymbol{k})$. Under time reversal, we also have $\boldsymbol{k} \to -\boldsymbol{k}$, but in addition the wavefunction undergoes complex conjugation. The latter imparts an addition minus sign, so that $\mathcal{B}_n(-\boldsymbol{k}) = -\mathcal{B}_n(\boldsymbol{k})$. These two conditions are compatible only if

$$\mathcal{B}_n(\boldsymbol{k}) = 0, \qquad \text{with } TR \times I. \tag{76}$$

Eq. (76) is true provided the smoothness and non-crossing condition of eigenstates, which we assumed, is obeyed. This means it is true for all $\boldsymbol{k}$ *except the Dirac points*. At the Dirac points, the crossing means that the Berry gauge field is not well-defined, as the eigenstate associated with each band is also not defined.

However, we can consider a loop encircling a Dirac point,

$$\Theta = \oint_K d\boldsymbol{k} \cdot \boldsymbol{\mathcal{A}}_n(\boldsymbol{k}), \tag{77}$$

where the subscript K indicates the line integral is taken around the Dirac point at (say) the K point of the Brillouin zone. This is a Berry phase: it gives the phase evolved under adiabatic evolution of a wavefunction through this loop. The quantity is invariant under single-valued gauge transformations, because it is the integral of a gradient, but changes under large but smooth gauge transformations, e.g. $\chi(\boldsymbol{k}) = p\theta(\boldsymbol{k})$, where $\theta(\boldsymbol{k})$ is the angle of the $\boldsymbol{k}$ point measured from the location of the Dirac point, and p is an integer so that the gauge transformation is single valued. This means that Θ is defined modulo 2π. It turns out that for a Dirac electron, the value of theta is actually

$$\Theta = \pi (\text{mod } 2\pi). \tag{78}$$

This is easily worked out from the eigenfunction of the Dirac Hamiltonian, or microscopically from the Bloch Hamiltonian of the graphene model.

The non-trivial value of π for the Berry phase implies the stability of the band touching, as can be argued as a proof by contradition. Suppose the band touching were to be removed by a small perturbation. Then we would require Eq. (76) to hold everywhere, including at the former Dirac point. Then we could use Stokes' theorem to express Θ in Eq. (77) as the area integral of $\mathcal{B}_n$ inside the loop, which would immediately have to vanish. However, a small perturbation can make only small changes in the Bloch states far from a degeneracy point, and so the loop integral cannot change discontinuously. We conclude that the band touching cannot be lifted by any small perturbation

preserving time-reversal and inversion symmetry. What can in fact happen, if symmetry allows it, is for the Dirac point to move in $\boldsymbol{k}$ space under the effect of perturbations (this is allowed if we break the 3-fold lattice rotation symmetry). Then the two Dirac points can drift and annihilate.

By similar arguments, we can obtain the quantization of Θ, which must be a multiple of π (including 0) around *any* loop, modulo 2π, and also the "fermion doubling" result that there must be an even number of such Dirac points. I leave these as exercises to the reader.

4.2 *Weyl point*

The stability of the Weyl point can also be understood more deeply using the Berry phase ideas discussed above for the 2d Dirac case. In three dimensions, for non-degenerate bands away from the touching point, we can still introduce the Berry gauge field from Eq. (72), but with three components. Now it has the full structure of a conventional electromagnetic vector potential, so we can define the full analog of a three-dimensional magnetic field,

$$\boldsymbol{\mathcal{B}}_n = \boldsymbol{\nabla} \times \boldsymbol{\mathcal{A}}_n, \tag{79}$$

which is the three-dimensional Berry curvature. It is by definition divergence free

$$\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{B}}_n = 0, \tag{80}$$

away from any singularities like the Weyl point. This means the Berry flux forms field lines which can emanate or terminate only at band touchings like the Weyl point, which appears as a "monopole" of Berry flux.

To see this that the monopole charge indeed is non-zero, we can consider the integral explicitly for a surface around the Weyl point. For this purpose, let us take the simplest example of a Weyl point in which we take $v_\mu = v$ all equal in Eq. (57), and let us compute the integral over a spherical surface around the Weyl point, since the result is independent of the shape of the surface using Eq. (80) and Gauss' theorem. For this choice, the Bloch eigenfunction for the positive band (the negative band can be readily worked out by the same method) is determined by the equation

$$\begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix} |\phi\rangle = k|\phi\rangle. \tag{81}$$

This has the solution

$$|\phi\rangle = \begin{pmatrix} \sqrt{\frac{k+k_z}{2k}} \\ \frac{k_x+ik_y}{\sqrt{2k(k+k_z)}} \end{pmatrix}. \tag{82}$$

Note that this eigenfunction depends only on $\hat{\boldsymbol{k}}$ and not the magnitude of $\boldsymbol{k}$ as is expected, and is singular along the "south pole" $\hat{\boldsymbol{k}} = -\hat{\boldsymbol{z}}$. The eigenfunction

cannot be a global analytic function on the sphere, but necessarily has some spurious singularity in some direction. This is a gauge artifact, and is related to the famous "Dirac string". Physical quantities like the Berry curvature are non-singular everywhere, as we will readily see. From this eigenfunction, we can compute the Berry gauge field,

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix} -\frac{k_y}{2k(k+k_z)} \\ \frac{k_x}{2k(k+k_z)} \\ 0 \end{pmatrix}. \tag{83}$$

Since it is not gauge invariant, the Berry vector potential is also singular at $k_z = 0$. Now taking the curl, we finally obtain the simple and physical result

$$\boldsymbol{\mathcal{B}} = \frac{\boldsymbol{k}}{2k^3} = \frac{\hat{\boldsymbol{k}}}{2k^2} \tag{84}$$

The surface integral is then easily computed,

$$\int d\hat{\boldsymbol{k}} \cdot \boldsymbol{\mathcal{B}} = 4\pi k^2 \frac{1}{2k^2} = 2\pi. \tag{85}$$

We see that the Weyl point appears as a monopole of strength 2π, i.e. Eq. (80) can be replaced by

$$\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{B}} = 2\pi\delta(\boldsymbol{k}). \tag{86}$$

Notably, had we considered the lower band, we would have obtained a -2π strength monopole.

The stability of the Weyl point follows from similar arguments to those we used for the Dirac point in two dimensions. The non-zero integral over Berry curvature and the divergence-free condition away from band crossings implies that there must be a crossing inside the integration volume. Since the integral can be taken at a finite radius, far from the crossing, the Weyl point can at most move smoothly with a small perturbation. In this case, no symmetry at all is required for stability, other than the translational invariance required to define the bands themselves.

There are interesting constraints also on the number and types of Weyl points. We can assign them an integer charge in units of 2π. The total charge of all Weyl points must vanish. This is because the Brillouin zone is a closed manifold, and any field lines emerging at a "source" monopole must terminate at a corresponding "sink". Thus the minimal number of Weyl points is two. Furthermore, if time reversal symmetry is preserved, there must be at least four Weyl points. This is because, under time-reversal a Weyl point at $\boldsymbol{k} = \boldsymbol{K}$ is exchanged with another Weyl point at $\boldsymbol{k} = -\boldsymbol{K}$ of the same charge. There must be another set of oppositely charged Weyl points elsewhere to compensate the non-zero charge of these two Weyl points. The situation with the minimal number allowed of only two toyal Weyl points conversely must break

time-reversal symmetry. We will see soon that there are immediate physical consequences of this broken time-reversal.

5 Insulators and topology

From the low energy point of view, insulators appear completely trivial: there are simply no low energy states below the band gap. However, we can still ask the question: are there different types of qualitatively distinct gapped states? One way to formulate this is to ask if every band insulator can be smoothly transformed into every other one? The answer is no. Moreover, it turns out that if we relax the basic framework of periodic boundary conditions/infinite volume to consider finite volume with a boundary, then the distinctions between different band insulators can appear in the energy spectrum as edge states.

5.1 *Two Dirac masses*

The simplest such situation is in two dimensions. Let us return to the graphene model of Sec. 3.2 and add some perturbations that turn the Dirac semimetal into an insulator. For the moment, we will consider spinless Dirac electrons, governed by Eq. (53). We saw that, for spin-independent interactions, there are two possible "mass" terms which could be added that maintain the translational symmetry of the lattice. Consider the Hamiltonian with both these terms added:

$$H = \sum_{k} \psi_k^\dagger v \left(\mu^z \tau^x k_x + \tau^y k_y + m_1 \tau^z + m_2 \mu^z \tau^z \right) \psi_k. \tag{87}$$

Here the mass m_1 is time-reversal invariant, and could be realized by adding a staggered potential of opposite sign on the A and B sublattices. The mass m_2 is odd under time-reversal, and can be realized by adding a second neighbor hopping (dashed lines in Fig. 2) which is pure imaginary and has a positive (negative) sign for second neighbors reached by "turning" right (left) when walking two steps on the lattice. The honeycomb model with imaginary second neighbor hopping is known as the *Haldane model*, after Haldane introduced it for reasons to become clear below. Since μ^z commutes with the one-particle terms in Eq. (87), it is a constant of the motion and can be treated as equal to ± 1. Then the energy dispersion is easily calculated as a function of μ^z to be

$$\epsilon_{\pm,k}(m_1, m_2) = \pm \sqrt{v^2 k^2 + (m_1 + \mu^z m_2)^2}. \tag{88}$$

We see that either m_1 or m_2 alone introduces a gap; however, the gap vanishes if $|m_1| = |m_2|$, by taking $\mu^z = -\text{sign}(m_1/m_2)$. If one plots a "phase diagram" in the $m_1 - m_2$ plane, there are four gapped regions separated by "phase boundaries". At least in this model, it is not possible to pass from the "charge density wave" insulator with $m_1 \neq 0, m_2 = 0$ to the "time-reversal broken" insulator with $m_1 = 0, m_2 \neq 0$, without passing through a model in

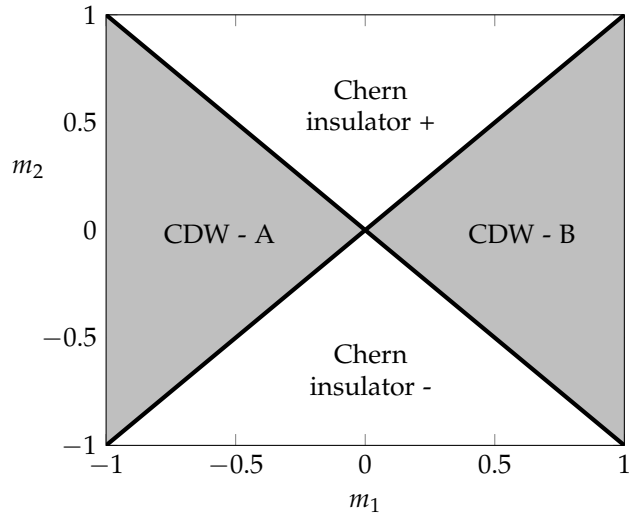


Figure 3: "Phase diagram" showing effects of masses on 2d Dirac fermions. The labels "CDW-A" and "CDW-B" indicate charge density wave regions in which the electrons are localized preferentially on the A or B sublattice sites, respectively.

which the gap vanishes. When the gap does vanish, on the $|m_1| = |m_2|$ lines, it does so for just one of the two Dirac points.

What is the physical meaning of this? It turns out that the two separated gapped insulators are indeed physically distinct phases. The "charge density wave" insulator is a simple band insulator, while the "time-reversal broken" insulator is a type of *topological insulator*, known as a *Chern insulator*, or *quantum Hall state*. The simplicity of the charge-density wave insulator can be seen by simply going back to the lattice model and increasing the staggered potential until it is very large. This process is smooth and no phase transitions occur: the gap increases monotonically as the potential is increased. When the potential is very strong, the insulator itself becomes atomic in nature: one electron resides each site of one of the sublattices (the one with much lower energy), while the other sublattice is empty. There is virtually no motion of the electrons.

5.2 *Edge state*

The Chern insulator, by contrast, does not have a simple atomic limit. This leads to interesting phenomena at an interface between the two. Let us consider modeling such an interface by the Dirac Hamiltonian but with masss $m_1(y), m_2(y)$ that are functions of y, with the interface located at $y = 0$. For $y \to \infty$, we have the charge density wave, and $m_1 > 0, m_2 = 0$, while for $y \to \infty$, we have the Chern insulator, and $m_1 = 0, m_2 > 0$. We assume the masses vary smoothly between the two regions, and write the Dirac equation

in the position representation in the y direction:

$$H = \sum_{k_x} \int dy\, \psi^\dagger_{k_x}(y) \left[v k_x \mu^z \tau^x - i v \tau^y \partial_y + (m_1(y) + m_2(y)\mu^z)\tau^z \right] \psi_{k_x}(y). \tag{89}$$

The single-particle eigenfunctions that diagonalize the Hamiltonian obey

$$\left[v k_x \mu \tau^x - i v \tau^y \partial_y + (m_1(y) + m_2(y)\mu)\tau^z \right] \phi_{k_x}(y) = \epsilon_{k_x} \phi_{k_x}(y). \tag{90}$$

Here we replaced $\mu^z \to \mu = \pm 1$ to indicate that we can treat the two eigenvalues of μ^z independently, as constants. Let us seek a solution in which ϕ is an eigenstate of τ^x, i.e. $\tau^x \phi = \tau \phi$, with $\tau = \pm 1$. We can rewrite $i\tau^y = \tau^z \tau^x = \tau^z \tau$ when acting on ϕ. Hence we have

$$\left[\tau \mu v k_x + \tau^z \left(-\tau v \partial_y + (m_1(y) + \mu m_2(y)) \right) \right] \phi_{k_x}(y) = \epsilon_{k_x} \phi_{k_x}(y). \tag{91}$$

This is consistent under the conditions:

Lecture 5 (1h 15mins)
January 30th, 2018

$$\epsilon_{k_x} = \tau \mu v k_x, \tag{92}$$

$$\left(-\tau v \partial_y + (m_1(y) + \mu m_2(y)) \right) \phi_{k_x}(y) = 0. \tag{93}$$

The second equation has a formal solution:

$$\phi_{k_x}(y) = A e^{\int_0^y dy' \frac{m_1(y') + \mu m_2(y')}{\tau v}}. \tag{94}$$

This solution is formal because this function is only normalizable if the exponential becomes large and negative at *both* $y \to +\infty$ and $y \to -\infty$. This requires $(m_1 + \mu m_2)/\tau < 0$ as $y \to +\infty$ and $(m_1 + \mu m_2)/\tau > 0$ as $y \to -\infty$. In turn this implies that the sign of $m_1 + \mu m_2$ is opposite at $y = \pm\infty$. The interface between the Chern and band insulator satisfies this condition. Specifically, in the band insulator at $y = +\infty$, $m_1 > 0$ and $m_2 = 0$, so the sign $m_1 + \mu m_2$ is positive, while in the Chern insulator, $m_1 = 0$ and $m_2 > 0$, so the sign of $m_1 + \mu m_2$ is the sign of μ. Hence for $\mu = -1$, the sign is different, and we obtain convergence for $\tau = -1$. So we obtain a *single branch* of modes (those with $\mu = \tau = -1$ which have such a special eigenstate, for which the dispersion relation is

$$\epsilon_{k_x} = v k_x. \tag{95}$$

This is a one-dimensional branch of states, whose wavefunction is exponentially localized at the interface between the Chern and band insulator. The mode resides *inside* the band gap, which is required for exponential localization, and which means that its low energy states reside at the Fermi energy even when the bulk of both insulators exhibit a gap. Importantly, the mode is *chiral*, in that the group velocity in the x direction, parallel to the interface, is positive. This is called a chiral edge state, and is characteristic of the integer quantum Hall effect.

The chiral edge state is the only low energy mode in this system. So below

some energy scale (roughly the bulk gap), the low energy effective theory just includes this one mode:

$$H_{\text{eff}} = \sum_{k_x} v k_x \, \psi^\dagger_{k_x} \psi_{k_x} = \int dx \; -iv\psi^\dagger \partial_x \psi. \tag{96}$$

The chirality of the edge state gives it a great deal of robustness. Perturbations at the edge, including disorder, cannot make a low energy electron turn around, because all the available states propagate in the same direction. We say that there is no backscattering possible. This means that the edge state cannot become localized by disorder, and in fact has an *infinite conductivity* (but not infinite conductance - we will come back to this).

5.3 *Chern number*

The gapless edge state appearing at the boundary between the charge density wave and Chern insulators suggests there is something qualitatively different about the two phases. Indeed there is, and the distinction is topology. We can understand it based on the Berry phase discussion we began earlier in Sec. 3.2. Let us consider the total Berry curvature of a filled band, which is a gauge independent quantity:

$$\Theta = \int_{BZ} d^2\boldsymbol{k} \, \mathcal{B}_n(\boldsymbol{k}), \tag{97}$$

where the integral is taken over the full Brillouin zone. This is actually a famous object, which is known to be a quantized topological invariant: 2π times the *Chern Number*,

$$\Theta = 2\pi C, \tag{98}$$

where C is an integer. Chern proved a general result that a "curvature" integrated over a two-dimensional closed manifold is quantized. Here the curvature is $\mathcal{B}$, and the manifold is the Brillouin zone, which is a torus. Eq. (97) can be regarded as the integral of the Berry flux normal to the surface of the torus.

One can understand this quantization more directly here by using Stoke's theorem to rewrite it as the line integral around some *arbitrary* "boundary" of the Brillouin zone:

$$\Theta = \oint_{\partial(BZ)} d\boldsymbol{k} \cdot \boldsymbol{\mathcal{A}}_n(\boldsymbol{k}). \tag{99}$$

For example for a square Bravais lattice with unit spacing we can take $-\pi < k_x < \pi$ and $-\pi < k_y < \pi$, and the line integral in Eq. (99) becomes an integral around the square. Now we can take advantage of gauge invariance to choose a specific gauge. We can definitely choose the "Landau gauge" where $\mathcal{A}_y = 0$.

Then the integral becomes

$$\Theta = \int_{-\pi}^{\pi} dk_x \mathcal{A}_x(k_x, -\pi) - \int_{-\pi}^{\pi} dk_x \mathcal{A}_x(k_x, \pi) = \theta_x(-\pi) - \theta_x(\pi) \tag{100}$$

This is a difference of two line integrals, $\theta_x(\pm\pi)$ which are actually defined on *loops* in parameter space, since $k_x = \pm\pi$ are equivalent points. Thus each $\theta_x(k_y)$ is actually itself a gauge-invariant Berry phase, and furthermore $k_y = \pi$ and $k_y = -\pi$ are equivalent. This means that these physical quantities must be equal up to a multiple of 2π, i.e. $\theta_x(-\pi) = \theta_x(\pi) + 2\pi C$. This shows the desired quantization.

There are a number of implications of a non-zero Chern number. One is that it is an *obstruction* to the construction of a smooth, periodic set of Bloch functions, over the full Brillouin zone. This is because if such a set exists, then $\boldsymbol{\mathcal{A}}$ and $\mathcal{B}$ are single valued, and therefore the integral, Eq. (97) of a curl over a continuous periodic surface without boundary (the torus) is necessarily zero (equivalently, opposite sides of the line integration in Eq. (99) or Eq. (100) must cancel exactly. Another view of the Chern number is from Eq. (100), which shows that it can be considered a "winding number" of $\theta_x(k_y)$. In fact, $\theta_x(k_y)$ has the physical interpretation of a "polarization", and the winding number of this polarization is related to something called a Thouless pump. Not sure if I will talk about this.

5.4 *Hall conductivity*

Now we are going to show that the Chern number is directly related to an easily measured quantity: the Hall conductivity. To do so, we first derive a general formula for the conductivity called the Kubo formula. This follows the general problem of linear response theory. We apply a small perturbation to the Hamiltonian of a system – in this case an electric field – and observe its effect upon the expectation value of another quantity – in this case the current density. The standard way to do this is to choose a gauge with zero scalar potential, so that the electric field is $\boldsymbol{E} = -\partial_t \boldsymbol{A}$, where $\boldsymbol{A}$ is the vector potential. For a spatially constant but in general AC electric field, we can take $\boldsymbol{A}(t) = \mathrm{Re}\,[\boldsymbol{E}/(i\omega)e^{-i\omega t}]$. The vector potential may be included by the minimal coupling procedure, which amounts to replacing $\boldsymbol{k} \to \boldsymbol{k} + e\boldsymbol{A}$, i.e. using the Hamiltonian

$$H(A) = \sum_{\boldsymbol{k}} \hat{h}_{ss'}(\boldsymbol{k} + e\boldsymbol{A}) c^\dagger_{s\boldsymbol{k}} c_{s'\boldsymbol{k}}. \tag{101}$$

The current density is defined by the derivative of the Hamiltonian (or of the action in the field theory) with respect to the vector potential, hence

$$\boldsymbol{j} = -e\frac{1}{V}\sum_{\boldsymbol{k}} \frac{\partial \hat{h}_{ss'}(\boldsymbol{k} + e\boldsymbol{A})}{\partial \boldsymbol{k}} c^\dagger_{s\boldsymbol{k}} c_{s'\boldsymbol{k}}, \tag{102}$$

where V is the system volume. Note that there is some explicit dependence on the vector potential in the current. For small electric fields, we can expand it:

$$j_\mu = -e\frac{1}{V}\sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}}\left[\frac{\partial \hat{h}}{\partial k_\mu} + e\frac{\partial^2 \hat{h}}{\partial k_\mu \partial k_\nu}A_\nu\right] c_{\boldsymbol{k}}, \tag{103}$$

where now $\hat{h}$ is evaluated with zero vector potential. Working to linear order in the electric field, and taking expectation values in the system with the field, we have

$$\begin{aligned} \langle j_\mu\rangle &= -e\frac{1}{V}\sum_{\boldsymbol{k}}\left[\left\langle c^\dagger_{\boldsymbol{k}}\frac{\partial \hat{h}}{\partial k_\mu}c_{\boldsymbol{k}}\right\rangle_1 + eA_\nu\left\langle c^\dagger_{\boldsymbol{k}}\frac{\partial^2 \hat{h}}{\partial k_\mu \partial k_\nu}c_{\boldsymbol{k}}\right\rangle_0\right] \\ &= \langle \mathrm{j}_\mu\rangle_1 - e^2 A_\nu \langle \mathrm{Q}_{\mu\nu}\rangle_0, \end{aligned} \tag{104}$$

with

$$\mathrm{j}_\mu = -e\frac{1}{V}\sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}}\frac{\partial \hat{h}}{\partial k_\mu}c_{\boldsymbol{k}}, \tag{105}$$

and

$$\mathrm{Q}_{\mu\nu} = \frac{1}{V}\sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}}\frac{\partial^2 \hat{h}}{\partial k_\mu \partial k_\nu}c_{\boldsymbol{k}}. \tag{106}$$

In Eq. (104) the subscript indicates the order to which the expectation value should be calculated in the vector potential.

Now we can use the linear response formalism to obtain the first term. This is a standard treatment, which we convered in Physics 217a (please see Sec. 5.4 of those notes). The standard result is that, in the presence of a time-dependent perturbation $H'(t)$ of a Hamiltonian, the first order shift of the expectation value of an operator $\mathcal{O}$ is

$$\langle \mathcal{O}(t)\rangle_1 = \langle \mathcal{O}(t)\rangle_0 - i\int dt' \,\langle\left[\mathcal{O}(t), H'(t')\right]\rangle_0 \,\theta(t-t'). \tag{107}$$

Taylor expanding the Hamiltonian in Eq. (101), we have

$$H'(t) = -V\boldsymbol{A}(t)\cdot\mathbf{j}(t). \tag{108}$$

So we obtain, using the fact that in equilibrium there is no current density $\langle \mathrm{j}\rangle_0 = 0$,

$$\langle \mathrm{j}_\mu(t)\rangle_1 = iV\left(\int dt' \langle\left[\mathrm{j}_\mu(t), \mathrm{j}_\nu(t')\right]\rangle_0 \theta(t-t')\right) A_\nu(t'). \tag{109}$$

Using the form of the vector potential in terms of electric field, we finally

obtain the conductivity:

$$\sigma_{\mu\nu}(\omega) = \frac{1}{\omega}\left[V\int_0^\infty dt\, e^{i\omega t}\langle\left[\mathrm{j}_\nu(0),\mathrm{j}_\mu(t)\right]\rangle + ie^2\langle \mathrm{Q}_{\mu\nu}\rangle_0\right]. \tag{110}$$

This is called the Kubo formula for the conductivity. The second term in the current (proportional to $\langle \mathrm{Q}\rangle$) is the so-called "diamagnetic" contribution. It is manifestly symmetric in μ,ν, and consequently does not contribute to the Hall conductivity, which is *defined* as the anti-symmetric part of the conductivity tensor. In two dimensions, there is just one component $\sigma_H = (\sigma_{xy}-\sigma_{yx})/2$. It is instructive to write the Kubo formula for σ_H in a spectral representation, by just inserting complete sets of states:

(111)

$$\begin{aligned}
\sigma_H(\omega) &= \frac{V}{2\omega}\int_0^\infty dt\frac{e^{i\omega t}}{Z} \\
&\quad \mathrm{Tr}\Big[e^{-\beta H}\left(\mathrm{j}_y e^{iHt}\mathrm{j}_x e^{-iHt} - e^{iHt}\mathrm{j}_x e^{-iHt}\mathrm{j}_y - \mathrm{j}_x e^{iHt}\mathrm{j}_y e^{-iHt} + e^{iHt}\mathrm{j}_y e^{-iHt}\mathrm{j}_x\right)\Big] \\
&= -\frac{V}{\omega}\int_0^\infty dt\frac{e^{i\omega t}}{Z}\sum_{mn} e^{-\beta E_m}\epsilon_{ij}\langle m|\mathrm{j}_i|n\rangle\langle n|\mathrm{j}_j|m\rangle\cos(E_n-E_m)t \\
&= V\sum_{mn}\frac{e^{-\beta E_m}}{Z}\epsilon_{ij}\langle m|\mathrm{j}_i|n\rangle\langle n|\mathrm{j}_j|m\rangle\frac{1}{2i\omega}\left[\frac{1}{\omega+E_m-E_n}+\frac{1}{\omega+E_n-E_m}\right].
\end{aligned}$$

We are interested in the low frequency limit. Taylor expanding the term in the square brackets, the dc limit is

Lecture 6 (1h 15mins)
February 1st, 2018

$$\sigma_H = V\sum_{m\neq n}\frac{e^{-\beta E_m}}{Z}\frac{i\epsilon_{ij}\langle m|\mathrm{j}_i|n\rangle\langle n|\mathrm{j}_j|m\rangle}{(E_n-E_m)^2}. \tag{112}$$

We can take $m\neq n$ because the numerator vanishes for $m=n$ (and the denominator's singular is regularized by the limit $\omega\to 0$). This expression is in terms of the many-body eigenstates and many-body energy levels. For free fermions, we can now proceed to re-express it in terms of single-particle states. For this, we start with Eq. (105) and apply the change of basis formula, $c_{ks} = \sum_n \phi^{(n)}_{k,s} c_{kn}$ to convert to the basis of Bloch eigenstates n. Keeping the index s of the sites/orbital symbolic, we can write this as

$$c_{\boldsymbol{k}} = \sum_n |\phi^{(n)}_{\boldsymbol{k}}\rangle c_{\boldsymbol{k},n}, \tag{113}$$

where now n sums over Bloch eigenstates/bands. The current operator is then

$$\mathrm{j}_\mu = -e\frac{1}{V}\sum_{\boldsymbol{k}}\sum_{nn'}\langle\phi^{(n')}_{\boldsymbol{k}}|\frac{\partial\hat{h}}{\partial k_\mu}|\phi^{(n)}_{\boldsymbol{k}}\rangle c^\dagger_{\boldsymbol{k},n'}c_{\boldsymbol{k},n} \tag{114}$$

Inserting this into Eq. (112), we see that because we have $m \neq n$, the only contributions arise from $n' \neq n$ in the current operators. Physically, the Fock state $|n\rangle$ must be obtained by removing one electron from single particle state n and adding one to state n'. So we obtain

$$\sigma_H = e^2 \frac{1}{V} \sum_{\boldsymbol{k}} \sum_{nn'} \frac{i\epsilon_{ij} \langle \phi_{\boldsymbol{k}}^{(n)} | \frac{\partial \hat{h}}{\partial k_i} | \phi_{\boldsymbol{k}}^{(n')} \rangle \langle \phi_{\boldsymbol{k}}^{(n')} | \frac{\partial \hat{h}}{\partial k_j} | \phi_{\boldsymbol{k}}^{(n)} \rangle}{(\epsilon_{n\boldsymbol{k}} - \epsilon_{n'\boldsymbol{k}})^2} n_F(\epsilon_{n\boldsymbol{k}})(1 - n_F(\epsilon_{n'\boldsymbol{k}})), \tag{115}$$

where $n_F(\epsilon)$ is the Fermi function. This is valid at any temperature for free fermions. Now by differentiating the Schrödinger equation for the Bloch functions, we obtain the identity

$$\langle \phi_{\boldsymbol{k}}^{(n)} | \frac{\partial \hat{h}}{\partial k_i} | \phi_{\boldsymbol{k}}^{(n')} \rangle = (\epsilon_{n\boldsymbol{k}} - \epsilon_{n'\boldsymbol{k}}) \langle \frac{\partial}{\partial k_i} \phi_{\boldsymbol{k}}^{(n)} | \phi_{\boldsymbol{k}}^{(n')} \rangle = -(\epsilon_{n\boldsymbol{k}} - \epsilon_{n'\boldsymbol{k}}) \langle \phi_{\boldsymbol{k}}^{(n)} | \frac{\partial}{\partial k_i} \phi_{\boldsymbol{k}}^{(n')} \rangle. \tag{116}$$

Using this identity for both matrix elements in the numerator, we can cancel the denominator and obtain

$$\begin{aligned} \sigma_H &= \frac{e^2}{V} \sum_{\boldsymbol{k}} \sum_{nn'} i\epsilon_{ij} \langle \frac{\partial}{\partial k_i} \phi_{\boldsymbol{k}}^{(n)} | \phi_{\boldsymbol{k}}^{(n')} \rangle \langle \phi_{\boldsymbol{k}}^{(n')} | \frac{\partial}{\partial k_j} \phi_{\boldsymbol{k}}^{(n)} \rangle n_F(\epsilon_{n\boldsymbol{k}})(1 - n_F(\epsilon_{n'\boldsymbol{k}})) \\ &= \frac{e^2}{V} \sum_{\boldsymbol{k}} \sum_{n} i\epsilon_{ij} \langle \frac{\partial}{\partial k_i} \phi_{\boldsymbol{k}}^{(n)} | \frac{\partial}{\partial k_j} \phi_{\boldsymbol{k}}^{(n)} \rangle n_F(\epsilon_{n\boldsymbol{k}}). \end{aligned} \tag{117}$$

In going from the first line to the second, we noticed that the term proportional to two Fermi functions vanishes due to symmetry of the matrix element product in $i \leftrightarrow j$ while multiplied by the ϵ_{ij} factor. For the other term, the sum over n' is free and becomes a resolution of the identity. Now we can take the infinite volume limit, which converts the result to

$$\sigma_H = e^2 \sum_n \int \frac{d^2\boldsymbol{k}}{(2\pi)^2} \mathcal{B}_n(\boldsymbol{k}) n_F(\epsilon_{n\boldsymbol{k}}). \tag{118}$$

This formula is valid for any free electron system, including both metals and insulators. It was actually derived long ago by Karplus and Luttinger who were concerned with the Hall effect in ferromagnetic metals. There was a big controversy about this but the modern view is that the explanation based on Eq. (118) is largely correct in metals.

For insulators, the Fermi function at zero temperature selects occupied bands, and the integrals are proportional to the Chern numbers of these filled bands. One then obtains from this that (putting back the factor of $\hbar$ set to one throughout to get units correct)

$$\sigma_H(T=0)^{\text{insulator}} = \frac{e^2}{2\pi\hbar} \sum_{n|\epsilon_n<0} C_n = \frac{e^2}{h} \sum_{n|\epsilon_n<0} C_n. \tag{119}$$

This is the celebrated TKKN formula. We have proven the quantization of the

Hall conductivity!

5.5 *Laughlin's argument*

The TKKN formula is beautiful but its origin is a bit opaque. One may also worry that it assumes a perfect periodic solid so that the inevitable imperfections in a real material will mess up the quantization. There is a very appealing and physical argument due to Laughlin that clarifies the physics of the quantized Hall conductivity and shows why it is robust, at least to imperfections.

Laughlin's argument neglects interactions between electrons, but not disorder. It goes something like this. We consider a two dimensional system at zero temperature, and assume that it has a well-defined local conductivity tensor $\sigma_{\mu\nu}$. We further assume that there are no extended states at the Fermi energy. In a clean system, this implies that the system is a band insulator, but we can also allow for disorder, which may induce states at the Fermi energy, provided that in the bulk – i.e. away from any boundaries – those states are localized. In condensed matter physics we say a state is localized if its wavefunction decays exponentially in space away from some region specific to that state. One can think roughly of localized states as states bound to some impurities. We may talk about localization in more detail later. The assumption is basically that the system has no mobile states at the Fermi energy with which to dissipate energy.

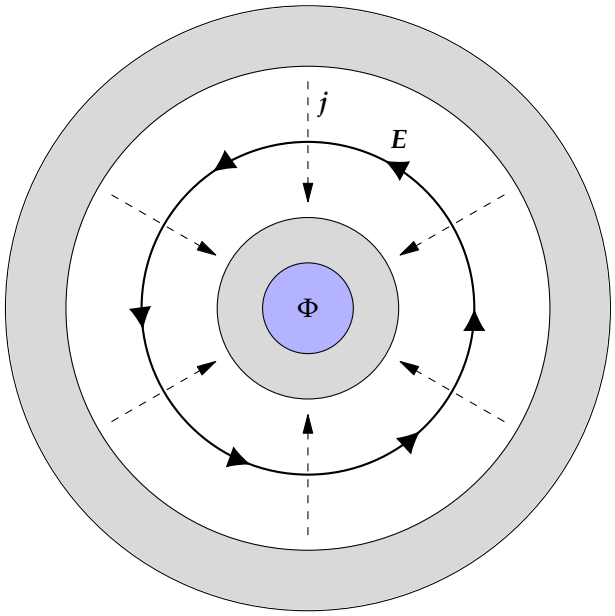


Figure 4: Corbino geometry: the sample is an annulus, with a flux Φ inserted inside the inner hole. No magnetic field penetrates the sample. The time-dependence of the flux during the insertion creates a circumferential electric field $\boldsymbol{E}$. Due to the Hall conductivity a radial current $\boldsymbol{j}$ is produced.

This implies that the symmetric parts of the conductivity tensor vanish, be-

cause the power dissipated in an electric field E_μ is $\sigma_{\mu\nu}E_\mu E_\nu$ which vanishes by assumption. This implies the conductivity tensor in 2d has just two elements $\sigma_H = \sigma_{xy} = -\sigma_{yx}$, the Hall conductivity. Now Laughlin's argument further constrains the magnitude of the Hall conductivity under these assumptions. We can use the conductivity tensor to compute linear response in any geometry, and so choose what is sometimes called the Corbino geometry, which consists of a ring-shaped sample or annulus (one can also formulate the argument using a cylinder). Imagine slowly turning on a magnetic field inside the inner hole of the ring, so that no field at all penetrates the sample itself, but a net flux $\Phi(t)$ passes through the hole. The flux is increased from zero to the flux quantum $\Phi = h/e$ very slowly, so that the response of the system is adiabatic.

Let us first analyze the effect of the flux using linear transport. A time dependent flux is accompanied according to Faraday's law by an electric field, in the azimuthal direction. The electric field is $E_\phi = -\partial_t\Phi/(2\pi r)$, at a radius r from the center of the hole. Accordingly, this creates a radial current $I = 2\pi r\sigma_H E_\phi = -\sigma_H\partial_t\Phi$. Integrating the current over time, we obtain a total transfer of charge from the outer to inner radius of

$$Q = -\sigma_H(\Phi(t_f) - \Phi(0)) = -\frac{h}{e}\sigma_H. \tag{120}$$

Now we will argue that the transferred charge must be an integer multiple of the elementary charge e. To see this we use quantum mechanics. The flux is included in quantum mechanics by a vector potential $A_\phi(r) = \Phi(t)/(2\pi r)$ along the tangential direction at radius r, which is included via minimal coupling as usual. After the flux is increased to h/e, the Hamiltonian reaches a form which is equivalent up to a gauge transformation, $\psi \to e^{i\phi}\psi$, where ϕ is the azimuthal angle in the plane, to the one with zero flux. At the single-particle level, we may write that

$$\mathcal{H}(\Phi = \frac{h}{e}) = e^{-i\phi}\mathcal{H}(\Phi = 0)e^{i\phi}, \tag{121}$$

where $\mathcal{H}$ is the single-particle Hamiltonian, and ϕ is the operator representing the azimuthal angle. This is a unitary transformation, which implies that the energy levels and single particle states (up to phases) are the same before and after the flux insertion. However, in the middle of the insertion process, the energies and states can have evolved. Since the process is assumed adiabatic, we can follow these individual levels through the flux evolution, and they must evolve in such a way that each eigenstate at zero flux evolves into another eigenstate at one flux quantum, i.e. the levels may permute. Note that this argument works for the full finite system, edges included.

A given single particle state s evolves through the flux insertion into another level s' after the insertion. This is called "spectral flow". It is perfectly possible for $s' = s$, but sometimes this is not the case. If both levels s and s' are occupied initially, then the evolution of $s \to s'$ does not change the occupation of the level s', and hence does not change the contribution of this level to the charge density, and specifically to the charge on either boundary.

If both levels are empty, the conclusion is the same. However, if s is occupied and s' is empty, or vice versa, then the level occupation of s' is changed, and the charge density may be modified. Now since we are making a very small change of flux in a large system, we expect that the energy level shifts over the flux insertion will be very small (indeed classically there is no work done by the Hall transport). So the contributions from spectral flow only occur for levels near the Fermi energy. Now the assumption that any states at the Fermi

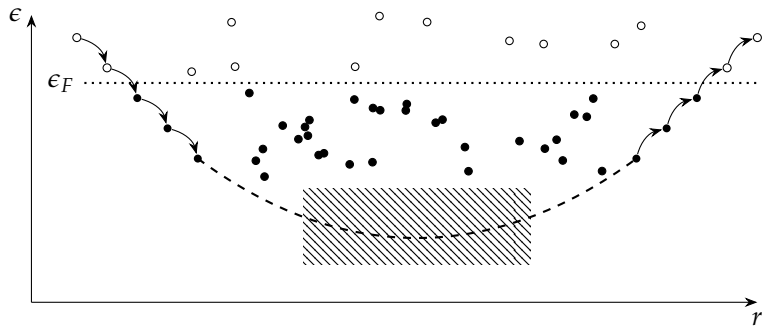


Figure 5: Sketch of spectral flow of single particle levels in the flux insertion process. Initially empty and full states are shown as open and filled circles, respectively. The horizontal axis is the radial distance, with circles showing the centroid of the corresponding levels. States which are extended around the annulus undergo spectral flow near the Fermi energy at the boundaries of the sample. Levels that are localized do not undergo spectral flow, and are indicated as circles without arrows. Some extended states must persist in the bulk, indicated by the dashed line. The spectral flow of levels across the Fermi level determines the number of electrons transferred, n.

level in the bulk are localized comes into play. The Aharonov-Bohm effect is only operative for states which are extended fully around the circumference of the disk, so that an electron in this state is able to sense the phase. For any localized state, the energy and wavefunction must be, up to a phase factor, completely independent of the flux. This implies there is no spectral flow for the levels at the Fermi energy in the bulk.

Knowing this, we therefore understand that any spectral flow at the Fermi level comes entirely from levels at the two edges. The net result can only be a change of population of electrons by some integer n at either edge, and by charge conservation the change must be equal and opposite, so that n electrons are transferred from one edge to another. Equating the charge Q transferred in Eq. (120) to $-ne$ we obtain finally the Hall quantization condition

$$\sigma_H = n\frac{e^2}{h}. \tag{122}$$

The Laughlin argument is powerful because it includes the effects of disorder. It helps to understand the global structure of the extended states, and makes a connection between the IQHE and pumping. A good homework problem is to actually check that pumping occurs in a simple model, by calcu-

Lecture 7 (1h 15mins)
February 6th, 2018

lating the spectral flow explicitly, for example for the Hamiltonian of an edge state obtained in Sec. 5.2.

5.6 *Many-body Chern Invariant*

Laughlin's argument gives a great understanding of how the IQHE is robust against disorder. It is less clear that it is robust against interactions. One way to see this is to start with the edge theory and try to add interactions. Another argument is to generalize the Chern number (and relation to the Hall conductivity) to a many-body formula, without reference to Bloch states. We do this by combining aspects of Laughlin's argument with the Kubo formula.

Let us return to the spectral representation of the Hall conductivity, Eq. (112), and take the zero temperature limit:

$$\sigma_H = \frac{1}{V}\sum_{n>0}\frac{i\epsilon_{ij}\langle 0|\mathsf{J}_i|n\rangle\langle n|\mathsf{J}_j|0\rangle}{(E_n-E_0)^2}, \tag{123}$$

where we defined the "total current operator" $\boldsymbol{J} = V\boldsymbol{j}$. Now we will try to reproduce these matrix elements of the current operator by some physical process. We recall that the current is the derivative of the Hamiltonian with respect to vector potential. We can introduce vector potential without magnetic field in the sample following the Laughlin construction by inserting flux. Consider the usual toroidal sample, but with flux inserted through both "holes" of the torus. This corresponds to taking

$$A_x = \frac{\Phi_x}{L_x}, \qquad A_y = \frac{\Phi_y}{L_y}. \tag{124}$$

This changes the Hamiltonian according to

$$H(\Phi_x,\Phi_y) = H(0,0) - \sum_{i=x,y}\frac{\Phi_i}{L_i}\mathsf{J}_i. \tag{125}$$

Now we have a Hamiltonian as a function of two paramters Φ_x, Φ_y, so we can contemplate the Berry phases accumulated as we move through this two dimensional parameter space. Note that inserting flux is very similar to varying momentum, as a flux (which is a fraction of the flux quantum) can be gauged away at the cost of changing the boundary conditions, which in turn leads to a shift in the allowed quantized discrete momenta. Now consider an infinitesimal change in the flux Φ_i. Standard perturbation theory implies that the change in the ground state wavefunction is

$$\frac{\partial}{\partial\Phi_i}|0\rangle = -\frac{1}{L_i}\sum_{n\neq 0}\frac{\langle n|J_i|0\rangle}{E_n-E_0}|n\rangle. \tag{126}$$

Taking the hermitian conjugate of this equation, and then the overlap of the

two, we obtain

$$\left(\frac{\partial}{\partial\Phi_j}\langle 0|\right)\frac{\partial}{\partial\Phi_i}|0\rangle = \frac{1}{L_iL_j}\sum_n \frac{\langle 0|J_j|n\rangle\langle n|J_i|0\rangle}{(E_n-E_0)^2}. \tag{127}$$

Recognizing $L_xL_y = V$, we get from Eq. (123) that

$$\sigma_H = \hbar i\epsilon_{ij}\left(\frac{\partial}{\partial\Phi_j}\langle 0|\right)\frac{\partial}{\partial\Phi_i}|0\rangle, \tag{128}$$

where we returned the necessary factor of $\hbar$ to make the units correct. We can rewrite this following the Berry phase conventions by defining the gauge connection

$$\mathcal{A}_i(\theta_x,\theta_y) = i\langle 0|\partial_{\theta_i}|0\rangle, \tag{129}$$

where we define the 2π-periodic angles

$$\theta_i = 2\pi\frac{\Phi}{\varphi_0} = \frac{e}{\hbar}\Phi, \tag{130}$$

in SI units where $\varphi_0 = h/e$. Then

$$\sigma_H = \frac{e^2}{\hbar}\mathcal{B}(\theta_x,\theta_y), \tag{131}$$

with

$$\mathcal{B}(\theta_x,\theta_y) = \frac{\partial}{\partial\theta_x}\mathcal{A}_y - \frac{\partial}{\partial\theta_y}\mathcal{A}_x \tag{132}$$

defining the many-body Berry curvature. Eq. (131) shows that the Hall conductivity is a Berry curvature! Now we appeal to the thermodynamic limit: in a large system, the Hall conductivity should not depend upon the value of some tiny flux put through the holes of the torus, i.e. on the boundary conditions. This is a little subtle, but is pretty clear for an insulator, and is maybe even some kind of definition of an insulator. Anyway, we can expect that $\mathcal{B}$ is independent of the angles θ_x,θ_y. We can replace it by its average, so that

$$\sigma_H = \frac{e^2}{\hbar}\int\frac{d^2\theta}{(2\pi)^2}\mathcal{B}(\theta_x,\theta_y) = \frac{e^2}{h}C, \tag{133}$$

where C is the many body Chern number

$$C = \frac{1}{2\pi}\int d^2\theta\,\mathcal{B}(\theta_x,\theta_y), \tag{134}$$

which is quantized to an integer. This shows quantization of the Hall conductivity, without any reference to non-interacting particles, or of translational symmetry for that matter.

5.7 *Chern insulators: summary and bulk-boundary correspondence*

In the prior parts of this section we have come to understand that there are classes of insulators in two dimensions, called Chern insulators, that are non-trivial and cannot be deformed into trivial ones. We described them in a number of ways:

- An example of a Chern insulator occurs in the Haldane model of a honeycomb lattice, which realizes time-reversal breaking opposite mass terms for the two Dirac fermions at the K and K' points.
- The Chern insulator in this example has a chiral edge state.
- The Hall conductivity is quantized and equal to e^2/h times an integer C known as the Chern number. The Chern number may be expressed in various ways, for non-interacting and interacting electrons.
- Laughlin's argument shows that this quantization can be understood as a consequence of spectral periodicity under insertion of a pure flux equal to the flux quantum, and that C describes a spectral flow at the edges of the sample. Equivalently, C gives the number of electrons pumped across the sample when a flux quantum is inserted. A non-zero C requires that there are extended states at the boundaries of the sample.
- The quantization of the Hall conductivity is robust to both disorder and interactions, but occurs only in the limit of zero temperature.

One point we did not comment on explicitly is the *bulk-boundary correspondence*, which is implied in some way by Laughlin's argument. We saw that the Chern insulator in graphene has a single chiral fermion edge state at the boundary to a trivial insulator. It is not too hard to show that it also has a unit Chern number $C = \pm 1$. In fact, this correspondence is general, and there is an identity relating the Chern number to the number of left and right moving modes, N_R and N_L, respectively, at a boundary:

$$C = N_R - N_L. \tag{135}$$

(This equation requires some definition of what "right" and "left" mean but let us not belabor it).

One way to argue for Eq. (135) is to use the fact that the Hall conductivity is given by $e^2/h \times C$, and then to calculate the Hall voltage directly from the low energy model of edge states, and compare the two results. The latter calculation is quite simple. Consider a Hall bar which is infinite in the x direction and boundary by $y = 0, L$ in the vertical direction. Suppose a voltage V_y applied between the top and bottom edges. This induces a shift in the chemical potential for the top modes from equilibrium of μ_L and those at the bottom of μ_0, with $\mu_L - \mu_0 = eV_y$. Now for each mode, the shifted chemical potential induces a change in the density of electrons. This occurs because when the chemical potential is shited by μ, the states between $k = 0$ and $k = -\mu/\hbar|v|$ change their occupation (v is the velocity of the mode). The change in the

electron density for mode a is

$$n_a = -\frac{\mu_a}{2\pi\hbar|v_a|}. \tag{136}$$

Note that electrons are always added with negative μ_a, irrespective of the direction of the velocity of the mode. This is why there is an absolute value here. Now the current induced in this mode is given by $I_a = -n_a e v_a$, which implies

$$I_a = \frac{e}{h}\frac{v_a}{|v_a|}\mu_a \tag{137}$$

Then the total current on a single edge is

$$I_{L/0} = \frac{e}{h}\mu_{L/0}\sum_a \frac{v_a}{|v_a|}. \tag{138}$$

Now we can get the full current in the x direction by taking $I_x = I_L - I_0$,

$$I_x = \frac{e}{h}(\mu_L - \mu_0)\sum_a \frac{v_a}{|v_a|} = \frac{e^2}{h}V_y\sum_a \frac{v_a}{|v_a|}. \tag{139}$$

The final sum is exactly the difference in the number of right and left moving modes, so we see that $I_x = G_{xy}V_y$ with

$$G_{xy} = \frac{e^2}{h}(N_R - N_L). \tag{140}$$

The quantity G_{xy} is the Hall *conductance* rather than the Hall *conductivity*, i.e. it is the ratio of the current to the voltage, rather than the ration of the current density to electric field. However, one can easily show that these are equal in two dimensions. Thus $\sigma_{xy} = G_{xy}$ in this case, and by comparing to the formula Eq. (133) of the Hall conductivity in terms of Chern number, we prove the bulk-boundary correspondence, Eq. (135).

In the second homework, you are asked to show the existence of spectral flow for a chiral edge state under the insertion of the single flux quantum. This can provide another basis for the bulk-boundary correspondence, using the connection of the number of electrons pumped under the flux insertion to the Hall conductivity/Chern number.

5.8 *From Chern to Time-Reversal Symmetric Topological Insulators*

We can use the bulk-boundary correspondence in different ways. One way is to regard the boundary property, i.e. the difference $N_R - N_L$, as the definition of the topological invariant. If we can argue independently of the bulk that this quantity is itself indeed topologically invariant, i.e. it is unchanged by smooth deformations of the Hamiltonian which do not cause a bulk phase transition, then we may not need the bulk definition. This turns out to be possible, and when we generalize beyond the Chern insulators, may be much

easier than the bulk approach. This will lead us to the Z_2 topological insulator with time-reversal symmetry in two dimensions.

Chern insulator and chirality of the edge

To do so, we first think through how we can argue for the edge invariant in the case of the Chern insulator, in a non-interacting picture. This is the "chirality" $N_R - N_L$. Consider a semi-infinite sample in the upper half-plane $y > 0$, with axes chosen so that translational symmetry is maintained along the x direction. Then we can still label states by quasimomentum k_x. The spectrum at a fixed k_x will consist of bulk states, which are extended (scattering) wavefunctions that are not bound to the wall, and bound states. The bulk states can have variable energy even at fixed k_x because the momentum transverse to the wall can change, so these appear as continuous regions in the k_x–ϵ plane (ϵ is the single-particle energy). Since we consider an insulator, the bulk states are separated at all k_x by a non-zero gap. The bound states appear as discrete states at fixed k_x, which then form dispersing curves $\epsilon_n(k_x)$. They must lie within the gap, or they would mix with the continuum states and lose their identity.

Since we are interested in topological features, we can imagine deforming the Hamiltonian so that the conduction and valence bands become horizontal at their edges – this does not close the gap so it is allowed. Then a given set of edge modes consists of a set of curves, the bound state dispersions, lying within the gap. These curves must obey certain rules:

1. A curve cannot end except by passing into the continuum.

2. The total number of discrete bound states at fixed k_x changes only when the end of a curve tied to the continuum passes through this k_x. This just means that discrete states do not appear or disappear at energies away from the continuum.

3. Curves must be smooth except when they intersect (this is just the smoothness of non-degenerate eigenvalues we have already discussed several times).

4. Subject to these rules, the curves may be smoothly deformed, and new curves may be added by smoothly drawing them out of a continuum (the latter corresponds to formation of a bound state).

We may start by considering a "trivial" insulator, by which we mean one which can be deformed to the case with no bound states at all. From this we may pull edge state branches out of the conduction or valence bands. Now we study the numbers N_R and N_L of edge states crossing a particular energy insider the gap. As a new branch is created and pulled across this energy, N_R and N_L change but always do so together, so that $N_R - N_L$ is unchanged. One can convince one's self that this remains true for all deformations allowed by the above rules.

In a similar way, we can consider starting with a situation with one right-moving edge state crossing the gap, so that $N_R - N_L = 1$. Once again, deforming this mode or adding new modes may give rise to additional pairs of right and left moving states at some energies, but the chirality $N_R - N_L$ remains fixed. At least at the level of pictures, we can convince ourselves that $N_R - N_L$ is a topological invariant.

Time-reversal invariant TIs and Z_2 invariant

Lecture 8 (1h 15mins)
February 8th, 2018

For a time-reversal invariant system, the Chern number must be zero. One can readily see that time-reversal symmetry (TRS) implies $\mathcal{B}(\boldsymbol{k}) = -\mathcal{B}(-\boldsymbol{k})$, which forces $C = 0$. Similarly, under TRS, a right-moving edge mode becomes a left-moving edge mode and so $N_R - N_L = 0$ (so the bulk-boundary correspondence in Eq. (135) is still valid but trivial).

However, it turns out that there is a still a topological invariant that survives in the presence of TRS. This is easiest to understand in terms of edge modes. Consider again the semi-infinite sample with translational symmetry and momentum k_x a good quantum number. The presence of the boundary does not spoil TRS, which takes $k_x \to -k_x$. Thus edge modes must come in degenerate pairs at k_x and $-k_x$. In general there are two values of k_x which are time-reversal invariant: $k_x = 0$ and $k_x = Q/2$ where Q is the smallest reciprocal lattice vector of the boundary Brillouin zone. At these time-reversal invariant wavevectors, a two-fold Kramer's degeneracy is required. Apart from these conditions we require the same ones as for the prior case without TRS.

Since the spectrum at k_x is identical to that at $-k_x$, it is sufficient to plot the spectrum for $0 \leq k_x \leq Q/2$. At both ends of this interval, any bound state modes must occur in pairs. Out of the energies within the gap at $k_x = 0$ and $k_x = Q/2$, two edge modes must emanate. Additional modes may emerge from the conductance and/or valence bands. Consider a fixed energy within the band gap and count the number of modes crossing the horizontal line at that energy. Now imagine varying that energy, which sweeps that line up or down. The number of modes crossing may change as that line crosses the local maxima or minima of edge modes, or by crossing the endpoints at $k_x = 0, Q/2$. However, when it does so, the number always changes by a multiple of 2. Thus the parity of the number of modes crossing the line is independent of the energy within the gap. Similarly, we may vary the edge modes rather than the energy at which we count, and the parity conservation holds. Thus we have identified a $\mathbb{Z}_2$ topological invariant, which is just the parity of the number of modes crossing a constant energy line over half the surface Brillouin zone.

This argument leaves many things unresolved. It is not immediately obvious that the invariant defined this way is independent of the choice of surface (it is – though the generalization to three dimensions is not). What is the bulk definition of the invariant, and a bulk-boundary correspondence? We are not going to address these questions now, though we will definitely come back to some related things.

6 Path integral methods

We are going to change gears now and develop some more field theory ideas. Specifically, we will introduce the path integral for fermions. This is a bit of a technical exercise. You need to see it, but perhaps do not need to really remember the details all that often. The results we arrive at in the end will be useful enough to remember, however, as is the general idea of how to get there. These things are covered in many textbooks. The classic reference is Negele and Orland's book, but these days you can find many notes online. Some of them might be helpful to you.

6.1 *Technical details*

Fermion coherent states and Grassmann numbers

To develop field theory in the path integral formulation, we would like to parallel the development for bosonic theories. That began with coherent states, which are eigenstates of the annihilation operator. Now we need to do that for fermions. Start with the case of a single mode, described by operators $c, c^\dagger$ with as usual $\{c, c^\dagger\} = 1$. We seek a state such that

$$c|\mathsf{c}\rangle = \mathsf{c}|\mathsf{c}\rangle, \tag{141}$$

where c is not an operator but a number, and $|\mathsf{c}\rangle$ is the coherent state. We notice a weird property required by fermions, since $c^2 = 0$. This means $c\mathsf{c}|\mathsf{c}\rangle = 0$. If we assume c is an ordinary number that commutes c, then we will find that $\mathsf{c}^2 = 0$. This is a contradiction for ordinary numbers, which implies c is not an ordinary number.

What turns out to work is for c to be what is called a Grassmann number. This is just some abstract object which commutes with ordinary numbers but anticommutes with other Grassmann numbers and with fermion operators. This implies in particular that $\mathsf{c}^2 = 0$ and makes Eq. (141) consistent with fermions. Recall that coherent states of bosons were Gaussian wavefunctions, and could be written as exponentials of creation operators on the vacuum. Solving Eq. (141) is easier than this. When working with Grassmann numbers, Taylor expansion is a powerful thing. Any expansion always terminates at a finite order, because $\mathsf{c}^2 = 0$. For the single fermion mode, one has just

$$|\mathsf{c}\rangle = |0\rangle - \mathsf{c}|1\rangle, \tag{142}$$

where $|0\rangle$ and $|1\rangle$ are the occupation number eigenstates. Another way to write this is

$$|\mathsf{c}\rangle = e^{-\mathsf{c}c^\dagger}|0\rangle, \tag{143}$$

which can be seen to be equal to Eq. (142) by Taylor expanding it. We can also define the bra

$$\langle\bar{\mathsf{c}}| = \langle 0|e^{-c\bar{\mathsf{c}}}, \tag{144}$$

which has the property that

$$\langle \bar{c}|c^\dagger = \langle \bar{c}|\bar{c}. \tag{145}$$

It is important to note that $\bar{c}$ is not the complex conjugate of c and that $\langle \bar{c}|$ is not the hermitian conjugate of $|c\rangle$. Actually $\bar{c}$ has exactly the same status as c: it is just a second Grassmann number. We can find the overlap of the coherent state bra and ket:

$$\langle \bar{c}|c\rangle = e^{\bar{c}c}. \tag{146}$$

Eqs. (141,143,144-146) readily generalize to many fermionic modes, just by adding an appropriate index.

Grassmann calculus

What we've describe so far is enough to do algebra. For example there is a Grassmann algebra which is built by linear combinations of the Grassmann numbers and their products, with complex coefficients. When we multiply states with these numbers we have enlarged the Hilbert space. Anyway, the next step is to learn to integrate and differentiate.

We just define these as linear operations, which have some weird properties

$$\frac{\partial}{\partial c}(a_0 + a_1 c) = a_1, \tag{147}$$

$$\int (a_0 + a_1 c)dc = \int dc(a_0 - a_1 c) = a_1. \tag{148}$$

The differentiation rule seems to make sense, while the integration one is just strange. The logic is that we are trying to emulate integration of well-behaved function on an infinite or periodic interval, for which the integral of a derivative is zero. The integration rule ensures this. If you compare, you will see that "integration is the same as differentiation".

Now we can write the Gaussian integral

$$\int e^{-a\bar{c}c} d\bar{c}dc = \int d\bar{c}dc\, e^{-a\bar{c}c} = a. \tag{149}$$

Work it out! Be careful about the order: $\int d\bar{c}dc = -\int dcd\bar{c}$. Note that this looks superficially similar to the result of an ordinary Gaussian integral over a complex variable except that it is proportional to a rather than $1/a$. You can either work out directly or get the following by differentiating the previous equation by a:

$$\int d\bar{c}dc\, e^{-a\bar{c}c}\bar{c}c = -1. \tag{150}$$

From this we define in the usual way expectation values

$$\langle \mathsf{c}\bar{\mathsf{c}}\rangle = -\langle \bar{\mathsf{c}}\mathsf{c}\rangle = \frac{-\int d\bar{\mathsf{c}}d\mathsf{c}\, e^{-a\bar{\mathsf{c}}\mathsf{c}}\bar{\mathsf{c}}\mathsf{c}}{\int d\bar{\mathsf{c}}d\mathsf{c}\, e^{-a\bar{\mathsf{c}}\mathsf{c}}} = \frac{1}{a}. \tag{151}$$

The result of the expectation value looks the same as that for ordinary Gaussian integrals, so long as one takes the proper order: $\langle \mathsf{c}\bar{\mathsf{c}}\rangle = +1/a$. Now we want to generalize the Gaussian integration formulae to many variables. In the case of real/complex variables we do this by making a change of variables in the path integral to diagonalize the exponential. Change of variables is a little different in Grassmann integrals. Specifically, if we change from variables c_a to d_a, *and the transformation is "odd"*, i.e. c_a is a function expressed as a linear combination of terms each of which contains an odd number of Grassmann numbers d_b, then

$$\int f(\mathsf{c}_a) d\mathsf{c}_1 \cdots d\mathsf{c}_n = \int f(\mathsf{c}_a(\mathsf{d}_b))\, [\det J_{ab}]^{-1}\, d\mathsf{d}_1 \cdots d\mathsf{d}_n, \tag{152}$$

where the Jacobean is

$$J_{ab} = \frac{\partial \mathsf{c}_a}{\partial \mathsf{d}_b}. \tag{153}$$

You can notice this formula is *not* intuitive for integration: in an ordinary integral one would the inverse Jacobean factor. One can also see that something like this is necessary from the simple Gaussian integral in Eq. (149), if you want the answer to be consistent with rescaling fields by $1/\sqrt{a}$. Another way to understand it is to remember that integration is the same as differentiation, so you should use the Jacobean from differentiation.

Using this formula, you can prove the general Gaussian integral identity:

$$\int d\bar{\mathsf{c}}d\mathsf{c}\, e^{-\bar{\mathsf{c}}\cdot A\cdot \mathsf{c}} = \det A, \tag{154}$$

where we used a vector notation where c and $\bar{\mathsf{c}}$ are n-component vectors of Grassmann numbers, and A is an $n \times n$ matrix. Implicitly $d\mathsf{c} = d\mathsf{c}_1 \cdots d\mathsf{c}_n$ etc. Another more general identity is the extension of this one, but with sources. One has

$$\int d\bar{\mathsf{c}}d\mathsf{c}\, e^{-\bar{\mathsf{c}}\cdot A\cdot \mathsf{c} + \bar{\mathsf{c}}\cdot \mathsf{d} + \bar{\mathsf{d}}\cdot \mathsf{c}} = (\det A)\, e^{\bar{\mathsf{d}}\cdot A^{-1}\cdot \mathsf{d}}. \tag{155}$$

From this, we can obtain by (Grassmann) differentiation the general form of all polynomial expectation values. The simplest is

$$\langle \mathsf{c}_a \bar{\mathsf{c}}_b\rangle = \left[A^{-1}\right]_{ab}. \tag{156}$$

One can obtain all the higher polynomial expectation values using Wick's theorem, keeping in mind signs arising from anti-commutations.

6.2 *Trotterization*

Lecture 9 (1h 15mins)
February 13th, 2018

Now we have most of what we need, math-wise. We want to apply it to treat the partition function, $Z = \mathrm{Tr}\, e^{-\beta H}$, as usual by breaking this into many small (imaginary) time intervals and then inserting complete sets of states. We will need both a resolution of the identity and a formula for the trace. It's not hard to work out the resolution of the identity. Let's do it by guessing and proving it is correct. Our guess is

$$\mathbb{I} = \int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} |\mathsf{c}\rangle\langle\bar{\mathsf{c}}|. \tag{157}$$

Let's check:

$$\begin{aligned}
\int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} |\mathsf{c}\rangle\langle\bar{\mathsf{c}}| &= \int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} \left(|0\rangle - \mathsf{c}|1\rangle\right) \left(\langle 0| - \langle 1|\bar{\mathsf{c}}\right) \\
&= \int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} \left(|0\rangle - \mathsf{c}|1\rangle\right) \left(\langle 0| + \bar{\mathsf{c}}\langle 1|\right) \\
&= \int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} \left(|0\rangle\langle 0| - \mathsf{c}|1\rangle\langle 0| + \bar{\mathsf{c}}|0\rangle\langle 1| + \mathsf{c}\bar{\mathsf{c}}|1\rangle\langle 1|\right) \\
&= \int d\bar{\mathsf{c}} d\mathsf{c}\, \left((1 - \bar{\mathsf{c}}\mathsf{c})|0\rangle\langle 0| - \mathsf{c}|1\rangle\langle 0| + \bar{\mathsf{c}}|0\rangle\langle 1| + \mathsf{c}\bar{\mathsf{c}}|1\rangle\langle 1|\right) \\
&= |0\rangle\langle 0| + |1\rangle\langle 1|. \qquad (158)
\end{aligned}$$

So it works! We can prove similarly the somewhat funny looking formula for the trace:

$$\mathrm{Tr}\, \mathcal{O} = \int d\bar{\mathsf{c}} d\mathsf{c}\, e^{-\bar{\mathsf{c}}\mathsf{c}} \langle -\bar{\mathsf{c}}|\mathcal{O}|\mathsf{c}\rangle. \tag{159}$$

This is valid for any bosonic operator $\mathcal{O}$. Note the minus sign inside the bra, the meaning of which might not be so obvious:

$$\langle -\bar{\mathsf{c}}| = \langle 0|e^{\mathsf{c}\bar{\mathsf{c}}}. \tag{160}$$

OK now we are in business! Ready to Trotterize. There are a standard bunch of steps. They look *very* similar to those we did for bosons in Sec.6 of the 217a notes. I will not show the steps in these notes, but maybe do some in class. The result is pretty much what you might guess:

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int [d\bar{\mathsf{c}} d\mathsf{c}] e^{-S}, \tag{161}$$

where the integral is over functions of τ which ranges from 0 to β that obey *anti-periodic* boundary conditions: $\bar{\mathsf{c}}(\beta) = -\bar{\mathsf{c}}(0)$ and $\mathsf{c}(\beta) = -\mathsf{c}(0)$. The action is

$$S = \int_0^\beta d\tau\, \left[\bar{\mathsf{c}}\partial_\tau \mathsf{c} + H(\bar{\mathsf{c}}, \mathsf{c})\right], \tag{162}$$

where in the action the Hamiltonian as a function of the operators $c, c^\dagger$ has been replaced by the same function of Grassmann variables. Similarly, we can calculate observables in the usual way:

$$\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}\hat{T}_\tau \mathcal{O}_1(\tau_1)\cdots\mathcal{O}_n(\tau_n)\right) = \frac{1}{Z}\int [d\bar{c}dc]\mathcal{O}_1(\tau_1)\cdots\mathcal{O}_n(\tau_n)e^{-S}, \tag{163}$$

where $\mathcal{O}(\tau) = e^{H\tau}\mathcal{O}e^{-H\tau}$ are imaginary-time evolved Heisenberg operators, and in going from the left-hand side to the right-hand side we replace operators by fields. A few comments are in order. There are lots of potential subtleties in these naïve continuum expressions, and in principle you should go back to discretization to resolve them. The Hamiltonian should be normal ordered before replacing operators by Grassmanns. And of course, again, the order matters for signs, so take care! After all these warnings, Eqs. (161-163) are pretty nice - they look just like their bosonic counterparts. This makes it all nice and easy to remember!

So far in this section I have been relatively careful to use (sightly!) different symbols for the Grassmann numbers and the fermion operators. In the future, I will be less careful, and when working with path integrals often use the same symbol as I use for the operator in the Hamiltonian formalism. It is usually clear from the context.

6.3 *Simple examples*

Let's show some simple examples of how the path integral for fermions works. Consider free fermions. Then the action is

$$S = \int d\tau \left[\bar{c}_i\partial_\tau c_i + h_{ij}\bar{c}_i c_j\right]. \tag{164}$$

The natural object to consider is the electron Green's function

$$G_{ij}(\tau-\tau') = \langle c_i(\tau)\bar{c}_j(\tau')\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}\hat{T}_\tau\, c_i(\tau)c_j^\dagger(\tau')\right). \tag{165}$$

This has various sorts of information in it. If we take the limit $\tau' \to \tau + 0^+$ and $i = j$, the time-ordering reconstructs the number operator for site i, we will get *minus* (the time-ordering operator requires the appropriate sign for the permutation used in the ordering process) the thermally averaged number of electrons on site i. Alternatively, we may analytically continue the Green's function to real time and obtain a spectral density that informs us about the single-electron excitations of the system.

Let us calculate the thing for free fermions, using the action in Eq. (164). We can simplify it by going to Fourier space. Introduce the Fourier series

$$c_i(\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n} e^{-i\omega_n\tau}c_i(i\omega_n), \qquad \bar{c}_i(\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n} e^{i\omega_n\tau}\bar{c}_i(i\omega_n). \tag{166}$$

Here importantly, to satisfy the anti-periodic boundary conditions on the path

integral, we need to take the "fermionic" Matsubara frequencies

$$\omega_n^{\text{fermion}} = \frac{2\pi}{\beta}(n + \tfrac{1}{2}). \tag{167}$$

In Eq. (166) one should remember that in the path integral, c_i and $\bar{c}_i$ are *not* conjugates in any way, so the choice of the opposite sign of the phase in the definition of the Fourier transform is purely convention, but it is a convenient one. You can regard Eq. (166) as an example of the change of variables formula for the Grassmann integral (this is a linear change of variables, hence "odd"). Putting these series into the action in Eq. (164), we get

$$S = \sum_{i\omega_n} \left[-i\omega_n \delta_{ij} + h_{ij}\right] \bar{c}_i(i\omega_n) c_j(i\omega_n). \tag{168}$$

The action has been block-diagonalized into independent blocks at each Matsubara frequency. Let's further consider the case of a single band and apply the Fourier transformation in space as well:

$$c_i(i\omega_n) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i} c_{\boldsymbol{k}}(i\omega_n), \qquad \bar{c}_i(i\omega_n) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}_i} \bar{c}_{\boldsymbol{k}}(i\omega_n) \tag{169}$$

Now the action is fully diagonalized:

$$S = \sum_{i\omega_n} \sum_{\boldsymbol{k}} \left[-i\omega_n + \epsilon_{\boldsymbol{k}}\right] \bar{c}_{\boldsymbol{k}}(i\omega_n) c_{\boldsymbol{k}}(i\omega_n). \tag{170}$$

Using the Gaussian integral formula, we have

$$\begin{aligned} \langle \hat{n}_{\boldsymbol{k}} \rangle &= -\langle c_{\boldsymbol{k}}(\tau) \bar{c}_{\boldsymbol{k}}(\tau + 0^+) \rangle = -\frac{1}{\beta} \sum_{\omega_n} e^{i\omega_n 0^+} \langle c_{\boldsymbol{k}}(\omega_n) \bar{c}_{\boldsymbol{k}}(\omega_n) \rangle \\ &= -\frac{1}{\beta} \sum_{\omega_n} \frac{e^{i\omega_n 0^+}}{-i\omega_n + \epsilon_{\boldsymbol{k}}} \end{aligned} \tag{171}$$

To calculate this sum, we need to be careful of convergence: the frequency sum should be logarithmically divergent at large ω_n, and it is only the exponential that saves it. To do the sum one uses some standard trick. Consider the following integral:

$$I(C) = \oint_C \frac{dz}{2\pi i} \frac{1}{e^{\beta z} + 1} \frac{e^{0^+ z}}{-z + \epsilon}, \tag{172}$$

where C is a circle of radius R around the origin in the complex plane (choosing R so that it never passes right through a pole). Along this circle, the first factor in the integrand is small when the real part of z is large (the exponential in the denominator blows up), and the second factor is small when the real part of z is negative. This is enough to ensure the convergence as R is taken large. Note that this works only because of the 0^+! Now if we take $R \to \infty$, the integral just becomes zero. We can also evaluate the integral differently, by

summing all the residues of the poles inside this infinite circle. There is one set of poles of the first function, at $z = i\omega_n$, and another pole at $z = \epsilon$. The result is

$$I(C \to \infty) = 0 = -\frac{1}{\beta}\sum_{\omega_n} \frac{e^{i\omega_n 0^+}}{-i\omega_n + \epsilon} - \frac{1}{e^{\beta\epsilon}+1}. \tag{173}$$

So we conclude that

$$\frac{1}{\beta}\sum_{\omega_n} \frac{e^{i\omega_n 0^+}}{-i\omega_n + \epsilon} = -\frac{1}{e^{\beta\epsilon}+1} = -n_F(\epsilon). \tag{174}$$

We obtain the expected result

$$\langle \hat{n}_{\boldsymbol{k}} \rangle = n_F(\epsilon_{\boldsymbol{k}}). \tag{175}$$

Note that the result was entirely determined by the 0^+ sign, and we had to cleverly choose the function $1/(e^{\beta z}+1)$ to obtain convergence of the integral in Eq. (172) and to have poles with constant residue $(1/\beta)$ at the fermionic Matsubara frequencies. If we put a 0^- instead in the sum, we would have needed to choose a different function.

Now let us look at the electron spectral function. There are some nice general rules for obtaining such spectral functions from the correlation functions calculated by the path integral. The standard way is to calculate the spectral function which is defined from the imaginary part of the retarded Green's function,

$$\rho(\omega) = -2\mathrm{Im}\, G_R(\omega), \tag{176}$$

where the retarded Green's function was defined for bosonic operators in the 217a notes in real time as the expectation value of a commutator, along with step function to impose causality. For fermionic operators, the definition is the same except that the commutator should be replaced by an anti-commutator. For the electron operators, we define

$$G_R(t) = -i\left\langle \{c_{\boldsymbol{k}}(t), c^\dagger_{\boldsymbol{k}}(0)\} \right\rangle \theta(t). \tag{177}$$

If you take the Fourier transform of $G_R(t)$, you will find that it can be written as

$$G_R(\omega) = \int \frac{d\omega'}{2\pi} \frac{\rho(\omega')}{\omega - \omega' + i\delta'}, \tag{178}$$

where $\delta = 0^+$, and $\rho(\omega)$ is the spectral function, which is

$$\rho(\omega) = \frac{1+e^{-\beta\omega}}{Z}\sum_{mn} |\langle m|c_{\boldsymbol{k}}|n\rangle|^2 e^{-\beta E_m} \times 2\pi\delta(\omega - E_n + E_m). \tag{179}$$

Note that the analogous formula for bosonic operators is nearly identical, ex-

cept that there would be a relative minus sign in the two terms in the numerator of the prefactor of the sum. This makes the fermionic spectral function slightly "nicer" insofar as it is always positive. From Eq. (178) we can see that it is easy to extract the spectral function from the retarded Green's function:

$$\rho(\omega) = -2\mathrm{Im}\, G_R(\omega). \tag{180}$$

Now how to get the retarded function? This is where the magic happens. By explicitly computing the spectral decomposition of the Matsubara Green's function, one can show that

$$G(i\omega_n) = \langle c_{\boldsymbol{k}}(\omega_n)\bar{c}_{\boldsymbol{k}}(\omega_n)\rangle = -\int \frac{d\omega'}{2\pi}\frac{\rho(\omega')}{i\omega_n - \omega'}, \tag{181}$$

so we can see that, comparing with Eq. (178),

$$G_R(\omega) = -G(i\omega_n \to \omega + i\delta). \tag{182}$$

Hence we get, finally

$$\rho(\omega) = 2\mathrm{Im}\,\left[G(i\omega_n \to \omega + i\delta)\right]. \tag{183}$$

These formulas, Eqs. (176)- (183), are general for any fermionic (odd in the number of fermions) operator. But that of course includes the non-interacting case. For that case we have

$$G(i\omega_n) = \frac{1}{-i\omega_n + \epsilon_{\boldsymbol{k}}}. \tag{184}$$

Applying Eq. (183) and using the standard identity $1/(x - i\delta) = P/x + i\pi\delta(x)$, we get that

$$\rho(\omega) = 2\pi\delta(\omega - \epsilon_{\boldsymbol{k}}). \tag{185}$$

The presence of a delta function is the sign of a particle excitation with energy $\epsilon_{\boldsymbol{k}}$. The prefactor 2π is the maximum possible, and indicates that this is a non-interacting system.

6.4 *Quasiparticles and the self energy*

The theory of solids is built on the foundation of free fermions. For much of the prior content of this class, we in fact relied on the free fermion model. Yet, in fact, the electrons in a solid are pretty far from free, and interact quite strongly with one another. So why does the non-interacting approach work? What exactly does it get right?

The basic explanation comes from Landau. He introduces the idea of an electronic quasiparticle. The Landau quasiparticle picture is one of "smooth" or "adiabatic" evolution of the low energy states of a system with increasing interactions. Consider a non-interacting fermion system. The many-body ground state (best to think of the chemical potential subsumed into the Hamil-

tonian) consists of a set of occupied levels below the Fermi energy, and empty levels above it. The low energy excitations consist of modifying the ground state by occupying a small number of levels above the Fermi energy, and/or emptying a small number of levels below the Fermi energy. If the "small number" is unity, we have what are called *elementary* excitations, electrons and holes, for a single added or removed electron, respectively.

The electronic system has typically a few conserved quantities which can be used to label these states. The charge, or electron number, is one, which of course distinguishes the ground state (neutral if we include the ions), the electrons (charge $-e$) and the holes (charge $+e$). If we have a periodic lattice, then translational symmetry allows us to assign (quasi-)momentum $\boldsymbol{k}$. The ground state typically has $\boldsymbol{k} = 0$, while the electrons and holes have a continuous momentum label. There might also be a spin quantum number if we do not have spin-orbit coupling, etc, and there can be other discrete quantum numbers like a band index.

Once all these quantum numbers are fixed, the energy of the electron or hole state is unique and non-degenerate (but dependent on the specific free Hamiltonian). If we proceed to higher energy states involving more than one excited electron and/or hole, this cease to be true. But we focus in Landau's picture on the elementary excitations, and view the higher energy states as built from these.

Lecture 10 (1h 15mins)
February 15th, 2018

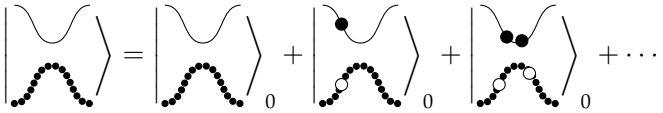
Now consider introducing interactions. Landau postulates that, as interactions are smoothly increased from zero, we can follow the original low energy states smoothly as well: their energies and wavefunctions may evolve, but they remain identifiable and qualitatively similar to their non-interacting counterparts. One may imagine carrying out this smooth continuation via simple perturbation theory in quantum mechanics. In perturbation theory, an isolated level (one without others near it that can mix strongly with it) indeed evolves smoothly. Using ordinary non-degenerate perturbation theory, one obtains a series

$$|n\rangle = |n\rangle_0 + \sum_{m\neq n} \frac{{}_0\langle m|H'|n\rangle_0}{E_n^{(0)} - E_m^{(0)}} |m\rangle_0 + \cdots \tag{186}$$

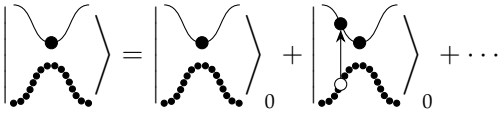
The state $|n\rangle_0$ is an eigenstate of the non-interacting system, and $|n\rangle$ is an exact eigenstate of the interacting Hamiltonian containing interactions H'. Non-smooth evolution may happen when there is a degeneracy in the spectrum, so the idea works best if this is minimized. The best case scenario is in an insulator, where there is a minimum energy (a "gap") required to create an electron or hole excitation, and the lowest energy state so created is indeed unique. In this case, perturbation theory for the elementary excitations, at least those near the bottom of their bands, is very well-behaved.[1]

[1] We are intentionally ignoring a subtlety of many-body systems which is that the sums appearing in naïve perturbation theory contain a huge number of terms – the total number of eigenstates is the exponential of the total entropy so exponentially large in the volume – and so there could be divergences that are purely due to the thermodynamic limit. The physical expectation is that such divergences cancel if one considers local quantities and energy differences between states, rather than absolute energies, at least for simple systems like insulators. Ultimately this belief

Even when perturbation theory is well-behaved, the interacting eigenstates are still linear combinations of the free ones. These combinations are restricted by symmetry. For example, a state obtained by adiabatic continuation of the free ground state can be expressed as a superposition of the free ground state and terms with an equal number of electrons and holes, with zero net momentum. Pictorially,

(187) $|0\rangle =$ 

Similarly, for the exact one quasiparticle state will be a superposition of the bare one electron state, plus ones with additional electron hole pairs of zero net momentum:

(188) $|\boldsymbol{k}\rangle =$ 

One can see in both these cases that for the free system, the terms beyond the first would require additional energy to create, e.g. to make the vertical transition shown by an arrow in the last term in Eq. (188). This means that the coefficients of these terms have a non-zero dominator of this additional energy.

For higher energy states, for example an electron in a highly excited band of the free system, nature is not so kind. Such a single particle state typically has the same energy and momentum as many multiple particle states (with more than one excited electron and hole). This degeneracy makes perturbation theory problematic, and the original particle state may "merge" into the continuum and become imperfectly defined with interactions. Another way of thinking about this merging is that the (high energy) electron can *decay* into a lower energy electron state by emitting one or more electron-hole pairs. For an insulator, such decay is forbidden just by energy conservation for the lowest energy electrons and holes. If we move from insulators to gapless systems like semi-metals or metals, then even for low energy electrons near the Fermi energy, decay is possible, and the situation is subtle.

We can try to see Landau's adiabatic approximation in action by studying the electron spectral function, $\rho(\omega)$. From Eq. (179), we can take the zero temperature limit to obtain

$$\rho(\omega, T=0) = \begin{cases} \sum_n \left|\langle n|c_{\boldsymbol{k}}^\dagger|0\rangle\right|^2 2\pi\delta(\omega - E_n + E_0) & \omega > 0 \\ \sum_m \left|\langle m|c_{\boldsymbol{k}}|0\rangle\right|^2 2\pi\delta(\omega - E_0 + E_m) & \omega < 0 \end{cases} . \tag{189}$$

You can see from here that for $\omega > 0$, the spectral function has contributions

relies upon locality of the Hamiltonian, i.e. that interactions are not too long range. A more precise approach is possible by replacing naïve perturbation theory by the concept of equivalence by local unitaries or finite-depth unitary circuits. Anyway, I think that we don't really need this here and we should be satisfied with a simpler physical understanding.

from "electron" excitations, i.e. states $|n\rangle$ with one more electron than the ground state $|0\rangle$ and a quasi-momentum larger by $\boldsymbol{k}$ than the ground state. For $\omega < 0$, it instead detects "hole" excitations with one less electron than the ground state. The total charge and momentum of the states $|n\rangle$ and $|m\rangle$ is fixed by symmetry, but otherwise any state with these quantum numbers may contribute to the sums.

Following Landau's arguments, we can think of each of the low energy contributions $|n\rangle$ to the electron sum as an exact eigenstate obtained by adiabatic continuation of some eigenstate of the free electron system, and $|0\rangle$ as the exact ground state which is an adiabatic continuation fo the free one. In the case of an insulator, as we discussed, the low energy quasiparticle states have nothing to mix with, and thus are protected from decay. The first term in the spectral function is therefore

$$\rho(\omega > 0) = \left|\langle \boldsymbol{k}|c_{\boldsymbol{k}}^\dagger|0\rangle\right|^2 2\pi\delta(\omega - \epsilon_{\boldsymbol{k}}) + \cdots \tag{190}$$

Thus we expect the δ-function we found for the free case, Eq. (185), remains, but with in general a reduced coefficient. The energy will also be shifted to some renormalized dispersion. Higher energy $|n\rangle$ may not be *adiabatically* continuous from the corresponding free states, but descend from them nonetheless. These higher terms, which give the $\cdots$ in Eq. (190), generally give *continuum* contributions to the spectral function, for example from states of two fully interacting electrons plus a hole, etc.

Let us check this understanding by calculating the spectral function in perturbation theory. The strategy is to use the path integral approach, which naturally calculates the imaginary time Green's function, and then obtain the retarded correlation function and hence $\rho(\omega)$ by analytic continuation. The methodology is very similar to what you should already have done for bosons in physics 217a. Suppose the quadratic Hamiltonian is diagonalized,

$$H_0 = \sum_{n,\boldsymbol{k}} \epsilon_{n\boldsymbol{k}} c_{n\boldsymbol{k}}^\dagger c_{n\boldsymbol{k}}. \tag{191}$$

A general four-fermion interaction U respecting translational symmetry is then

$$H' = \frac{1}{2V} \sum_{n_1\cdots n_4} \sum_{\boldsymbol{k}_1\cdots\boldsymbol{k}_4} U_{n_1n_2n_3n_4}(\boldsymbol{k_1}\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4) c_{n_1\boldsymbol{k}_1}^\dagger c_{n_2\boldsymbol{k}_2}^\dagger c_{n_3\boldsymbol{k}_3} c_{n_4\boldsymbol{k}_4}\, \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}. \tag{192}$$

In the path integral action, this becomes

$$S_0 = \sum_{n,\boldsymbol{k},\omega_n} \bar{c}_{n\boldsymbol{k}}(\omega_n)\,(-i\omega_n + \epsilon_{n\boldsymbol{k}})\, c_{n\boldsymbol{k}}(\omega_n), \tag{193}$$

and

$$S' = \frac{1}{2\beta V} \sum_{1\cdots 4} U(1234)\bar{c}_1\bar{c}_2 c_3 c_4\, \delta_{1+2,3+4}, \tag{194}$$

where we introduced some (hopefully self-explanatory) notation to keep the latter equation brief.

We are going to calculate the Green's function,

$$G(\boldsymbol{k}, i\omega_n) = \langle c_{n\boldsymbol{k}}(\omega_n)\bar{c}_{n\boldsymbol{k}}(\omega_n)\rangle\,, \tag{195}$$

(c.f. Eq. (181) for a single band), perturbatively in S', by just expanding the integrand of the path integral order by order in S', which generates standard diagrammatic perturbation theory. It is convenient to "resum" the diagrams that appear in the form of the self-energy $\Sigma_n(\boldsymbol{k}, i\omega_n)$, which is defined by

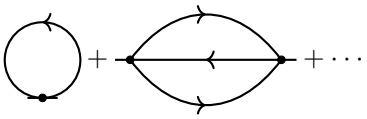
$$G_n(\boldsymbol{k}, i\omega_n) = \frac{1}{-i\omega_n + \epsilon_{n\boldsymbol{k}} + \Sigma_n(\boldsymbol{k}, i\omega_n)}. \tag{196}$$

Note that any function G can be represented in this form, and we can always invert this to obtain $\Sigma(G)$. In general the Green's function and the self-energy need not be diagonal in the band index, so that they become matrices, but we will neglect this complication.

In diagrammatic terms, the interaction is represented by a vertex with two incoming and outgoing lines, the direction of the arrows on the lines indicating whether it represents a $\bar{c}$ field (outgoing) or c field (incoming):

(197) $S' =$ 

The self-energy has the nice property that it is obtained in perturbation theory by summing only the *one-particle irreducible* diagrams (those which cannot be broken into disconnected parts by cutting a single line), and truncating the external legs.

(198) $\Sigma =$ 

The first term is a "tadpole" and gives a trivial constant. The second term is the first non-trivial term in the self-energy. By appropriately labeling the lines we get (taking the zero temperature limit for simplicity, which turns Matsubara frequency sums into integrals)

$$\Sigma_n(k, i\omega_n) = \frac{2}{V}\sum_{mpp'}\sum_{\boldsymbol{q},\boldsymbol{q}'}\int \frac{d\Omega_n d\Omega'_n}{(2\pi)^2}\Gamma_{nmpp'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{q}') \times \frac{1}{-i\Omega_n + \epsilon_{p\boldsymbol{q}}}\frac{1}{-i\Omega'_n + \epsilon_{p'\boldsymbol{q}'}}\frac{1}{-i(\omega_n + \Omega_n + \Omega'_n) + \epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}}}, \tag{199}$$

where

$$\Gamma_{nmpp'}(\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}') = U_{nmpp'}(\boldsymbol{k},\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}')U_{p'pmn}(\boldsymbol{q}',\boldsymbol{q},\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k},\boldsymbol{k}) \tag{200}$$

is some complicated function of band indices and momentum which is smooth and non-divergent for all parameters if the interactions are short-ranged. The two frequency integrals can be done successively by contours. The result is

$$\Sigma_n(k,i\omega_n) = \frac{2}{V}\sum_{mpp'}\sum_{\boldsymbol{q},\boldsymbol{q}'}\Gamma_{nmpp'}(\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}')\frac{\theta(\epsilon_{p\boldsymbol{q}})\theta(\epsilon_{p'\boldsymbol{q}'})\theta(-\epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}})+(\epsilon\leftrightarrow-\epsilon)}{i\omega_n+\epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}}-\epsilon_{p\boldsymbol{q}}-\epsilon_{p'\boldsymbol{q}'}}. \tag{201}$$

This result is quite nice, because it can be easily analytically continued, taking $i\omega \to \omega + i\delta$. Since everything but the $i\delta$ is real, we readily see that the imaginary part of the self-energy is simple (the real part is not so simple):

$$\begin{aligned}\mathrm{Im}\Sigma(\boldsymbol{k},\omega+i\delta) = -2\pi\sum_{mpp'}\int\frac{d^d\boldsymbol{q}d^d\boldsymbol{q}'}{(2\pi)^{2d}}\Gamma_{nmpp'}(\boldsymbol{k},\boldsymbol{q},\boldsymbol{q}')\left[\theta(\epsilon_{p\boldsymbol{q}})\theta(\epsilon_{p'\boldsymbol{q}'})\theta(-\epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}})+(\epsilon\leftrightarrow-\epsilon)\right]\\ \times\delta(\omega+\epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}}-\epsilon_{p\boldsymbol{q}}-\epsilon_{p'\boldsymbol{q}'}).\end{aligned} \tag{202}$$

One physical interpretation obtains if we take $\omega = \epsilon_{\boldsymbol{k}}$ – this is called the "on-shell" condition. We can think of this as representing an electron with energy $\omega > 0$ and momentum $\boldsymbol{k}$, which may decay into two electrons with momentum $\boldsymbol{q}, \boldsymbol{q}'$ and a hole with (missing) momentum $\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}$. The theta functions enforce that the states are available for the two electrons produced, i.e. they are above the Fermi energy and so initially empty, and likewise the hole state is initially occupied – had we chosen $\omega < 0$ the electrons and holes are swapped. The self-energy gives the rate of the decay process.

To see that this physical interpretation is sensible, consider the retarded Green's function including the self-energy

$$G_R(\boldsymbol{k},\omega) = \frac{1}{\omega-\epsilon_{\boldsymbol{k}}-\Sigma(\boldsymbol{k},\omega)-i\delta}. \tag{203}$$

Expressing $\Sigma = \Sigma' + i\Sigma''$ in terms of real and imaginary parts, and taking the imaginary part of G_R, we obtain

$$\rho(\boldsymbol{k},\omega) = \frac{-2\Sigma''(\boldsymbol{k},\omega)}{(\omega-\epsilon_{\boldsymbol{k}}-\Sigma'(\boldsymbol{k},\omega))^2+(\Sigma''(\boldsymbol{k},\omega))^2}. \tag{204}$$

From this, when the imaginary part of the self-energy is small, there is a sharp peak in the spectral function at the renormalized energy $\omega = \varepsilon_{\boldsymbol{k}}$ which is the solution of

$$\varepsilon_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} + \Sigma'(\boldsymbol{k},\varepsilon_{\boldsymbol{k}}). \tag{205}$$

We may expand around this solution in the vicinity of the peak, assuming

$\omega - \varepsilon_k \ll \omega, \epsilon_k$, to obtain to leading order

$$\rho(\boldsymbol{k}, \omega) = \frac{-2Z_k\gamma_k}{(\omega - \varepsilon_k)^2 + \gamma_k^2}, \tag{206}$$

where

$$\gamma_k = \frac{\Sigma''(\boldsymbol{k}, \varepsilon_k)}{1 - \partial_\omega \Sigma'(\boldsymbol{k}, \varepsilon_k)}, \tag{207}$$

and

$$Z_k = \frac{1}{1 - \partial_\omega \Sigma'(\boldsymbol{k}, \varepsilon_k)}. \tag{208}$$

This describes a Lorentzian peak whose width is γ_k and weight is reduced from the 2π of Eq. (185) for free fermions by the factor Z_k. A Lorentzian is the Fourier transform of an exponential, indicating that the quasiparticle decays with a decay rate of order this width. This confirms that interpretation.

It is interesting to check how this works out for a band insulator, using the perturbative result for the self-energy in Eq. (202). Consider the imaginary part of the self-energy for an electron at the bottom of the lowest conduction band, $\Sigma_c''(\boldsymbol{k}, \omega = \epsilon_{c,k})$, with $\boldsymbol{k}$ the band minimum, where since we are working perturbatively, we may to leading order ignore the shift of the band energy with interactions. Then the delta-function in Eq. (202) gives non-zero contributions only when

$$\omega = \epsilon_{c,k} = \epsilon_{p\boldsymbol{q}} + \epsilon_{p'\boldsymbol{q}} - \epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}}. \tag{209}$$

Furthermore, for $\omega > 0$ only the term for which the theta functions select $\epsilon_{p\boldsymbol{q}}, \epsilon_{p'\boldsymbol{q}'} > 0$ and $\epsilon_{m,\boldsymbol{q}+\boldsymbol{q}'-\boldsymbol{k}} < 0$ can contribute. However, if $\epsilon_{c\boldsymbol{k}}$ is the minimum energy of the conduction band, the right hand side of Eq. (209) is strictly larger than the left, so the delta-function condition can never be satisfied, and we find that Σ'' is strictly zero.

The other extreme, where decay is always possible, is in a metal. Here there are generally contributions to Eq. (202) even when n is taken to be the band at the Fermi energy, $\boldsymbol{k}$ is a momentum just outside the Fermi surface, and $\omega = \epsilon_{\boldsymbol{k}}$ is on-shell. These occur because there are states in which m, p, p' are also from this band and the corresponding momenta are all near the Fermi surface. An asymptotic analysis of the integral in Eq. (202) shows that the result, while non-zero, is parametrically small in the energy above the Fermi level, at least for dimensions $d \geq 2$:

$$\mathrm{Im}\Sigma(\boldsymbol{k}, \omega \approx \epsilon_{\boldsymbol{k}}) \sim \begin{cases} \text{const} \times \omega^2 & d > 2 \\ \text{const} \times \omega^2 \ln(1/\omega) & d = 2 \end{cases}. \tag{210}$$

In the perturbative expression, the constant is obviously quadratic in the strength of interactions. Landau supposes that, even beyond perturbation theory, the same frequency dependence holds, while the prefactor may not be small. This means that for small enough ω, the decay rate of the quasiparticle

becomes small, and indeed much smaller than its energy. Ultimately this is a key ingredient in Landau's justification of the quasiparticle approach.

One should note that Eq. (204) is just an exact rewriting, and so it is also valid away from the peak, i.e. when ω is not close to the quasiparticle energy. Then the expansion leading to the Lorentzian form is invalid. In that case, there is no sharp peak, but rather a smooth imaginary part whose frequency dependence comes largely from that of Σ'' itself (modulo the denominator). This does not have to do with decay. Rather the interpretation is that the self-energy is picking up contributions from higher excited (exact) multi-quasiparticle states to the spectral decomposition. That is, in the interacting system the state created by acting with a creation operator on the vacuum, i.e. $c_{\boldsymbol{k}}^\dagger|0\rangle$, is a sum of terms including some smooth amplitude for multiparticle states. Consequently, these continuum excitations, which were already present in the free system but gave zero contributions to the Green's function in that case, are "lit up" by interactions and produce a smooth continuum weight. This "off-shell" part of the self-energy is generally non-zero above some frequency, even for the band insulator case.

Figure 6: Spectral function. It would be nice to have a sketch.

Incidentally, both the quasiparticle peak and the continuum weight are typical features observed in Angle Resolved Photo-Emission Spectroscopy (ARPES), a measurement in which shoots high energy photons at a solid with enough energy to kick electrons out. The ejected electrons are collected and by resolving their momentum and energy, one can determine the spectral function $\rho(\boldsymbol{k}, \omega)$. This has become one of the most powerful and widespread probes of electronic materials.

6.5 *Electromagnetic response from the effective action*

We've already talked about conductivity, and especially the Hall conductivity, in many terms, and in particular as a linear response quantity. A closely related point of view which is formulated in the language of field theory is the idea of an effective electromagnetic action. The simplest way to think about this is to imagine coupling the electrons in a system to an electromagnetic gauge field A_μ (including both the time component - the scalar potential - and the spatial components), by minimal coupling. This gauge field may be called a "probe" field. We call it a probe because we do not a priori wish to give it any dynamics. It might be considered an external classical field that we can vary at our convenience. Then we can ask how the partition function of the system depends upon the space-time configuration of the gauge field. In equations,

$$Z[A_\mu(\boldsymbol{x}, \tau)] = \int [d\bar{c}dc] e^{-S[\bar{c}, c, A_\mu]}. \tag{211}$$

In principle we can define this in the original quantum theory in terms of operators as well, but it is awkward. Now it is convenient to define the logarithm

of this partition function to be the *effective action* of the gauge field:

$$Z[A_\mu(\boldsymbol{x},\tau)] = e^{-S_{\text{eff}}[A_\mu(x,\tau)]}. \tag{212}$$

The reason for the name is that if we *were* to regard the gauge field as another quantum field instead of just the classical probe one, we would have integrated over it as well as the fermions. We could do this functional integral in stages, and after first integrating out the fermions, the result would be a new path integral with exactly S_{eff} in the role of the action (plus any other terms explicitly involving the electromagnetic field we saw fit to add).

Now there is a certain logic that leads us to expect a simple form of the effective action in some situations. In particular, if the fermionic system we are describing has a gap to all bulk excitations, then we expect the fermions sustain no power-law correlations. Consequently, the path integral over them should be as "finite" as a path integral ever is, and the effective action should therefore be an analytic and local *functional* of the probe gauge field. This is usually what we assume when we write down Lagrangians in field theory.

This situation applies to band insulators of all types, including the Chern insulators we studied previously. It is interesting to see how the physics of the quantum Hall effect manifests itself in the electromagnetic effective action. We will do this via an explicit calculation. Consider the Haldane honeycomb model related to graphene, which we studied in Sec. 5.1. We wll ignore spin, i.e. consider spinless fermions. The low energy Hamiltonian we derived there, Eq. (87), consists of two Dirac fermions, labeled there by $\mu^z = s = \pm 1$, physically corresponding to the two valleys. Let us rewrite this as

$$H = \sum_s \sum_{\boldsymbol{k}} \psi^\dagger_{s,\boldsymbol{k}} \left(s\tau^x v k_x + \tau^y v k_y + \tilde{m}_s \tau^z \right) \psi_{s,\boldsymbol{k}}, \tag{213}$$

where $\tilde{m}_s = m_1 + s m_2$ are two Dirac masses. It is convenient to make the canonical transformation $\psi_- \to \tau^y \psi_-, \psi^\dagger_- \to \psi^\dagger_- \tau^y$. This removes the s factor in front of the τ^x and transfers it to the masses:

$$H \to \sum_s \sum_{\boldsymbol{k}} \psi^\dagger_{s,\boldsymbol{k}} \left(\tau^x v k_x + \tau^y v k_y + m_s \tau^z \right) \psi_{s,\boldsymbol{k}}, \tag{214}$$

with $m_s = s\tilde{m}_s$. Note that after this transformation and redefinition of masses, in the Chern insulator the two masses have the same sign, i.e. $m_+ m_- > 0$, while for the CDW insulator they have opposite sign. The corresponding action is just the sum of two terms, $S = S_+ + S_-$, with

$$S_s = \int d\tau \sum_{\boldsymbol{k}} \bar{\psi}_{s,\boldsymbol{k}} \left(\partial_\tau + v\tau^i k_i + m_s \tau^z \right) \psi_{s,\boldsymbol{k}}. \tag{215}$$

Transforming back to real space, we can add in the probe gauge field according to the minimal coupling prescription:

$$S_s = \int d\tau d^2x \, \bar{\psi}_s \left(\partial_\tau - ieA_0 - iv\tau^i (\partial_i - ieA_i) + m_s \tau^z \right) \psi_s. \tag{216}$$

Since the actions for the two Dirac points are decoupled, we can treat them separately. The resulting effective action will be the sum of the effective actions from each Dirac point. It is convenient to first make small changes of variables, to simplify the equations. Let

$$\psi \to e^{-i\frac{\pi}{4}\tau^z}\psi, \qquad \bar{\psi} \to i\bar{\psi}e^{-i\frac{\pi}{4}\tau^z}. \tag{217}$$

Note that this transformation is allowed in the path integral since ψ and $\bar{\psi}$ are independent fields. This brings the action into a simpler form:

$$S_s = \int d^3x\, \bar{\psi}_s \left(v_\mu \tau^\mu(\partial_\mu - ieA_\mu) + m_s\right)\psi_s, \tag{218}$$

where we let $\tau \to z$ appear as a third euclidean coordinate, with $v_z = 1$. This is pretty much the quantum field theory conventions. Now we are ready to compute the effective action. For convenience, we are going to choose units so that $v_\mu = 1$. We have $S_{\text{eff}}[A] = \sum_s S^{\text{dirac}}_{\text{eff}}[A, m_s]$, since the only dependence on s appears through the mass. Using the formula for the Grassman integral, we have formally that

$$S^{\text{dirac}}_{\text{eff}} = -\ln\det\left(\tau^\mu(\partial_\mu - ieA_\mu) + m_s\right) = -\text{Tr}\ln\left(\tau^\mu(\partial_\mu - ieA_\mu) + m_s\right). \tag{219}$$

We can rearrange this according to

$$\begin{aligned} S^{\text{dirac}}_{\text{eff}} &= -\text{Tr}\ln\left(\tau^\mu\partial_\mu + m_s - ieA_\mu\tau^\mu\right) = -\text{Tr}\ln\left(G^- - ieA_\mu\tau^\mu\right) \\ &= -\text{Tr}\ln G^- - \text{Tr}\ln\left(1 - ieGA_\mu\tau^\mu\right) \\ &= \text{const.} + ie\text{Tr}\left(GA_\mu\tau^\mu\right) - \frac{e^2}{2}\text{Tr}\left(GA_\mu\tau^\mu GA_\nu\tau^\nu\right) + O(A^3). \end{aligned} \tag{220}$$

Here we defined the Green's function,

$$G = \left(\tau^\mu\partial_\mu + m_s\right)^{-1}. \tag{221}$$

It can be readily written in momentum space as

$$G(k) = \left(-ik_\mu\tau^\mu + m_s\right)^{-1} = \frac{ik_\mu\tau^\mu + m}{k^2 + m^2}. \tag{222}$$

In Eq. (220), the constant term can be neglected, and the term linear in the gauge field vanishes. The quadratic term is most easily evaluated in momentum space. The trace should be interpreted as a full operator trace, which means in this case a momentum integration and a matrix trace. We have

$$\begin{aligned} &S^{\text{dirac}}_{\text{eff}} = \\ &\frac{e^2}{2}\int\frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}\,\text{Tr}\left[\frac{m + i(q_a + k_a/2)\tau^a}{m^2 + (q + k/2)^2}\tau^\mu\frac{m + i(q_b - k_b/2)\tau^b}{m^2 + (q - k/2)^2}\tau^\nu\right]A_\mu(k)A_\nu(-k) \\ &\equiv \frac{1}{2}\int\frac{d^3k}{(2\pi)^3}\Pi_{\mu\nu}(k)A_\mu(k)A_\nu(-k). \end{aligned} \tag{223}$$

We can carry out the trace in Eq. (223) (which is now just the matrix trace) using identities for Pauli matrices:

$$\operatorname{Tr}\tau^a\tau^b = 2\delta^{ab}, \qquad \operatorname{Tr}\tau^a\tau^b\tau^c = 2i\epsilon^{abc},$$
$$\operatorname{Tr}\tau^a\tau^b\tau^c\tau^d = 2\left(\delta^{ab}\delta^{cd} + \delta^{ad}\delta^{bc} - \delta^{ac}\delta^{bd}\right). \tag{224}$$

This gives

$$\Pi_{\mu\nu}(k) = e^2 \int \frac{d^3q}{(2\pi)^3} \frac{2m^2\delta^{\mu\nu} - 2m\epsilon^{\mu\nu\lambda}k_\lambda - 2\left(2q_\mu q_\nu - \frac{1}{2}k_\mu k_\nu - (q^2 - k^2/4)\delta^{\mu\nu}\right)}{(m^2 + (q+k/2)^2)(m^2 + (q-k/2)^2)}. \tag{225}$$

We are interested in the small momentum behavior of $\Pi_{\mu\nu}(k)$, which controls long-wavelength universal physics. Due to the presence of the mass in the denominators, the integral has no infra-red divergences, and should be a smooth function of momentum (some terms may require a large q cut-off to make them finite, but this is physical anyway). Furthermore, Eq. (225) has O(3) rotational symmetry in the Euclidean plane. This restricts the form of the Taylor expansion of $\Pi_{\mu\nu}$ in k_μ. The leading term is naïvely a constant proportional to $\delta^{\mu\nu}$, but this must vanish by gauge invariance, since it would represent a mass for A_μ. The next term is linear in k_μ, and must be proportional to the ϵ symbol by O(3) symmetry. We neglect higher $O(k^2)$ contributions. The anti-symmetric linear term arises *solely* from the explicit $\epsilon^{\mu\nu\lambda}k_\lambda$ in the numerator – expansion of the rest of the expression in powers of k can only lead to symmetric terms, which cannot contribute at linear order (one can see this for example by using the Feynman trick). To obtain the leading contribution we may therefore keep only this term and set $k = 0$ in the denominator. This gives

$$\Pi_{\mu\nu}(k) = -2e^2\epsilon_{\mu\nu\lambda}mk_\lambda \int \frac{d^3q}{(2\pi)^3}\frac{1}{(q^2+m^2)^2} = -\frac{e^2}{4\pi}\frac{m}{|m|}\epsilon_{\mu\nu\lambda}k_\lambda. \tag{226}$$

Re-inserting this into Eq. (223) we obtain finally

$$S_{\text{eff}}^{\text{dirac}} = -i\frac{e^2}{8\pi}\frac{m}{|m|}\int d^3x\, \epsilon_{\mu\nu\lambda}A_\mu\partial_\nu A_\lambda. \tag{227}$$

Please note the factor of i. This arose from the k_λ factor in Eq. (226), which in real space is $i\partial_\lambda$. With our condensed matter conventions, which are natural for the thermodynamic partition function with imaginary time, is defined as $e^{-S_{\text{eff}}}$, so that the factor in the exponential is intrinsically imaginary. The total effective action is the sum of the two contributions from both Dirac points, whence $S_{\text{eff}} = S_{\text{CS}}$, with

$$iS_{\text{CS}}[A] = \frac{ke^2}{4\pi}\int d^3x\, \epsilon_{\mu\nu\lambda}A_\mu\partial_\nu A_\lambda, \tag{228}$$

where

$$k = \frac{1}{2}\left(\frac{m_+}{|m_+|} + \frac{m_-}{|m_-|}\right) \tag{229}$$

is an integer. Eq. (228) is the famous *Chern-Simons* action. The integer k is called the *level* of the Chern-Simons theory, and physically has the meaning of the Hall conductivity, in units of e^2/h. There are deep field theory arguments which require k to be quantized to an integer for any "simple" insulator without some more subtle structure (such subtle structure does arise in the *fractional* quantum Hall effect). The Haldane/graphene model is physical and so this happens automatically. If we just accept the field theory arguments (which we may discuss...) that k is quantized, then this is enough to ensure the stability of the quantum Hall effect. In QFT terms, the quantized Hall state is perhaps just defined by the presence of a Chern-Simons term in the effective action.

6.6 *Chern-Simons theory*

Lecture 11 (1h 15mins)
February 20th, 2018

The effective action in Eq. (228) is the simplest example of Chern-Simons (CS) theory, which in turn is what is known as a topological quantum field theory (TQFT). It is the beginning of a vast subject. I'd like to touch a bit on it, at the most basic level, to get a glimpse of this alternative point of view on the quantum Hall effect.

We derived the CS action from a specific microscopic model. This at least proves there are physical problems where it occurs with non-zero k. We can, however, take an alternative point of view and obtain the CS term from general arguments. If we do not care about microscopics, this is sufficient and very general. The argument is as follows. Suppose that we have a large system consisting of electrons which has a gapped and unique ground state in the bulk. Below the energy scale of the gap, there are no bulk degrees of freedom which can be excited. Consequently, the process of integrating out the electrons is innocuous in the sense that it cannot generate any non-analytic terms in the probe gauge field, and we can safely do it without missing any low energy excitations. Then there is a consistent description of the system in terms of an analytic and local effective action in $A_\mu(x,\tau)$.

Such an analytic and local action can be addressed by expanding the lagrangian density in powers of A_μ and its derivatives. The terms in this expansion are constrained by symmetry (not so important, as symmetries can be broken) and gauge invariance (important!). Apart from any linear terms in A_μ which can be removed by a shift, the lowest order term, counting powers of A_μ and of derivatives, which may occur is the CS term (an $A_\mu A_\nu$ term without derivatives is not gauge invariant). Actually the CS term itself is not *obviously* gauge invariant, since it involves a gauge field without a derivative acting on it. How is it ok? A gauge transformation takes $A_\mu \to A_\mu + \frac{1}{e}\partial_\mu \chi$.

Under this transformation, the variation of the Chern-Simons term is

$$\begin{aligned} iS_{\mathrm{CS}}[A] &\to iS_{\mathrm{CS}}[A] + \frac{ke}{4\pi}\int d^3x\, \epsilon_{\mu\nu\lambda}\partial_\mu\chi\partial_\nu A_\lambda \\ &= iS_{\mathrm{CS}}[A] + \frac{ke}{4\pi}\int d^3x\, \partial_\mu\left(\epsilon_{\mu\nu\lambda}\chi\partial_\nu A_\lambda\right). \end{aligned} \tag{230}$$

If we are allowed, as we often sloppily do, to neglect boundary terms, then the CS term is invariant, because its variation is the integral of a total derivative. This is fine on a closed manifold, e.g. if we take periodic boundary conditions in space and consider the $T > 0$ partition function and impose periodic boundary conditions on χ and on the field strength $\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda$.

Quantization of the Chern-Simons level

The last point is subtle. It is pretty clear we need periodic boundary conditions on the field strength, because it is physical. But there is no good reason we need periodic boundary conditions on χ (or on A_μ for that matter). What we really need is to maintain the anti-periodic boundary conditions on the electrons, but since they transform by the phase factor $\psi \to e^{i\chi}\psi$, we may allow χ to wind by a multiple of 2π. For such a topologically non-trivial gauge transformation, the invariance of the CS term is not obvious. Let us consider this variation more carefully. We start by rewriting the CS term more explicitly

$$iS_{CS}[A] = \frac{ke^2}{4\pi}\int d^3x\, \left[A_0\epsilon_{ij}\partial_i A_j - \epsilon_{ij}A_i\partial_0 A_j + \epsilon_{ij}A_i\partial_j A_0\right]. \tag{231}$$

Now what we will do is to consider a minimal non-trivial gauge field configuration in a periodic system and see how the action transforms under a gauge transformation. The simplest such configuration has a constant A_0 and a constant magnetic flux through a spatial cross-section,

$$\Phi = \int d^2x\, \epsilon_{ij}\partial_i A_j. \tag{232}$$

With periodic boundary conditions, there is a Dirac quantization condition imposed on the flux: it must be an integer multiple of the flux quantum, $\Phi = nh/e = 2\pi n/e$. This is necessary for consistent quantum mechanics of charge e particles. Let us denote the constant $A_0 = s/(e\beta)$, where s/e is equal to the integral of A_0 over imaginary time. The variable s is nice because it behaves simply under a gauge transformation with non-zero winding: for $\chi = 2\pi\tau/\beta$, we have $s \to s + 2\pi$. Now we can try to evaluate Eq. (231) for this gauge field configuration. The second term is zero because the spatial components of the gauge field are constant. The last term might appear zero but this is actually false because with a non-zero flux A_i cannot be single-valued. Instead we should integrate by parts in space after which the last

term becomes equal to the first. The result is that

$$iS_{\rm CS}[A_0 = s/\beta, \Phi] = \frac{ke^2}{2\pi}\int d^3x A_0 \epsilon_{ij}\partial_i A_j = \frac{ke}{2\pi} s\Phi = kns. \tag{233}$$

Under the large gauge transformation which takes $s \to s + 2\pi$, this changes by $2\pi kn$. The partition function is unchanged if this is a multiple of 2π (remember the i!). This implies that *the CS term is properly gauge invariant only when k is an integer*. This is remarkable because we obtain a quantization condition from just gauge invariance and the discreteness of charge in units of e.

Equations of motion

We can use the Chern-Simons theory to discuss the linear response of the system. To do this, we should analytically continue to real time. This requires taking $\tau \to it$, $A_0 \to -iA_0$, and $S \to iS$. We obtain the real-time action

$$S^{\rm rt}_{\rm CS} = \frac{ke^2}{4\pi}\int d^2x\, dt\, \left[A_0\epsilon_{ij}\partial_i A_j - \epsilon_{ij}A_i\partial_t A_j + \epsilon_{ij}A_i\partial_j A_0\right], \tag{234}$$

which is pretty much just a rewrite of Eq. (231). Now we can obtain the current by

$$j_i = -\frac{\delta S}{\delta A_i} = -\frac{ke^2}{2\pi}\epsilon_{ij}\left(\partial_j A_0 - \partial_t A_j\right) = -\frac{ke^2}{2\pi}\epsilon_{ij}E_j = -\frac{ke^2}{h}\epsilon_{ij}E_j. \tag{235}$$

This is exactly the current-field relation of a system with a Hall conductivity $\sigma_H = ke^2/h$ and *zero* diagonal conductivity $\sigma_{xx} = \sigma_{yy} = 0$. So in the field theory approach the quantization of the CS level is the quantization of the Hall conductivity. The vanishing diagonal conductivity was implicit in the more physical discussion of the previous sections, but it comes for free in the field theory approach. In fact, the smooth analytic assumption for the effective action precludes the possibility of a dissipative conductivity.

6.7 *Fractional Quantum Hall Effect*

I can't leave CS theory behind without saying a *very* quick word about the fractional quantum Hall effect. It was discovered experimentally that quantized Hall plateaus occur not only for integer multiples of e^2/h but also rational fractional multiples, most famously the Laughlin sequence $\sigma_H = \nu e^2/h$, with $\nu = 1/(2m+1)$, one over an odd integer. The description in terms of the CS theory, Eq. (228), seems impossible since the level k must be an integer to satisfy gauge invariance.

Field theory has a glib answer for this, which misses a huge amount of physics, but is satisfying in its minimalism. We made an assumption in writing down Eq. (228) that there were no low energy bulk degrees of freedom. This is not quite true in fractional quantum Hall states. Instead, some low energy degrees of freedom must be kept (they are zero energy on the torus). These are described by an *emergent* gauge field a_μ which is not a probe field but a real one representing physical degrees of freedom. Because we do not have

so much time left in the course, I am going to ask you to just accept that it is possible for a gauge field to emerge like this. The low energy description of the physical degrees of freedom will include *only* this gauge field.

For an electronic system, this implies there must be a description of the physical electrical (3-)current j_μ in terms of a_μ. To satisfy the continuity equation, the only possible choice is

$$j_\mu = \alpha \epsilon_{\mu\nu\lambda} \partial_\nu a_\lambda. \tag{236}$$

Here α is some constant. Naïvely we can choose α arbitrarily by just rescaling a_λ. However, we should also impose a periodic equivalence on the emergent gauge field: otherwise we will not be able to have any net charge in a closed system with periodic boundary conditions. This total charge, which is the integral of j_0, can of course be a non-zero multiple of e. If we choose the periodicity of a_μ to be $2\pi/e$ like it is for our probe gauge field, then the flux quantization is in units of h/e and so we should take $\alpha = e^2/h = e^2/(2\pi\hbar) = e^2/2\pi$ in units with $\hbar = 1$:

$$j_\mu = \frac{e^2}{2\pi} \epsilon_{\mu\nu\lambda} \partial_\nu a_\lambda. \tag{237}$$

Please note this is the physical current j_μ, which is a source for a physical electromagnetic field with gauge field A_μ: the charge which is the integral of j_0 is the physical electromagnetic one. By introducing the emergent gauge field a_μ, we also should acknowledge the possible existence of gauge charges, which are sources of the internal gauge field, and which experience forces mediated by a_μ. However, we are going to assume that all such charges have a gap in the bulk, and first study the physics below that gap.

Now we postulate an action for the emergent gauge field

$$S[a; A] = \int d^3x \left[\frac{pe^2}{4\pi} \epsilon_{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda - j_\mu A_\mu \right]. \tag{238}$$

We postulated a CS term for the emergent gauge field, and included the usual $\boldsymbol{j} \cdot \boldsymbol{A}$ term in the action, so that we can describe the effects of a physical electromagnetic field. This looks a lot like what we did for the integer quantum Hall effect, but it is important that here the CS term is for the internal not the probe gauge field. The level p of this internal CS term is distinct from the level k that appeared in the effective action for A_μ. I omitted the "effective" label for $S[a; A]$ in Eq. (238), because I wanted to emphasize that not all the degrees of freedom in the bulk have been integrated out. It might still be called an effective action though, because obviously the microscopic electrons are not in there, and actually almost all the bulk degrees of freedom have been got rid of.

To obtain the physical electromagnetic effective action, we can put Eq. (237) into Eq. (238), and integrate out the internal gauge field. This is a Gaussian integral and so it is equivalent to solving the equation of motion for a_μ. The

equation of motion is

$$\frac{\delta S[a;A]}{\delta a_\mu} = \frac{pe^2}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda - \frac{e^2}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda = 0, \tag{239}$$

which just has the solution

$$a_\mu = \frac{1}{p}A_\mu, \tag{240}$$

and substituting this back into the action gives finally

$$S_{\text{eff}}[A] = -\frac{e^2}{4\pi p}\int d^3x\, \epsilon_{\mu\nu\lambda}A_\mu\partial_\nu A_\lambda. \tag{241}$$

Note that by comparing to Eq. (228), we achieved $k \to 1/p$ in this process, so by carrying through the equation of motion analysis in Sec. 6.6, we see that this describes a fractional quantum Hall effect, $\sigma_H = \frac{1}{p}e^2/h$. This is the so-called *Laughlin sequence* of fractional quantum Hall states.

Lecture 12 (1h 15mins)
February 22nd, 2018

There are many questions to be asked here. A good one is how Eq. (241) can now be gauge invariant when we needed an integer level before? In fact it is still not gauge invariant, but Eq. (238) is. The problem is that in going to the final effective action we treated A_μ and a_μ like they were single valued, which in general they are not, e.g. Eq. (240) does not have solutions in all cases. However, if we are interested in infinitesimal A_μ the process is ok since such configurations are topologically trivial. So Eq. (241) is correct in this case and this is enough to obtain the Hall conductivity. However, we miss a lot of physics that is captured by Eq. (239), and is related to topologically non-trivial configurations of a_μ.

Another good question is how to get the "oddness" of the denominator p in the fractional quantum Hall effect? It seems like any integer p is ok from what we have discussed so far. This ultimately is related to the fermionic nature of the microscopic electrons, which has not played a role in this discussion up to now.

These questions and more are answered by thinking more carefully about the topological excitations of the emergent CS theory, and by the quasiparticles *above* the gap in the fractional quantum Hall state. There is no good way to do this justice in the time we have. But I'll give you a taste. Let's look at the topological excitations of the CS theory, Eq. (239), on a torus, with zero external probe field $A_\mu = 0$. We are interested in the path integral over a_μ. Let us rewrite the action explicitly, as we did in Eq. (234) for A_μ, but staying in imaginary time:

$$\begin{aligned} S_{\text{CS}} &= -i\frac{pe^2}{4\pi}\int d^2x d\tau\, \left[a_0\epsilon_{ij}\partial_i a_j - \epsilon_{ij}a_i\partial_\tau a_j + \epsilon_{ij}a_i\partial_j a_0\right] \\ &= \frac{pe^2}{2\pi}\int d^2x d\tau\, \left[-ia_0\,\epsilon_{ij}\partial_i a_j + ia_1\partial_\tau a_2\right]. \end{aligned} \tag{242}$$

Now if we compare this action to ones with which we are familiar, e.g. from quantum mechanics, we can recognize the second term. It is the same form as the $ip\partial_\tau x$ term which occurs between position and momentum. This "Berry phase" term induces canonical commutation relations between p and x, and likewise so does the one above between a_1 and a_2:

$$[a_1(\boldsymbol{x}), a_2(\boldsymbol{x}')] = \frac{2\pi}{pe^2} i\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{243}$$

The first term is different. We see that a_0 appears only here, and the integral over a_0 is very simple:

$$\int [da_0] e^{-i\frac{pe^2}{2\pi}\int d^2x d\tau\, a_0\, \epsilon_{ij}\partial_i a_j} = \delta\left[\frac{pe^2}{2\pi}\epsilon_{ij}\partial_i a_j\right], \tag{244}$$

where the right hand side indicates a functional delta function. This basically just enforces the constraint that the flux through the actual volume of the same is zero $\epsilon_{ij}\partial_i a_j = 0$.

The latter constraint means that there are actually no bulk gauge-invariant degrees of freedom. This is why CS theory is called a topological field theory. What is left? For the torus there are two non-trivial loops:

$$\phi_1 = \int dx\, a_x(x, 0), \qquad \phi_2 = \int dy\, a_y(0, y), \tag{245}$$

where we arbitrarily chose $y = 0$ in the first term and $x = 0$ in the second: the integral is independent of these choices due to the zero flux condition through the bulk (it is actually independent of any smooth deformation). These quantities can be interpreted as the gauge flux through the two holes of the torus. Now we can evaluate the commutator of these two flux operators using Eq. (243), which gives

$$[\phi_1, \phi_2] = \frac{2\pi}{pe^2} i \tag{246}$$

Now remembering that the gauge field is periodic, we should consider the exponentials of these fluxes, which are gauge invariant and respect the periodicity requirements:

$$W_i = e^{2\pi i \phi_i/\phi_0} = e^{ie\phi_i}, \tag{247}$$

with $\phi_0 = h/e = 2\pi\hbar/e = 2\pi/e$. The W_i operators are called "Wilson loops". They represent the discrete quantum degrees of freedom of the CS theory on the torus. Now Eq. (246) means that ϕ_1 and ϕ_2 are canonically conjugate, so that W_1 generates translations of ϕ_2 and vice-versa. Specifically,

$$W_2^{-1}\phi_1 W_2 = \phi_1 + \frac{2\pi}{pe} = \phi_1 + \frac{\phi_0}{p}, \tag{248}$$

and similarly

$$W_1^{-1}\phi_2 W_1 = \phi_2 - \frac{2\pi}{pe} = \phi_2 - \frac{\phi_0}{p}. \tag{249}$$

This finally implies

$$W_1 W_2 = e^{\frac{2\pi i}{p}} W_2 W_1. \tag{250}$$

The last equation is fully gauge invariant and expressed in terms of nice periodic quantities. It is actually a familiar thing in solid state physics: the magnetic translation algebra. It arises in a number of places. Most importantly, it is well-known that this algebra has no one dimensional representations, and in fact has representations of minimum dimension p. This is because if we consider an eigenstate of W_2, Eq. (250) implies that W_1 multiplies its eigenvalue under W_2 by $e^{\frac{2\pi i}{p}}$. So the level p dynamical CS theory on the torus has a p-fold degeneracy. This degeneracy does not affect any local gauge invariant operators (which are trivial in the CS theory), and so is topological.

What is the meaning of this degeneracy? Well we can understand it by thinking of an annulus *à la* Laughlin, instead of a torus, with a small hole on the inside. Let's think of x as the coordinate along the circumferential direction and y as the radial coordinate. Then ϕ_1 is the gauge flux through the hole of the annulus. Recall the physical electromagnetic current is related to the gauge flux from Eq. (237). So we can compute the charge inside the circle enclosed by ϕ_1 as

$$Q = \frac{e^2}{2\pi}\phi_1 = \frac{e}{\phi_0}\phi_1. \tag{251}$$

From Eq. (248), we get

$$W_2^{-1} Q W_2 = Q + \frac{e}{p}. \tag{252}$$

This tells us that the states related by the W_2 operator differ in the charge in the hole of the annulus by the *fraction* of an electron charge e/p. This is in very close analogy to Laughlin's flux insertion argument. Indeed, we can view W_2 as a flux insertion operator. However, the commutation relations imply that it inserts $1/p$ fraction of a gauge flux quantum. If you compare to Eq. (240), you can see that this corresponds, if we couple it to an external gauge field, to a single physical flux quantum. So this really does echo Laughlin's thought experiment.

We can imagine shrinking the size of the hole until it is microscopic in size. Then the hole is simply a place for a quasi-particle to live. The algebra of the Wilson loops is telling us that there are fractionally charged quasi-particles! One can think of the Wilson loop operator as representing the Aharonov-Bohm/Berry phase factor accumulated on adiabatically transporting an elementary quasi-particle of the system around the loop in question. What is

perhaps more fundamental than fractional charge is fractional statistics. The non-commutation of Wilson loops, Eq. (250), actually has the physical meaning that under adiabatic motion of one quasiparticle around another, the quantum state aquires a Berry phase of $2\pi/p$. (We actually discussed this in my 217a class – see Fig.18 of the 217a notes). A different derivation of this fact is to consider explicitly including quasiparticles in the bulk of the CS theory, by adding their three-current j_μ to the action:

$$(253)\quad iS_{\mathrm{CS}}[a,\mathrm{j}] = \int d^3x \left[\frac{pe^2}{4\pi}\epsilon_{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda - \mathrm{j}_\mu a_\mu\right].$$

Please compare to Eq. (238): here we write the *quasi-particle* current j_μ, which carries the emergent U(1) charge and hence is coupled to a_μ, rather than the electrical current j_μ which carries physical charge and hence is coupled to the external gauge field A_μ. We could also add the latter term but in the absence of external applied fields it is not important. Carrying out the integral over a_0 (or taking the equation of motion obtained by differentiating with respect to it) gives the relation

$$(254)\quad \frac{pe^2}{2\pi}\epsilon_{ij}\partial_i a_j = \mathrm{j}_0.$$

For a collection of stationary point particles, which have gauge charge in multiples of the fundamental charge e have $\mathrm{j}_0(\boldsymbol{x},t) = \sum_a n_a e\delta(\boldsymbol{x}-\boldsymbol{x}_a)$, which implies

$$(255)\quad \epsilon_{ij}\partial_i a_j = \frac{\phi_0}{p}\sum_a n_a\delta(\boldsymbol{x}-\boldsymbol{x}_a).$$

So each particle with gauge charge e is accompanied by a gauge flux of $1/p$ times a flux quantum. This gives rise to the Aharonov-Bohm phase of $2\pi/p$ upon taking one particle around the other (this is slightly subtle, but discussed in many places – see for example the David Tong notes). If we consider two identical quasi-particles, with the same (gauge) charge, this phase is twice the phase obtained by exchanging the two quasi-particles, so the exchange phase is π/p. For $p>1$ this is not a pure sign, and so they are rightly called "anyons".

With this observation, we can finally address the question of the parity of p. A requirement for an electronic system is that an excitation with the properties of an electron exists in the system. The electron has, obviously, fermionic statistics. So we can try to create it by making a composite of several anyons. If we take n anyons, it forms a composite particle which has exchange statistics of n^2 times the fundamental anyon statistics (for example this is understood by taking one composite around the other). The phase accumulated for exchanging these composites is then $n^2\pi/p$. The *physical* charge of this quasi-particle is just n times the charge of a single quasi-particle, i.e. ne/p. So to get the charge of the electron we need $n=p$, which makes the exchange phase equal to $p\pi$. This is equivalent to a Fermi minus sign only for p odd. Thus we arrive at the odd-denominator condition due to the underlying Fermi statistics

of electrons. Conversely, even denominator Laughlin states of bosons can be described by CS theory with p even.

At this point, we are going to leave Chern-Simons theory and the fractional quantum Hall effect behind. There is much more to this subject, but it is certainly specialized and I would like to move on to other topics.

Lecture 13 (1h 15mins)
February 27th, 2018

7 Renormalization group for Fermi systems

Topological phases, such as we have discussed before, are (locally) very robust and stable, because they have a spectral gap and because of their topological nature. A metal is in some sense the opposite situation, with a huge number of low energy excitations. It definitely has numerous possible instabilities. Landau's Fermi liquid idea is largely a guess, and works remarkably well. But it has a less than systematic feel to it. A more satisfactory approach is to regard a metal as a (quantum) critical state, i.e. a gapless continuum field theory, and ask if its perturbations are relevant or irrelevant in the renormalization group sense. We will try to formulate this idea now for various gapless Fermi systems, from Weyl and Dirac semimetals to the ultimate case of metals. A cautionary remark is in order: we will only partly succeed in regarding a metal as a continuum field theory, for reasons to be discussed, and consequently this nominally systematic approach is not quite that. For the Weyl and Dirac systems there are no issues.

7.1 *RG for nodal semimetals*

Set-up for nodal semi-metals

Let's start with the nodal semimetals. Here we may have a number of Weyl or Dirac points, located at various momenta in the Brillouin zone. We introduce continuum fields $\psi_{aA}(\boldsymbol{x})$ which represent the low energy electronic states near these points,

$$c_{ia} \sim \sum_A \psi_{aA}(\boldsymbol{x}_i) e^{-i\boldsymbol{K}_A \cdot \boldsymbol{x}_i}, \tag{256}$$

where i labels sites, a labels any other degrees of freedom such as orbitals, spin, etc., and A labels the nodal points. The linearized Hamiltonian takes the generic form

$$H_0 = \int d^d\boldsymbol{x} \psi^\dagger \left(-i \sum_\mu \Gamma_\mu \partial_\mu \right) \psi. \tag{257}$$

where we subsumed all spin/orbital/sublattice/K-point indices into an implicit spinor nature of ψ, and Γ_μ are some matrices which live in this spinor space. We will treat this using the path integral, and so study the correspond-

ing action

$$S_0 = \int d^d\boldsymbol{x}\, d\tau\, \bar{\psi}\left(\partial_\tau - i\sum_\mu \Gamma_\mu \partial_\mu\right)\psi. \tag{258}$$

This action has a scale invariance. One can take

$$\boldsymbol{x} \to b\boldsymbol{x}, \qquad \tau \to b\tau, \qquad \psi \to b^{-d/2}\psi, \tag{259}$$

and this leaves S invariant. We will want to add to the Hamiltonian some four-fermion interaction, we we assume to be local (for any short-range interaction we can expand it in terms of local terms plus derivatives which are less important):

$$H_1 = \int d^d\boldsymbol{x}\, \bar{\psi}\bar{\psi}\mathsf{M}\psi\psi, \tag{260}$$

where M is some four-index tensor. This gives rise to the action

$$S_1 = \int d^d\boldsymbol{x} d\tau\, \bar{\psi}\bar{\psi}\mathsf{M}\psi\psi. \tag{261}$$

The addition of this term, $S = S_0 + S_1$, to the action, spoils the scale-invariance of Eq. (259) (try it!). We want to understand the ultimate consequence of this breaking of scale-invariance on the low energy physics: does the scale invariance become a better or worse approximation at low energies? What is the long-distance fate of the system.

Renormalization group approach à la Wilson

The Renormalization Group (RG) gives a way to address this. It makes the notion of scale invariance more precise by regularizing the theory with a short-distance cut-off so that it is actually finite (i.e. the path integral does not suffer from short-distance definition problems) and then implementing this scale transformation. Let us state the basic idea before going into any detail of how it is implemented. The first important concept is that of a *scale-dependent effective action* $S^{\Lambda\to\Lambda'}$, which describes a system with a microscopic cut-off on the largest momenta in the system, Λ, *coarse-grained* to describe only those modes with momenta smaller than $\Lambda' < \Lambda$. So $S^{\Lambda\to\Lambda} = S^\Lambda$ is the microscopic action with a cut-off Λ. To carry out the RG we first separate out the modes with $|k| < \Lambda'$ and those with $\Lambda' < |k| < \Lambda$, and carry out the path integral over the latter:

$$\psi = \psi^< + \psi^>, \tag{262}$$

where

$$\psi_{\boldsymbol{k},\omega_n} = \psi^<_{\boldsymbol{k},\omega_n}\Theta(|k| < \Lambda') + \psi^>_{\boldsymbol{k},\omega_n}\Theta(\Lambda' < |k| < \Lambda), \tag{263}$$

and correspondingly for $\bar{\psi}$. Then the effective action is defined so that the correct partition function is obtained using it to define the weight for the

$$Z = \int [d\bar{\psi}][d\psi]\, e^{-S^\Lambda} = \int [d\bar{\psi}^<][d\psi^<][d\bar{\psi}^>][d\psi^>]\, e^{-S^\Lambda[\bar{\psi}^<,\psi^<,\bar{\psi}^>,\psi^<]} \tag{264}$$
$$= \int [d\bar{\psi}^<][d\psi^<] e^{-S^{\Lambda\to\Lambda'}[\bar{\psi}^<,\psi^<]},$$

where

$$e^{-S^{\Lambda\to\Lambda'}[\bar{\psi}^<,\psi^<]} \equiv \int [d\bar{\psi}^>][d\psi^>]\, e^{-S^\Lambda[\bar{\psi}^<,\psi^<,\bar{\psi}^>,\psi^<]}. \tag{265}$$

In this way we can define a renormalized effective action $S^{\Lambda\to\Lambda'}[\bar{\psi},\psi]$ for any $\Lambda' < \Lambda$, and indeed regard this as a continuous *flow* of the action functionals, taking $\Lambda' = \Lambda e^{-\ell}$, with $\ell \geq 0$. It is conventional, and useful, to make the actions at different ℓ easier to compare by rescaling the fields in such a way as to restore a fixed cut-off at all ℓ. This is done by changing variables in the path integral over the remaining fields:'

$$\psi^<_{\boldsymbol{k},\omega_n} = b^\chi \psi'_{b\boldsymbol{k},b^z\omega_n}, \qquad \bar{\psi}^<_{\boldsymbol{k},\omega_n} = b^\chi \bar{\psi}'_{b\boldsymbol{k},b^z\omega_n}, \tag{266}$$

with $b = e^\ell = \Lambda/\Lambda'$, so that the cut-off for the momenta of the $\psi', \bar{\psi}'$ fields is restored to Λ. The numbers χ and z are chosen in order to preserve nice features of the effective action after rescaling – see below. With this transformation we define the rescaled effective action by

$$S^{\Lambda,\ell}[\bar{\psi}',\psi'] = S^{\Lambda\to\Lambda e^{-\ell}}[\bar{\psi}^<,\psi^<]. \tag{267}$$

Note that the right-hand side should be evaluated by inserting Eq. (266) in it to express the functional in terms of the "primed" fields. By construction $S^{\Lambda,\ell=0}[\bar{\psi},\psi] = S^\Lambda[\bar{\psi},\psi]$, so Eq. (267) defines a family of actions with a fixed cut-off, parametrized by $\ell \geq 0$, whose low energy properties are all identical. This is the *renormalization group flow* in the space of actions, often called the space of theories. A scale invariant theory (like S_0) is a *fixed point* of the RG flow. It may be attractive, i.e. actions which are close to it evolve closer to it with increasing ℓ, or it may be repulsive – and like general dynamical systems one can find different "eigen-directions" in the flow for which perturbations of a fixed point decay or grow. Of most interest are the fully stable fixed points, since they govern the low energy properties of all nearby theories. Fixed points with a small number of unstable directions are also of interest, and describe situations in which scale invariance can be achieved by some kind of tuning, e.g. phase transitions.

Perturbative implementation

Now let us see how the RG is actually carried out perturbatively in interactions. For simplicity we directly work in the (almost – we will very occasionally need β and V to normalize extensive quantities) zero temperature

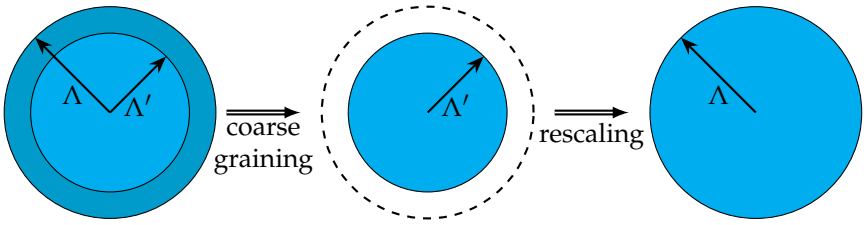


Figure 7: Wilsonian RG when the gapless modes lie at $\boldsymbol{k} = 0$, as in nodal semi-metals.

and infinite volume limit, so that momentum and Matsubara frequency sums become integrals. We choose a slightly different Fourier convention which is convenient in this limit:

$$\psi(\boldsymbol{x},\tau) = \int^{\Lambda} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}}\, \psi_{\boldsymbol{k},\omega_n} e^{-i\boldsymbol{k}\cdot\boldsymbol{x}-i\omega_n\tau}, \qquad \psi_{\boldsymbol{k},\omega_n} = \int d^d\boldsymbol{x}d\tau\, \psi(\boldsymbol{x},\tau) e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\omega_n\tau},$$

(268)

$$\bar\psi(\boldsymbol{x},\tau) = \int^{\Lambda} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}}\, \bar\psi_{\boldsymbol{k},\omega_n} e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\omega_n\tau}, \qquad \bar\psi_{\boldsymbol{k},\omega_n} = \int d^d\boldsymbol{x}d\tau\, \bar\psi(\boldsymbol{x},\tau) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}-i\omega_n\tau}.$$

The short-distance regularization appears as a cut-off on the maximum momentum, $|k| < \Lambda$, as indicated by the superscript on the integral. With this convention, the action is

$$S_0 = \int^{\Lambda} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}}\, \bar\psi_{\boldsymbol{k},\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi_{\boldsymbol{k},\omega_n}. \tag{269}$$

with the real space fields defined as just the Fourier transforms of their Fourier space counterparts. Because modes with different $\boldsymbol{k}$ are decoupled in S_0, we have

$$\begin{aligned} S_0 &= \int^{\Lambda'} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}}\, \bar\psi^{<}_{\boldsymbol{k},\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi^{<}_{\boldsymbol{k},\omega_n} + \int_{\Lambda'}^{\Lambda} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}}\, \bar\psi^{>}_{\boldsymbol{k},\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi^{>}_{\boldsymbol{k},\omega_n} \\ &= S_0^{<} + S_0^{>}. \end{aligned} \tag{270}$$

So without interactions, the coarse-graining step of the RG, Eq. (265), is simple:

$$\begin{aligned} S_0^{\Lambda\to\Lambda'} &= -\ln\left[\int [d\bar\psi^{>}][d\psi^{>}]\, e^{-S_0^{<}-S_0^{>}}\right] \\ &= S_0^{<} - \beta V \int_{\Lambda'}^{\Lambda} \frac{d^d\boldsymbol{k}d\omega_n}{(2\pi)^{d+1}} \mathrm{Tr}\ln(-i\omega_n + k_\mu\Gamma_\mu) = S_0^{<} - \beta V s^{>}. \end{aligned} \tag{271}$$

There is only a constant shift of the action. The rescaling step to restore the cut-off can now be made by applying Eq. (266) with $\chi = (d+2)/2$ and $z = 1$, which gives

$$\begin{aligned} S_0^<[\bar\psi^>, \psi^>] &= \int^{\Lambda/b} \frac{d^d\boldsymbol{k} d\omega_n}{(2\pi)^{d+1}}\, \bar\psi^<_{\boldsymbol{k},\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi^<_{\boldsymbol{k},\omega_n} \\ &= b^{-(d+2)} \int^{\Lambda/b} \frac{d^d\boldsymbol{k} d\omega_n}{(2\pi)^{d+1}}\, \bar\psi'_{b\boldsymbol{k},b\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi'_{b\boldsymbol{k},b\omega_n} \\ &= \int^{\Lambda} \frac{d^d\boldsymbol{k} d\omega_n}{(2\pi)^{d+1}}\, \bar\psi'_{\boldsymbol{k},\omega_n}\left(-i\omega_n + k_\mu\Gamma_\mu\right)\psi'_{\boldsymbol{k},\omega_n} = S_0[\bar\psi', \psi'], \end{aligned} \tag{272}$$

where in the last line we changed variables in the integral $\boldsymbol{k} \to \boldsymbol{k}/b, \omega_n \to \omega_n/b$. We see that for this case, using the definition in Eq. (267),

$$S^{\Lambda,\ell}[\bar\psi, \psi] = S_0[\bar\psi, \psi] + \text{const.} \tag{273}$$

This is the expression of scale-invariance of the quadratic theory. That is, S_0 is a fixed point of the RG.

Now let us see how to incorporate the interactions from S_1. We split the fields into slow and fast parts according to Eq. (262). Then we have

$$\begin{aligned} S_1 &= \int d^d\boldsymbol{x} d\tau\, [\bar\psi^<\bar\psi^<\mathsf{M}\psi^<\psi^< + \bar\psi^>\bar\psi^<\mathsf{M}\psi^<\psi^< + \bar\psi^<\bar\psi^<\mathsf{M}\psi^<\psi^> \\ &\quad + \bar\psi^>\bar\psi^>\mathsf{M}\psi^<\psi^< + \cdots] \\ &\equiv S_1^< + \mathcal{S}[\bar\psi^<, \psi^<, \bar\psi^>, \bar\psi^>], \end{aligned} \tag{274}$$

where we define $S_1^<$ to be all the terms which contain no "fast" fields (i.e. $S_1^< = S_1|_{\psi\to\psi^<}$), and put the rest into $\mathcal{S}$. In principle all combinations of slow and fast fields appear there. We must integrate out the fast fields, following Eq. (265). This leads formally to (dropping the constant contribution)

$$S^{\Lambda\to\Lambda'} = S_0^< + S_1^< + \Delta S^<, \tag{275}$$

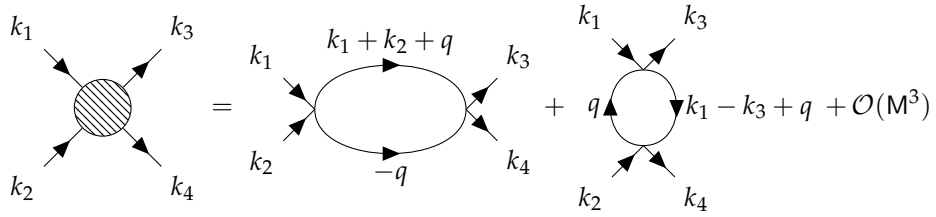
with

$$\Delta S^< = -\ln\left\langle e^{-\mathcal{S}[\bar\psi^<,\psi^<,\bar\psi^>,\bar\psi^>]}\right\rangle_> . \tag{276}$$

Here the final expectation value is the result of doing the integral over fast fields. This must be evaluated perturbatively in $\mathcal{S}$, i.e. perturbatively in M. This expansion has a nice diagrammatic representation. We indicate the slow fields $\bar\psi^<, \psi^<$ by "external lines" which are not contracted, and fast fields $\bar\psi^>, \psi^>$ become internal lines, as they are integrated out according to the rules of Gaussian integration. Terms with two external lines are potential corrections to S_0: these "tadpole diagrams" vanish at leading order if we have properly

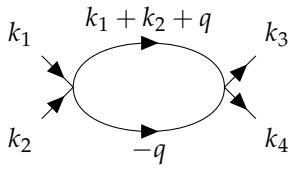
normal-ordered the terms in the interaction Hamiltonian H_1. Terms with four external lines give corrections to S_1. They have the form

(277)



Here we have indicated $d+1$-momenta on the various lines, i.e. combined momentum and frequency into a single variable. Each diagram represents a distinct contribution to $\Delta S^<$ in Eq. (276). We will not work them out in detail, because this requires specifying the Γ_μ matrices more precisely. However, it is instructive to consider the first diagram a little further, in order to understand the process:

$$\Delta S^<_{\text{pp}} = \quad \text{(278)}$$



$$= -2 \int^{<} \prod_{i=1}^{4} \frac{d^{d+1}k_i}{(2\pi)^{d+1}} \bar{\psi}_{k_1,\alpha} \bar{\psi}_{k_2,\beta} \psi_{k_3,\gamma} \psi_{k_4,\lambda} (2\pi)^{d+1} \delta(k_1 + k_2 - k_3 - k_4)$$

$$\times \int \frac{d^{d+1}q}{(2\pi)^{d+1}} \mathsf{M}_{\alpha\beta\eta\sigma} \mathsf{M}_{\sigma'\eta'\gamma\lambda} G^>_{\eta\eta'}(k_1 + k_2 + q) G^>_{\sigma\sigma'}(-q). \quad \text{(278)}$$

Here the "pp" indicates this diagram is in the "particle-particle" channel, i.e. that the arrows inside the loop flow in the same direction. The equation contains $G^>$, which is the Green's function for the Gaussian theory governed by $S^>_0$, i.e.

$$G^>_{\eta\eta'}(k = (\omega_n, \boldsymbol{k})) = \left[(-i\omega_n + k_\mu \Gamma_\mu)^{-1} \right]_{\eta\eta'} \Theta\left(\frac{\Lambda}{b} < |k| < \Lambda \right). \quad \text{(279)}$$

Warning: to get the sign correct in Eq. (278), one must carefully consider the fermion contractions and keep track of minus signs incurred on anti-commuting Grassmann fields: this is reflected here in the order of the "contracted" indices σ, σ' and η, η'. The terms on the final line of Eq. (278) may be expanded in a series in k_i, which gives a correction to M at zeroth order with $k_i = 0$, and higher order terms generating irrelevant gradient operators. Keeping just the $k_i = 0$ contribution, one obtains the correction to M of the

form

$$\Delta \mathsf{M}^{\mathrm{pp}}_{\alpha\beta\gamma\lambda} = -2 \int_{\Lambda/b}^{\Lambda} \frac{d^{d+1}q}{(2\pi)^{d+1}} \mathsf{M}_{\alpha\beta\eta\sigma} \mathsf{M}_{\sigma'\eta'\gamma\lambda} G^{>}_{\eta\eta'}(q) G^{>}_{\sigma\sigma'}(-q). \tag{280}$$

The integral is restricted to the shell in momentum space defining the fast modes. Thus it is guaranteed to be finite, since the singularity in the Green's function occurs only at $\omega_n = \boldsymbol{k} = 0$, which is outside the integration domain. The integral can be explicitly carried out in many cases. If we take the rescaling to be infinitesimal,

$$b = e^{\delta\ell}, \qquad 0 < \delta\ell \ll 1, \tag{281}$$

then the integral itself becomes linear in $\delta\ell$, since this gives the thickness of the momentum shell. Consequently, in this limit, the result of the integration is of the form

Lecture 14 (1h 15mins)
March 1st, 2018

$$\Delta \mathsf{M} = -\Lambda^{d-1} \delta\ell \left[\mathsf{M}\Gamma_{\mathrm{pp}}\mathsf{M} + \mathsf{M}\Gamma_{\mathrm{ph}}\mathsf{M} \right], \tag{282}$$

where we included contributions from both diagrams. Here Γ_{pp}, Γ_{ph} are tensors that encode the contractions that follow from each diagram, and the Λ^{d-1} prefactor follows dimensionally.

So finally, including these terms that we have generated, we find

$$S^{\Lambda\to\Lambda'} = S_0^{<} + \int d^d\boldsymbol{x} d\tau\, \bar{\psi}^{<}\bar{\psi}^{<} \left(\mathsf{M} + \Delta\mathsf{M}\right) \psi^{<}\psi^{<} + \mathcal{O}(\mathsf{M}^3). \tag{283}$$

Following this, we should redefine fields according to Eq. (266), to re-express the new expression for the partition function and now effective action in terms of ψ'. Note that by Fourier transformation, the definition of the new fields in real space corresponding to Eq. (266) with $\chi = (d+2)/2$ and $z = 1$ is

$$\psi^{<}(\boldsymbol{x}, \tau) = b^{-d/2} \psi'(\boldsymbol{x}/b, \tau/b), \tag{284}$$

which one can check agrees with Eq. (259). This leads to a new effective action of the form

$$S^{\Lambda,\ell}[\psi'] = S_0[\psi'] + b^{1-d} \int d^d\boldsymbol{x} d\tau\, \bar{\psi}'\bar{\psi}' \left(\mathsf{M} + \Delta\mathsf{M}\right) \psi'\psi' + \mathcal{O}(\mathsf{M}^3). \tag{285}$$

Since $b > 1$, for $d > 1$ the interaction term appears like before but *smaller*. This is what is meant by an *irrelevant* interaction. Comparing to the original action, and considering the infinitesimal scaling defined in Eq. (281), then the new

term has the same form as the old but with $\mathsf{M} \to \mathsf{M} + \delta\mathsf{M}$, with

$$\begin{aligned} \mathsf{M} + \delta\mathsf{M} &= e^{(1-d)\delta\ell}\,(\mathsf{M} + \Delta\mathsf{M}) + O(\mathsf{M}^3)\delta\ell \\ &= \mathsf{M} + (1-d)\delta\ell\mathsf{M} - \Lambda^{d-1}\delta\ell\left[\mathsf{M}\Gamma_{\rm pp}\mathsf{M} + \mathsf{M}\Gamma_{\rm ph}\mathsf{M}\right] + \cdots, \end{aligned} \tag{286}$$

working to $O(\delta\ell)$, and using Eq. (282) in the second line.

We can repeat this rescaling to iterate to a total rescaling of $\ell = \int \delta\ell$ and a scale-dependent coupling that obeys

$$\frac{\partial \mathsf{M}}{\partial \ell} = -(d-1)\mathsf{M} - \Lambda^{d-1}\left[\mathsf{M}\Gamma_{\rm pp}\mathsf{M} + \mathsf{M}\Gamma_{\rm ph}\mathsf{M}\right] + \cdots \tag{287}$$

Only through some hard work can we obtain the tensors $\Gamma_{\rm pp}$ and $\Gamma_{\rm ph}$ to fully define the quadratic terms in this (tensor) equation. Work that hard is reserved for your homework – ☺. However, we can see that for $d > 1$, the quadratic terms are not very important at large ℓ, at least if M is initially small, since the flow will take M to progressively smaller values (if M is not initially small we are out of luck, and the whole procedure cannot be carried out analytically – we need to rely on guesses or other knowledge).

Summary

We conclude for $d > 1$, weak interactions are *irrelevant* for Dirac and Weyl semimetals. The scale invariance of the free fermion theory is restored at low energies. This may be considered a version of Fermi liquid theory for this case: the low energy excitations are asymptotically free quasiparticles.

We can see that, while our concrete formulation used momentum space, it did not play a major role in the conclusion. Actually we could have applied other RG schemes with different types of cut-off, e.g. a real space cut-off, or your favorite scheme from quantum field theory such as dimensional regularization, and obtained physically identical results. This is because our effective theory has low energy modes only at zero momentum, and so the action is a Taylor expansion around this point. Order by order, polynomials of momentum Fourier transform directly back into derivatives in real space, so we can just as well think in real space. The argument pretty much relies just on "power counting": the rescaling in Eq. (284) or Eq. (259) is dictated by dimensional analysis, and it determined the important $d-1$ factor. This dimension counting is the same for Weyl and Dirac fermions, and so we conclude that all *local* interactions are irrelevant for Weyl and Dirac fermions in two and three dimensions.

There are some interesting problems where interactions are not irrelevant. We can see that one dimension is such a case: here the power-counting term vanishes and the interaction appears to be scale invariant. This scale invariance is not exact however, and the quadratic terms become crucial. We say that the interactions are "marginal" in this case. Another is a quadratic band touching, where the Hamiltonian involves second (spatial) derivatives rather that first order ones. It turns out that short-range interactions in two dimen-

sions are marginal for such a quadratic band touching. We may also consider long-range interactions. Coulomb $1/r$ interactions is an important case. One can easily check that $1/r$ interactions are marginal for the Weyl/Dirac problems in both two and three dimensions.

7.2 *RG for metals*

One-dimensionality of the kinetic energy

With the simpler case of nodal semi-metals under our belt, we are ready to tackle the problem of RG for a Fermi surface. This follows a rather well known review article by R. Shankar. We are interested in perturbations of a free action of the form

(288)
$$S_0 = \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \bar{\psi}_k \left(-i\omega_n + \epsilon_{\boldsymbol{k}}\right) \psi_k.$$

For simplicity we are going to neglect any band/spin indices for this subsection. To carry out the Wilsonian RG, we need to include some cut-off Λ into this action, such that reducing Λ is equivalent to focusing on lower energy degrees of freedom. The tricky aspect is that the low energy states in this case correspond to those on the Fermi surface, i.e. $\epsilon_{\boldsymbol{k}} = 0$, which is in general an extended object in momentum space, and so we cannot just describe it by a Taylor expansion. The natural way to describe it is instead to the cut-off by a shell of thickness 2Λ around this surface, which is sensible provided Λ is small compared to the typical radius, k_F, of the Fermi surface. The RG consists of progressively "thinning" this shell down towards the ideal limit of a true $d-1$ dimensional surface.

For simplicity, we will consider the case of spherical symmetry with $O(d)$ rotational symmetry of the Hamiltonian, so that $\epsilon_{\boldsymbol{k}}$ is a function of $|\boldsymbol{k}|$ only, and the Fermi surface is a true sphere with radius k_F. We can work in spherical coordinates so that

(289)
$$\boldsymbol{k} = \hat{\boldsymbol{K}}(k_F + q),$$

where $\hat{\boldsymbol{K}}$ is a unit vector giving the direction in momentum space, and q is the distance from the Fermi surface normal to the surface. We can define new fields in these variables: The free action is

$$S_0 = \int \frac{d\omega_n d\hat{\boldsymbol{K}} dq \, (k_F+q)^{d-1}}{(2\pi)^{d+1}} \bar{\psi}_{\hat{\boldsymbol{K}}(k_F+q),\omega_n} \left(-i\omega_n + \epsilon_{k_F+q}\right) \psi_{\hat{\boldsymbol{K}}(k_F+q),\omega_n}$$

(290)
$$\approx \frac{k_F^{d-1}}{(2\pi)^{d+1}} \int d\hat{\boldsymbol{K}} dq d\omega_n \, \bar{\psi}_{\hat{\boldsymbol{K}}(k_F+q),\omega_n} \left(-i\omega_n + v_F q\right) \psi_{\hat{\boldsymbol{K}}(k_F+q),\omega_n},$$

with v_F the Fermi velocity. From here redefine the field variables to be in terms

of $\hat{\boldsymbol{K}}$ and q, and with a natural normalization

(291)
$$\bar{\psi}_{\hat{\boldsymbol{K}}(k_F+q),\omega_n} = \left(\frac{(2\pi)^{d-1}}{k_F^{d-1}S_{d-1}}\right)^{1/2} \bar{\psi}_{\hat{\boldsymbol{K}},q,\omega_n}, \qquad \psi_{\hat{\boldsymbol{K}}(k_F+q),\omega_n} = \left(\frac{(2\pi)^{d-1}}{k_F^{d-1}S_{d-1}}\right)^{1/2} \psi_{\hat{\boldsymbol{K}},q,\omega_n},$$

where S_d is the surface area of the d-sphere. This gives

$$S_0 = \int \frac{d\hat{\boldsymbol{K}}}{S_{d-1}} \int_{-\Lambda}^{\Lambda} \frac{dq}{2\pi} \int \frac{d\omega_n}{2\pi}\, \bar{\psi}_{\hat{\boldsymbol{K}},q,\omega_n} \left(-i\omega_n + vq\right) \psi_{\hat{\boldsymbol{K}},q,\omega_n}. \tag{292}$$

In this formula we have separated the variable which is cut-off, q, fully from the other variables. We can see that the fermionic propagator depends only on q and ω_n, and *not* on the angular variable $\hat{\boldsymbol{K}}$. The latter appears more like an internal "flavor" index in the fermion fields. From the point of view of the propagator, the low energy dynamics is effectively $1+1$-dimensonal, regardless of the physical dimension d! This is a source of very different behavior for the Fermi surface problem in comparison to the previous one.

In this form, the free action has a manifest scale invariance, just like S_0 for the nodal fermions in the previous subsection. Following the same procedure, we obtain a fixed point for the free theory if we take

$$\bar{\psi}^{>}_{\hat{\boldsymbol{K}},q,\omega_n} = b^{3/2}\bar{\psi}'_{\hat{\boldsymbol{K}},bq,b\omega_n}, \qquad \psi^{>}_{\hat{\boldsymbol{K}},q,\omega_n} = b^{3/2}\psi'_{\hat{\boldsymbol{K}},bq,b\omega_n}, \tag{293}$$

which is a special case of Eq. (266), if we view $\hat{\boldsymbol{K}}$ as an internal index. It is important to note that there is a subtlety in comparison to the situation of the previous subsection, because there are two important momentum scales in the problem: the cut-off Λ *and* the Fermi momentum k_F. The ratio k_F/Λ is dimensionless, and merely rescaling does not change it. So when we integrate out modes in the coarse-graining step, the ratio k_F/Λ is increased, and we cannot restore it by a rescaling. Since we choose to rescale to restore the cut-off to Λ, we effectively increase k_F. The important point is that the ratio k_F/Λ increases under the RG. Viewed globally, the low energy region becomes a narrower and narrower ring near the Fermi surface. This narrowness is physical and has consequences we will explore below.

Given that the propagator and the rescaling appears the same as in $1+1$ dimensions, we can expect that interactions also may behave similarly to that case. We saw that for 1d Dirac fermions short-range interactions are marginal, so it will not be surprising to find the same here. Nevertheless, there are significant differences from the $1+1$ dimensional case, as we will clearly see.

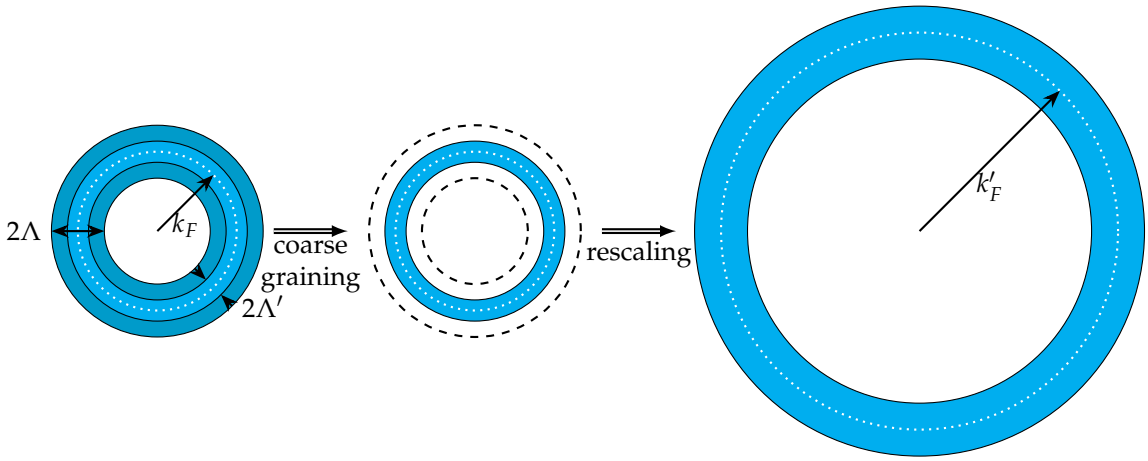


Figure 8: Wilsonian RG for a circular Fermi surface. By rescaling momenta to restore the thickness of the annulus around the Fermi surface, the Fermi momentum is effectively enlarged by a factor Λ'/Λ.

Phase space constraints and two types of interactions

We consider a general interaction involving four fermion operators, i.e. a two-body interaction, which satisfies translational invariance:

(294)
$$S_1 = \int \prod_{i=1}^{3} \frac{d^{d+1}k_i}{(2\pi)^{d+1}} U(\{k_i\}) \bar{\psi}_1 \bar{\psi}_2 \psi_3 \psi_4.$$

where we abbreviated $\bar{\psi}_1 = \bar{\psi}_{\boldsymbol{k}_i,\omega_{n,i}}$ etc., and there are only three independent integrals, so that

(295) $\boldsymbol{k}_4 = \boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}_3, \qquad \omega_{n,4} = \omega_{n,1} + \omega_{n,2} - \omega_{n,3}.$

Now we would like to transform this to spherical coordinates and impose the momentum shell cut-off. We write

$$S_1 = \prod_{i=1}^{3} \int \frac{d\hat{\boldsymbol{K}}_i}{S_d} \int_{-\Lambda}^{\Lambda} \frac{dq_i}{2\pi} \int \frac{d\omega_{n,i}}{(2\pi)^2} U(\{\hat{\boldsymbol{K}}_i\})$$

(296)
$$\times \bar{\psi}_{\hat{\boldsymbol{K}}_1,q_1,\omega_{n1}} \bar{\psi}_{\hat{\boldsymbol{K}}_2,q_2,\omega_{n2}} \psi_{\hat{\boldsymbol{K}}_3,q_3,\omega_{n3}} \psi_{\hat{\boldsymbol{K}}_4,q_4,\omega_{n4}} \Theta(\Lambda - ||\boldsymbol{k}_4| - k_F|).$$

Now in order to be sure that all four momenta lie inside the shell, we needed to introduce the Θ function to constrain the length of the fourth momentum. The expression for the fourth momentum in spherical coordinates is more

complicated than in Eq. (295):

(297)
$$\hat{\boldsymbol{K}}_4 = \frac{\hat{\boldsymbol{K}}_1(k_F+q_1)+\hat{\boldsymbol{K}}_2(k_F+q_2)-\hat{\boldsymbol{K}}_3(k_F+q_3)}{|\hat{\boldsymbol{K}}_1(k_F+q_1)+\hat{\boldsymbol{K}}_2(k_F+q_2)-\hat{\boldsymbol{K}}_3(k_F+q_3)|},$$

(298)
$$q_4 = \hat{\boldsymbol{K}}_4\cdot[\hat{\boldsymbol{K}}_1(k_F+q_1)+\hat{\boldsymbol{K}}_2(k_F+q_2)-\hat{\boldsymbol{K}}_3(k_F+q_3)]-k_F.$$

Notably, the solution of these equations does not generically have q_4 inside the shell, which is why the Θ function is needed in Eq. (296). Indeed, this means that the Θ function restricts the integration domain of the three otherwise free angular variables $\hat{\boldsymbol{K}}_1, \hat{\boldsymbol{K}}_2, \hat{\boldsymbol{K}}_3$. The physics here is that the four physical momenta vectors obey the constraint $\boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}_3+\boldsymbol{k}_4$, and at the same time lie very close to the Fermi surface. These two conditions are highly constraining. It is useful to think of the extreme case $q_i=0$, so all four vectors are exactly on the Fermi surface. This is simplest in two dimensions. There are really only two solutions to these constraints. First, we can have arbitrary $\hat{\boldsymbol{K}}_1$ and $\hat{\boldsymbol{K}}_2$, so that $\boldsymbol{k}_1+\boldsymbol{k}_2$ is a vector whose length is of order k_F. Then for the remaining two momenta to add to the same sum, we either need $\hat{\boldsymbol{K}}_3=\hat{\boldsymbol{K}}_1$ and $\hat{\boldsymbol{K}}_4=\hat{\boldsymbol{K}}_2$, or the same with $\hat{\boldsymbol{K}}_3$ and $\hat{\boldsymbol{K}}_4$ interchanged. For spinless electrons, these represent the same terms, since we can simply anticommute ψ_3 and ψ_4. We see that in this case while the first two unit vectors are free, the third is completely determined. The second possibility is to have $\hat{\boldsymbol{K}}_2=-\hat{\boldsymbol{K}}_1$, so that the sum vanishes. Then we can arbitrarily choose $\hat{\boldsymbol{K}}_3$ and take $\hat{\boldsymbol{K}}_4=-\hat{\boldsymbol{K}}_3$. Importantly, in this case too there are only two free $\hat{\boldsymbol{K}}_i$ directions, not three as one might naïvely expect.

The actual integral is over a non-zero range of q_i, so these conditions are not perfectly satisfied, and there is some non-zero measure for all three $\hat{\boldsymbol{K}}_i$ with $i=1,2,3$. However, when $\Lambda \ll k_F$, the integration region is all very near one of the two above situations. So we can separate the interaction into two terms, each including one of these regions: $S_1 = S_{1,V}+S_{1,W}$:

$$S_{1,V} = \int \frac{d\hat{\boldsymbol{K}}_1}{S_d}\frac{d\hat{\boldsymbol{K}}_2}{S_d}\int_{\hat{\boldsymbol{K}}_3\approx\hat{\boldsymbol{K}}_1}\frac{d\hat{\boldsymbol{K}}_3}{S_d}\prod_{i=1}^{3}\int_{-\Lambda}^{\Lambda}\frac{dq_i}{2\pi}\int\frac{d\omega_{n,i}}{(2\pi)^2}\,\mathsf{V}(\hat{\boldsymbol{K}}_1\cdot\hat{\boldsymbol{K}}_2)$$

(299)
$$\times\,\bar{\psi}_{\hat{\boldsymbol{K}}_1,q_1,\omega_{n1}}\bar{\psi}_{\hat{\boldsymbol{K}}_2,q_2,\omega_{n2}}\psi_{\hat{\boldsymbol{K}}_4,q_4,\omega_{n4}}\psi_{\hat{\boldsymbol{K}}_3,q_3,\omega_{n3}}\,\Theta(\Lambda-|q_4|),$$

$$S_{1,W} = \int \frac{d\hat{\boldsymbol{K}}_1}{S_d}\frac{d\hat{\boldsymbol{K}}_3}{S_d}\int_{\hat{\boldsymbol{K}}_2\approx-\hat{\boldsymbol{K}}_1}\frac{d\hat{\boldsymbol{K}}_2}{S_d}\prod_{i=1}^{3}\int_{-\Lambda}^{\Lambda}\frac{dq_i}{2\pi}\int\frac{d\omega_{n,i}}{(2\pi)^2}\,\mathsf{W}(\hat{\boldsymbol{K}}_1\cdot\hat{\boldsymbol{K}}_3)$$
$$\times\,\bar{\psi}_{\hat{\boldsymbol{K}}_1,q_1,\omega_{n1}}\bar{\psi}_{\hat{\boldsymbol{K}}_2,q_2,\omega_{n2}}\psi_{\hat{\boldsymbol{K}}_3,q_3,\omega_{n3}}\psi_{\hat{\boldsymbol{K}}_4,q_4,\omega_{n4}}\,\Theta(\Lambda-|q_4|).$$

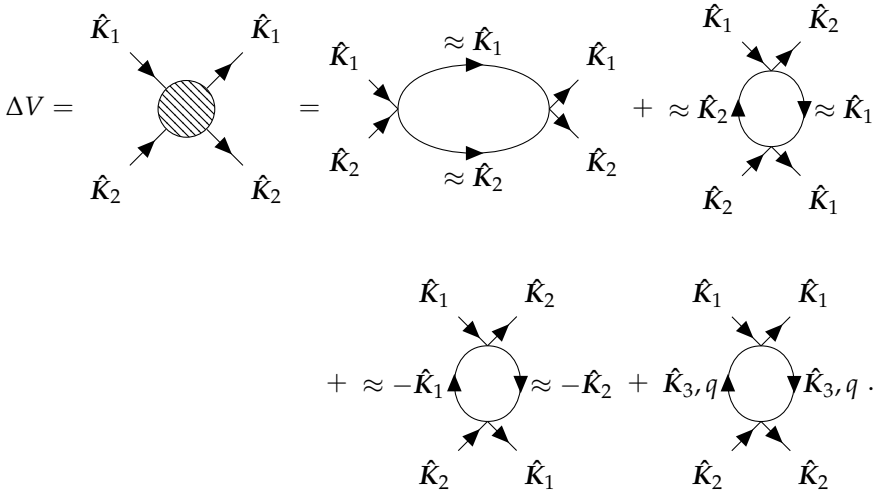
Here the interactions have been taken to be functions only of the "large" integration variables, since they are assumed smooth on the scale of k_F, and we have also used rotational invariance to write them in terms invariant inner product. We chose the order of the operators in the V term so that

$V > 0$ reflects a repulsive interaction. The result is that the interactions are parametrized by two functions V and W of one variable. These describe two "channels" of interactions. The first, V channel describes "forward scattering" of electrons: two incoming electrons are scattered by this interaction into states with momenta in the same two regions of the Fermi surface. The second, W channel describes "pair scattering": two electrons with nearly opposite momenta are scattered to another completely different pair of anti-podal points on the Fermi surface.

Lecture 15 (1h 15mins)
March 8th, 2018

RG for forward scattering interaction

Applying the scale transformation in Eq. (293) to Eq. (299), it is easy to see that the interactions V and W are indeed marginal at the rescaling level. The key then is to examine how they behave under the coarse-graining part of the RG. To do this, we return to the diagrams we studied in the previous subsection. In that case, we saw that the corrections to the interactions were to leading order obtained by diagrams in which all external momenta and frequencies were set to zero (because we are expanding around the divergent point of the Green's functions which occurs at zero momentum and frequency) and in which the momenta inside the loop are integrated over the shell. Here instead of to zero we should set the external momenta to lie exactly on the Fermi surface, which is analogous insofar as this is where the Green's functions diverge. In this way we obtain four diagrams that describe corrections to the V vertex:

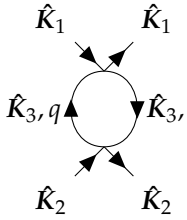


(300)

Let us examine these different diagrams. The first, second, and fourth each contain two V-type vertices, since the incoming legs at each vertex are not opposite. The third diagram contains two W vertices. Next, note the momentum labels on the first three diagrams: one can see that the angular component of the internal wavevectors are fixed by the external ones in all these cases. This means that when $\Lambda \ll k_F$, there is almost no integration volume for these diagrams. Thus they give asymptotically zero contribution in the scaling limit as $\Lambda' = \Lambda e^{-\ell} \to 0$.

All that is left is the fourth diagram. Here we have a free integration over the internal variables in the loop: $\hat{K}_3, q, \omega_n$. This is of the form

(301)



$$\propto \int \frac{d\hat{K}_3}{S_d} V(\hat{K}_1 \cdot \hat{K}_3) V(\hat{K}_3 \cdot \hat{K}_2) \int\limits_{\Lambda' < |q| < \Lambda} \frac{dq}{2\pi} \int \frac{d\omega_n}{2\pi} \frac{1}{(-i\omega_n + vq)^2} = 0.$$

The final result vanishes upon carrying out the frequency integral, because all singularities are on one side of the real axis, and the contour can be taken on the opposite side. This type of vanishing is a consequence of causality: basically the same excitation cannot travel both forward and backward. So we see that all contributions to the renormalization of V have vanished. Since V was also marginal at the rescaling level, we conclude that up to second order, this interaction does not flow:

$$\partial_\ell V = 0, \qquad \text{to } O[(V,W)^2]. \tag{302}$$

In fact it turns out that V is exactly marginal in the scaling limit. It is an example of what we call a *Fermi liquid interaction*, which Landau envisioned from a rather different argument.

To get an idea of why this interaction is marginal, let us re-arrange the operators in the expression, Eq. (299), for the V coupling:

$$S_{1,V} = \int \frac{d\hat{K}_1}{S_d} \frac{d\hat{K}_2}{S_d} \int\limits_{\hat{K}_3 \approx \hat{K}_1} \frac{d\hat{K}_3}{S_d} \prod_{i=1}^{3} \int_{-\Lambda}^{\Lambda} \frac{dq_i}{2\pi} \int \frac{d\omega_{n,i}}{(2\pi)^2} V(\hat{K}_1 \cdot \hat{K}_2)$$
$$\times \bar{\psi}_{\hat{K}_1, q_1, \omega_{n1}} \psi_{\hat{K}_3, q_3, \omega_{n3}} \bar{\psi}_{\hat{K}_2, q_2, \omega_{n2}} \psi_{\hat{K}_4, q_4, \omega_{n4}} \Theta(\Lambda - |q_4|). \tag{303}$$

Now we note that in this term $\hat{K}_3 \approx \hat{K}_1$ and $\hat{K}_4 \approx \hat{K})_2$, so let us make that replacement in the last line:

$$S_{1,V} \approx \int \frac{d\hat{K}_1}{S_d} \frac{d\hat{K}_2}{S_d} \int\limits_{\hat{K}_3 \approx \hat{K}_1} \frac{d\hat{K}_3}{S_d} \prod_{i=1}^{3} \int_{-\Lambda}^{\Lambda} \frac{dq_i}{2\pi} \int \frac{d\omega_{n,i}}{(2\pi)^2} V(\hat{K}_1 \cdot \hat{K}_2)$$
$$\times \bar{\psi}_{\hat{K}_1, q_1, \omega_{n1}} \psi_{\hat{K}_1, q_3, \omega_{n3}} \bar{\psi}_{\hat{K}_2, q_2, \omega_{n2}} \psi_{\hat{K}_2, q_4, \omega_{n4}} \Theta(\Lambda - |q_4|). \tag{304}$$

We can see from this that this term is expressed in terms of "number operators" $\bar{\psi}_{\hat{K}} \psi_{\hat{K}}$, so that the number of fermions at each direction of the Fermi surface is separately conserved. This vastly reduces the ability of this interaction to mix different states in the Fock space. So it is perhaps not surprising

that it does not renormalize.

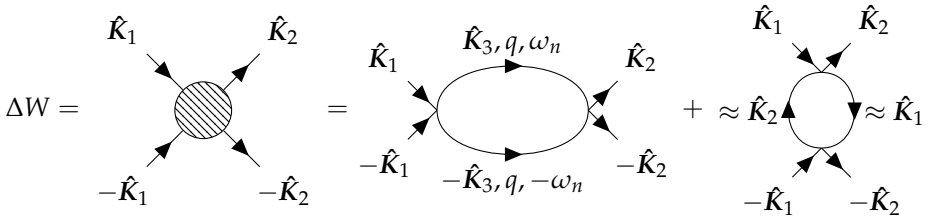
Landau introduced a version of this interaction in the Hamiltonian form which makes this conservation law even more explicit. The Landau Fermi liquid Hamiltonian is

(305)
$$H_{FL} = \sum_k \epsilon_k n_k + \frac{1}{2L^d} \sum_{k,k'} V_{k,k'} n_k n_{k'},$$

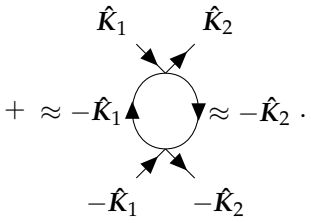
where $n_k = c_k^\dagger c_k$ is the number operator, and $V_{k,k'}$ is the analog of the V coupling above. Eq. (305) is trivially exactly soluble since n_k is a good quantum number for all momenta.

RG for pair scattering interaction

Let us turn to the renormalization of W. In this case we can draw three diagrams:



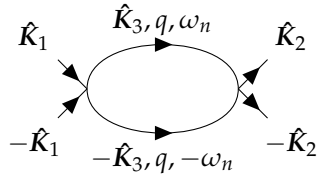
(306)



The first diagram represents two W vertices, while the second and third diagrams involve one V and one W vertex. The latter two terms vanish in the small Λ limit because their internal angles are constrained. One is left with

the first diagram:

$$\Delta W = \quad \propto \int \frac{d\hat{\boldsymbol{K}}_3}{S_d} W(\hat{\boldsymbol{K}}_1 \cdot \hat{\boldsymbol{K}}_3) W(\hat{\boldsymbol{K}}_3 \cdot \hat{\boldsymbol{K}}_2)$$



(307)

$$\times \int\limits_{\Lambda' < |q| < \Lambda} \frac{dq}{2\pi} \int \frac{d\omega_n}{2\pi} \frac{1}{(-i\omega_n + vq)(i\omega_n + vq)} \neq 0.$$

This time the internal frequency integral does not vanish, because there are poles symmetrically placed on both sides of the real axis. Thus the W interaction flows under the RG. With a little effort, one can get the sign, and the result is

$$\partial_\ell W(\hat{\boldsymbol{K}}_1 \cdot \hat{\boldsymbol{K}}_2) = -c \int \frac{d\hat{\boldsymbol{K}}_3}{S_d} W(\hat{\boldsymbol{K}}_1 \cdot \hat{\boldsymbol{K}}_3) W(\hat{\boldsymbol{K}}_3 \cdot \hat{\boldsymbol{K}}_2), \tag{308}$$

where c is a positive constant. The right hand side of Eq. (308) is basically a convolution. For example, in two dimensions, we can redefine the function via

$$\mathsf{W}(\theta) = W(\cos\theta), \tag{309}$$

and the RG equation becomes

$$\partial_\ell \mathsf{W}(\theta_1 - \theta_2) = -c \int \frac{d\theta'}{2\pi} \mathsf{W}(\theta_1 - \theta') \mathsf{W}(\theta' - \theta_2). \tag{310}$$

This allows us to Fourier transform it

$$\mathsf{W}(\theta) = \sum_m \mathsf{W}_m e^{im\theta}, \tag{311}$$

which gives

$$\partial_\ell \mathsf{W}_m = -c\mathsf{W}_m^2. \tag{312}$$

This clearly shows that each angular momentum channel is independent at this order. The system is when the interaction is repulsive in all channels, $\mathsf{W}_m > 0$: these interactions are called "marginally irrelevant". If even one of them is attractive, $\mathsf{W}_m < 0$, the metallic state becomes unstable: this interaction is "marginally relevant". This instability was discovered by Leon Cooper, and is often called the *Cooper instability*. It induces pairing and leads to superconductivity.

A comment here is in order. In the theory without spin, Fermi statistics places a strong constraint on the function $W(\hat{\boldsymbol{K}}_1 \cdot \hat{\boldsymbol{K}}_2)$: it must be odd under the interchange $\hat{\boldsymbol{K}}_1 \leftrightarrow \hat{\boldsymbol{K}}_2$. This translates in two dimensions to $\mathsf{W}(\theta + \pi) =$

$-\mathrm{W}(\theta)$, which requires $\mathrm{W}_m = 0$ for m even. That is, only odd angular momentum pairing interactions exist. If spin is included, the anti-symmetry required by Fermi statistics can be accommodated in other ways by the spin structure, both even and odd angular momentum pairings are possible.

8 Superconductivity

8.1 *Path integral formulation*

The RG we just discussed reveals an instability of the metallic state when interactions are attractive. This leads to superconductivity. We would like now to introduce field theory methods for the superconductivity problem. The RG is great for checking for instabilities, but not as good for calculating what they lead to. Basically, the RG is only controlled in the perturbative regime, but the instability means that the pair scattering interaction grows at low energies and develops non-perturbative effects.

We can treat these by some non-perturbative path integral technique, which is a version of mean field theory. But first we need to set this up. We return to our original Fourier conventions and consider the action including the pair-scattering interaction, $S = S_0 + S_1$, with

(313)
$$S_0 = \sum_{\boldsymbol{k},\omega_n} \bar{c}_{\boldsymbol{k},\omega_n,\alpha} \left(-i\omega_n + \epsilon_{\boldsymbol{k}}\right) c_{\boldsymbol{k},\omega_n,\alpha},$$

(314)
$$S_1 = -\frac{1}{2\beta V} \sum_{\{\boldsymbol{k}_i,\omega_{n,i}\}} U(\boldsymbol{k}_1 - \boldsymbol{k}_4) \bar{c}_{1\alpha} \bar{c}_{2\beta} c_{3\beta} c_{4\alpha}\, \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4} \delta_{\omega_{n1}+\omega_{n2}-\omega_{n3}-\omega_{n4}}.$$

Here α, β are spin-1/2 indices that take the values $1, 2 = \uparrow / \downarrow$. The minus sign in S_1 was introduced so that $U > 0$ constitutes an attractive interaction. We should require $U(\boldsymbol{k}) = U(-\boldsymbol{k})$ symmetric, since any antisymmetric component vanishes under the exchange $1 \leftrightarrow 2, 3 \leftrightarrow 4$. Note that we have not explicitly required the momenta to take the form they must for the pair-scattering interaction, but only taken the interaction to have the appropriate dependence. In principle the S_1 term therefore contains a forward-scattering part as well. However, this will not be important, and we will treat the interaction in a manner which singles out the Cooper channel. The idea is to use a Hubbard-Stratonovich transformation to rewrite the interaction as a quadratic theory with a fluctuating pairing order parameter. Let us massage the interaction first into a more promising form. We change summation variables and explicitly use the δ functions to get

(315)
$$S_1 = -\frac{1}{2\beta V} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \sum_{\omega_n,\omega_n',\bar{\omega}_n} U(\boldsymbol{k} - \boldsymbol{k}')\, \bar{c}_{-\boldsymbol{k}',-\omega_n',\beta} \bar{c}_{\boldsymbol{k}'+\boldsymbol{q},\omega_n'+\bar{\omega}_n,\alpha} c_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} c_{-\boldsymbol{k},-\omega_n,\beta},$$

where ω_n, ω_n' are fermionic Matsubara frequencies and $\bar{\omega}_n$ is a bosonic one.

We apply a Hubbard-Stratonovich transformation in the form

$$e^{-S_1} = \int [d\bar{\Delta} d\Delta] \exp\left(-\frac{\beta V}{2} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \sum_{\bar{\omega}_n} W_{\boldsymbol{k},\boldsymbol{k}'} \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \Delta^{\alpha\beta}_{\boldsymbol{k}',\boldsymbol{q},\bar{\omega}_n} \right)$$

(316)

$$\times \exp\left(\frac{1}{2} \sum_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \left[\bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \sum_{\omega_n} c_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} c_{-\boldsymbol{k},-\omega_n,\beta} + \Delta^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \sum_{\omega_n} \bar{c}_{-\boldsymbol{k},-\omega_n,\beta} \bar{c}_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} \right] \right)$$

Lecture 16 (1h 15mins)
March 9th, 2018

This reproduces the form of S_1 in Eq. (315) (up to a constant related to $\ln\det W$) provided we take $\left[W^{-1}\right]_{\boldsymbol{k},\boldsymbol{k}'} = U(\boldsymbol{k}-\boldsymbol{k}')$ (the inverse is in the matrix sense). Substituting this into the path integral, the full path integral is

(317)

$$Z = \int [d\bar{\Delta} d\Delta d\bar{c} dc] e^{-S},$$

with

$$S = \frac{\beta V}{2} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \sum_{\bar{\omega}_n} W_{\boldsymbol{k},\boldsymbol{k}'} \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \Delta^{\alpha\beta}_{\boldsymbol{k}',\boldsymbol{q},\bar{\omega}_n} + \sum_{\boldsymbol{k},\boldsymbol{q},\omega_n\bar{\omega}_n} \Big[(-i\omega_n + \epsilon_{\boldsymbol{k}}) \delta_{\boldsymbol{q},0} \delta_{\bar{\omega}_n,0} \bar{c}_{\boldsymbol{k},\omega_n,\alpha} c_{\boldsymbol{k},\omega_n,\alpha}$$

(318)

$$- \frac{1}{2} \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} c_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} c_{-\boldsymbol{k},-\omega_n,\beta} - \frac{1}{2} \Delta^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \bar{c}_{-\boldsymbol{k},-\omega_n,\beta} \bar{c}_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} \Big].$$

Now formally the Grassmann integral can be carried out since it is Gaussian. It yields

(319)

$$Z = \int [d\bar{\Delta} d\Delta] e^{-S_{\text{eff}}},$$

with

(320)

$$S_{\text{eff}} = \frac{\beta V}{2} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \sum_{\bar{\omega}_n} W_{\boldsymbol{k},\boldsymbol{k}'} \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} \Delta^{\alpha\beta}_{\boldsymbol{k}',\boldsymbol{q},\bar{\omega}_n} + \mathcal{S},$$

with

(321)

$$\mathcal{S} = -\ln\det\left[(-i\omega_n + \epsilon_{\boldsymbol{k}}) + \bar{\Delta} + \Delta \right],$$

where we left the structure of the matrix in Eq. (321) rather implicit.

8.2 *Saddle point*

At this point we are prepared to make our non-perturbative approximation. It is simply to make a saddle point evaluation of the path integral in Eq. (319),

i.e. with respect to $\bar{\Delta}, \Delta$. Taking the saddle point equations gives

(322)
$$\frac{\delta S_{\text{eff}}}{\delta \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n}} = 0 = \frac{\beta V}{2} \sum_{\boldsymbol{k}'} W_{\boldsymbol{k},\boldsymbol{k}'} \Delta^{\alpha\beta}_{\boldsymbol{k}',\boldsymbol{q},\bar{\omega}_n} - \frac{1}{2} \sum_{\omega_n} \left\langle c_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} c_{-\boldsymbol{k},-\omega_n,\beta} \right\rangle ,$$

(323)
$$\frac{\delta S_{\text{eff}}}{\delta \Delta^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n}} = 0 = \frac{\beta V}{2} \sum_{\boldsymbol{k}'} W_{\boldsymbol{k}',\boldsymbol{k}} \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k}',\boldsymbol{q},\bar{\omega}_n} - \frac{1}{2} \sum_{\omega_n} \left\langle \bar{c}_{-\boldsymbol{k},-\omega_n,\beta} \bar{c}_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} \right\rangle ,$$

which can be rewritten as

$$\Delta^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} = \frac{1}{\beta V} \sum_{\boldsymbol{k}'\omega_n} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle c_{\boldsymbol{k}'+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} c_{-\boldsymbol{k}',-\omega_n,\beta} \right\rangle .$$

(324)
$$\bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} = \frac{1}{\beta V} \sum_{\boldsymbol{k}'\omega_n} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle \bar{c}_{-\boldsymbol{k}',-\omega_n,\beta} \bar{c}_{\boldsymbol{k}'+\boldsymbol{q},\omega_n+\bar{\omega}_n,\alpha} \right\rangle .$$

It is natural to expect a solution that does not break translational symmetry in space or imaginary time. This corresponds to the condition $\boldsymbol{q} = \bar{\omega}_n = 0$. So we impose

(325)
$$\Delta^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} = \Delta^{\alpha\beta}_{\boldsymbol{k}} \delta_{\boldsymbol{q},0} \delta_{\bar{\omega},0}, \qquad \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k},\boldsymbol{q},\bar{\omega}_n} = \bar{\Delta}^{\alpha\beta}_{\boldsymbol{k}} \delta_{\boldsymbol{q},0} \delta_{\bar{\omega},0}.$$

Then the saddle point equations become

$$\Delta^{\alpha\beta}_{\boldsymbol{k}} = \frac{1}{\beta V} \sum_{\boldsymbol{k}',\omega_n} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle c_{\boldsymbol{k}',\omega_n,\alpha} c_{-\boldsymbol{k}',-\omega_n,\beta} \right\rangle .$$

(326)
$$\bar{\Delta}^{\alpha\beta}_{\boldsymbol{k}} = \frac{1}{\beta V} \sum_{\boldsymbol{k}',\omega_n} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle \bar{c}_{-\boldsymbol{k}',-\omega_n,\beta} \bar{c}_{\boldsymbol{k}',\omega_n,\alpha} \right\rangle .$$

The function $\Delta^{\alpha\beta}_{\boldsymbol{k}}$ is called the gap function, and these are the gap equations. The expectation values on the right hand side are known as "pair fields". The summation over ω_n is equivalent to taking the equal time expectation value:

$$\Delta^{\alpha\beta}_{\boldsymbol{k}} = \frac{1}{V} \sum_{\boldsymbol{k}'} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle c_{\boldsymbol{k}',\alpha}(\tau) c_{-\boldsymbol{k}',\beta}(\tau) \right\rangle .$$

(327)
$$\bar{\Delta}^{\alpha\beta}_{\boldsymbol{k}} = \frac{1}{V} \sum_{\boldsymbol{k}'} U(\boldsymbol{k}-\boldsymbol{k}') \left\langle \bar{c}_{-\boldsymbol{k}',\beta}(\tau) \bar{c}_{\boldsymbol{k}',\alpha}(\tau) \right\rangle .$$

8.3 *Solution of the gap equation*

Pairing symmetries

The gap function and pair field are antisymmetric under $\boldsymbol{k} \to -\boldsymbol{k}$ *and* $\alpha \leftrightarrow \beta$. Simple solutions push the antisymmetry into the orbital or spin part only. For example, a singlet superconductor has the form

$$\Delta_{\boldsymbol{k}}^{\alpha\beta} = \Delta_s(\boldsymbol{k})\epsilon_{\alpha\beta}, \tag{328}$$

where $\epsilon_{\alpha\beta} = i\sigma^y_{\alpha\beta}$ is the usual unit anti-symmetric 2×2 matrix. In this case, $\Delta_s(\boldsymbol{k}) = \Delta_s(-\boldsymbol{k})$ should be an *even* function. This is called an even parity superconductor. Such an even function can be expanded in a series of radial functions multiplying spherical harmonics $Y_{lm}(\hat{\boldsymbol{k}})$, with only even integer angular momentum $l = 0, 2, \cdots$, which are denoted s-wave, d-wave, etc. A triplet superconductor occurs if we take the spin part to be symmetric:

$$\Delta_{\boldsymbol{k}}^{\alpha\beta} = \boldsymbol{\Delta}_t(\boldsymbol{k}) \cdot (\sigma^y \boldsymbol{\sigma})_{\alpha\beta}\,. \tag{329}$$

Here $\boldsymbol{\Delta}_t(\boldsymbol{k})$ is a 3-component vector of complex order parameters known as the triplet order parameter. It is odd in momentum, $\boldsymbol{\Delta}_t(\boldsymbol{k}) = -\boldsymbol{\Delta}_t(-\boldsymbol{k})$, and hence has only spherical harmonics with odd $l = 1, 3, \cdots$ corresponding to p-wave, f-wave, and higher channels.

For simplicity, we will focus on the singlet superconducting case, for which we can write the quantity appearing the gap equation as

$$\langle c_{\boldsymbol{k},\alpha} c_{-\boldsymbol{k},\beta} \rangle = \psi(\boldsymbol{k})\epsilon_{\alpha\beta}, \tag{330}$$

where we suppressed the τ in the equal-time correlation function, and defined the "pair field" $\psi(\boldsymbol{k})$. The gap equation becomes

$$\Delta(\boldsymbol{k}) = \frac{1}{V}\sum_{\boldsymbol{k}'} U(\boldsymbol{k}-\boldsymbol{k}')\psi(\boldsymbol{k}'). \tag{331}$$

The function $\bar{\Delta}(\boldsymbol{k}) = \Delta^*(\boldsymbol{k})$ at the saddle point level.

Bogoliubov-de Gennes Hamiltonian

Eq. (331) is implicitly a non-linear equation because ψ has a complex dependence on Δ. To obtain it, we need to compute the expectation value in Eq. (330). This comes from the fermionic part of action S in Eq. (318), evaluated at the saddle point configuration of the gap function:

$$\begin{aligned} S_c = \sum_{\boldsymbol{k},\omega_n} \Big[& (-i\omega_n + \epsilon_{\boldsymbol{k}})\bar{c}_{\boldsymbol{k},\omega_n,\alpha} c_{\boldsymbol{k},\omega_n,\alpha} \\ & - \frac{1}{2}\bar{\Delta}(\boldsymbol{k})\epsilon_{\alpha\beta} c_{\boldsymbol{k},\omega_n,\alpha} c_{-\boldsymbol{k},-\omega_n,\beta} - \frac{1}{2}\Delta(\boldsymbol{k})\epsilon_{\alpha\beta}\bar{c}_{-\boldsymbol{k},-\omega_n,\beta}\bar{c}_{\boldsymbol{k},\omega_n,\alpha} \Big]. \end{aligned} \tag{332}$$

We recognize that the path integral over $\bar{c}, c$ with this action just represents the partition function of a quadratic fermion "mean field" Hamiltonian:

(333)
$$H_{\text{mf}} = \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} - \bar{\Delta}(\boldsymbol{k}) c^T_{\boldsymbol{k}} \frac{\epsilon}{2} c_{-\boldsymbol{k}} - \Delta(\boldsymbol{k}) c^\dagger_{-\boldsymbol{k}} \frac{\epsilon}{2} c^*_{\boldsymbol{k}} \right].$$

This is known as the Bogoliubov-de Gennes Hamiltonian. It is drastically different from the usual free fermion model in that it contains "anomalous" terms with a product of two annihilation operators or two creation operators, that do not conserve fermion number. This is a consequence of the fact that the superconducting order parameter (Δ or ψ) breaks the U(1) symmetry that generates charge conservation.

H_{mf} is still quadratic, so it can be diagonalized. There are many ways to do this. First let us write the spin sum explicitly:

(334)
$$H_{\text{mf}} = \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} \left(c^\dagger_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow} + c^\dagger_{\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\downarrow} \right) - \bar{\Delta}(\boldsymbol{k}) c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow} - \Delta(\boldsymbol{k}) c^\dagger_{-\boldsymbol{k}\downarrow} c^\dagger_{\boldsymbol{k}\uparrow} \right].$$

Here in the anomalous terms we used the fact that the gap function is even in $\boldsymbol{k}$ to combine the two terms in the spin sum (anti-commuting the operators and changing the sign of the momentum variable). For the form given here, we can adopt a simple prescription which is to define new d operators of the form

(335)
$$d_{\boldsymbol{k}\uparrow} = c_{\boldsymbol{k}\uparrow}, \qquad d_{\boldsymbol{k}\downarrow} = c^\dagger_{-\boldsymbol{k}\downarrow}.$$

This is a simpler version of what are called the Nambu operators. This is chosen so that the Hamiltonian in terms of d operators is no longer anomalous:

$$H_{\text{mf}} = \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} \left(d^\dagger_{\boldsymbol{k}\uparrow} d_{\boldsymbol{k}\uparrow} + d_{-\boldsymbol{k}\downarrow} d^\dagger_{-\boldsymbol{k}\downarrow} \right) - \bar{\Delta}(\boldsymbol{k}) d_{\boldsymbol{k}\uparrow} d^\dagger_{\boldsymbol{k}\downarrow} - \Delta(\boldsymbol{k}) d_{\boldsymbol{k}\downarrow} d^\dagger_{\boldsymbol{k}\uparrow} \right]$$

(336)
$$= \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} d^\dagger_{\boldsymbol{k}\uparrow} d_{\boldsymbol{k}\uparrow} + \epsilon_{-\boldsymbol{k}} (1 - d^\dagger_{-\boldsymbol{k}\downarrow} d_{-\boldsymbol{k}\downarrow}) + \bar{\Delta}(\boldsymbol{k}) d^\dagger_{\boldsymbol{k}\downarrow} d_{\boldsymbol{k}\uparrow} + \Delta(\boldsymbol{k}) d^\dagger_{\boldsymbol{k}\uparrow} d_{\boldsymbol{k}\downarrow} \right].$$

Assuming that the spectrum is inversion symmetric, $\epsilon_{-\boldsymbol{k}} = \epsilon_{\boldsymbol{k}}$, we obtain

(337)
$$H_{\text{mf}} = E_0 + \sum_{\boldsymbol{k}} d^\dagger_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} \sigma^z + \Delta(\boldsymbol{k}) \sigma^+ + \bar{\Delta}(\boldsymbol{k}) \sigma^- \right] d_{\boldsymbol{k}}.$$

where $E_0 = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}$ is a constant, we returned to the implicit notation for the spinor index, and $\sigma^\pm = (\sigma^x \pm i\sigma^y)/2$ are the spin-1/2 raising and lowering matrices. For each momentum, this has the form of the Hamiltonian for a

spin-1/2 particle in a Zeeman field,

(338)
$$H_{\rm mf} = E_0 + \sum_{\boldsymbol{k}} \boldsymbol{n}_{\boldsymbol{k}} \cdot d^\dagger_{\boldsymbol{k}} \boldsymbol{\sigma} d_{\boldsymbol{k}},$$

with

(339)
$$\boldsymbol{n}_{\boldsymbol{k}} = \begin{pmatrix} \mathrm{Re}\Delta(\boldsymbol{k}) \\ \mathrm{Im}\Delta(\boldsymbol{k}) \\ \epsilon_{\boldsymbol{k}} \end{pmatrix}.$$

This is easily diagonalized by choosing the spin quantization axis parallel to $\boldsymbol{n}_{\boldsymbol{k}}$. Let

(340)
$$d_{\boldsymbol{k}} = U_{\boldsymbol{k}} f_{\boldsymbol{k}},$$

with the unitary matrix $U_{\boldsymbol{k}}$ such that

(341)
$$\boldsymbol{n}_{\boldsymbol{k}} \cdot U^\dagger_{\boldsymbol{k}} \boldsymbol{\sigma} U_{\boldsymbol{k}} = E_{\boldsymbol{k}} \sigma^z,$$

with

(342)
$$E_{\boldsymbol{k}} = |\boldsymbol{n}_{\boldsymbol{k}}| = \sqrt{\epsilon^2_{\boldsymbol{k}} + |\Delta(\boldsymbol{k})|^2}.$$

Then

(343)
$$H_{\rm mf} = E_0 + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} f^\dagger_{\boldsymbol{k}} \sigma^z f_{\boldsymbol{k}} = E_0 + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} \left(f^\dagger_{\boldsymbol{k}+} f_{\boldsymbol{k}+} - f^\dagger_{\boldsymbol{k}-} f_{\boldsymbol{k}-} \right).$$

The result is a spectrum reminiscent of a semi-conductor, with a gap equal to (twice) the value of $|\Delta(\boldsymbol{k})$ at the Fermi momentum. Physically, the anomalous pairing terms mix the degenerate electron and hole states at the Fermi energy, and the resulting level repulsion opens a gap. The states precisely at the Fermi energy are equal mixtures of electrons and holes, while those further away are mostly electron-like or mostly hole-like.

Free energy and gap equation

Now we can address the gap equation, by calculating the pair field from this Hamiltonian. We will use a trick, which is not necessary but convenient. From

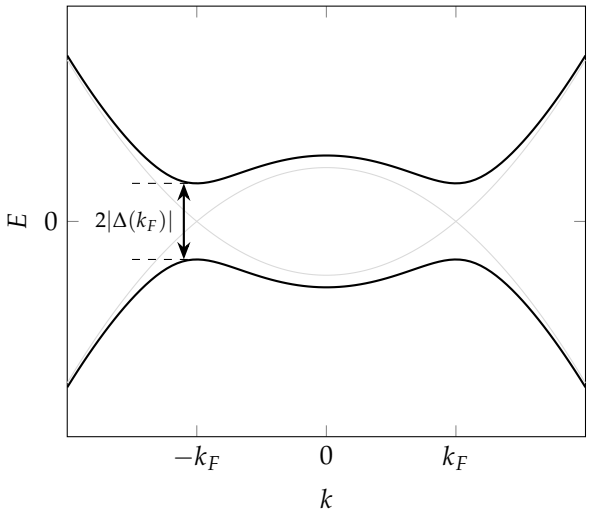


Figure 9: Bogoliubov-de Gennes quasiparticle spectrum. The faint gray lines are the spectrum in the normal state, the upward-opening and downward-opening parabolas corresponding to particle and hole excitations, respectively. Mixing particles and holes due to the anomalous terms in the BdG Hamiltonian leads to the spectrum $\pm E_{\boldsymbol{k}}$ shown by the solid lines.

Eq. (330), we can contract both sides with the ϵ tensor to obtain

(344)
$$\psi(\boldsymbol{k}) = \left\langle c_{\boldsymbol{k}}^T \frac{\epsilon}{2} c_{-\boldsymbol{k}} \right\rangle .$$

Comparing to Eq. (333), we see that this is precisely the coefficient of $-\bar{\Delta}(\boldsymbol{k})$ in the Hamiltonian. Since the integral over $\bar{c}, c$ just calculates the fermion partition function, we can recognize that the required expectation value is just a derivative of the logarithm of the partition function:

$$\psi(\boldsymbol{k}) = \frac{\operatorname{Tr}\left(\psi(\boldsymbol{k}) e^{-\beta H_{\mathrm{mf}}}\right)}{\operatorname{Tr}\left(e^{-\beta H_{\mathrm{mf}}}\right)} = \frac{\operatorname{Tr}\left(-\frac{\partial H_{\mathrm{mf}}}{\partial \bar{\Delta}(\boldsymbol{k})} e^{-\beta H_{\mathrm{mf}}}\right)}{\operatorname{Tr}\left(e^{-\beta H_{\mathrm{mf}}}\right)} = \frac{\operatorname{Tr}\left(\frac{1}{\beta}\frac{\partial}{\partial \bar{\Delta}(\boldsymbol{k})} e^{-\beta H_{\mathrm{mf}}}\right)}{\operatorname{Tr}\left(e^{-\beta H_{\mathrm{mf}}}\right)}$$

(345)
$$= \frac{1}{\beta}\frac{\partial}{\partial \bar{\Delta}(\boldsymbol{k})} \ln \operatorname{Tr}\left(e^{-\beta H_{\mathrm{mf}}}\right) = -\frac{\partial}{\partial \bar{\Delta}(\boldsymbol{k})} F_{\mathrm{mf}},$$

where F_{mf} is the free energy

(346)
$$F_{\mathrm{mf}} = -k_B T \ln \operatorname{Tr}\left(e^{-\beta H_{\mathrm{mf}}}\right).$$

The mean field free energy is simple to evaluate from Eq. (343). The partition function for a single fermion mode with energy ϵ is $z = 1 + \exp(-\beta\epsilon)$. Adding

all the modes, we obtain

$$\begin{aligned} F_{\mathrm{mf}} &= E_0 - k_B T \sum_{\boldsymbol{k}} \ln\left(1 + e^{-\beta E_{\boldsymbol{k}}}\right) + \ln\left(1 + e^{+\beta E_{\boldsymbol{k}}}\right) \\ &= E_0 - k_B T \sum_{\boldsymbol{k}} \left[\ln 2 + \ln\left(1 + \cosh \beta E_{\boldsymbol{k}}\right)\right] \\ &= E_0 - 2k_B T \sum_{\boldsymbol{k}} \left[\ln 2 + \ln \cosh \frac{\beta E_{\boldsymbol{k}}}{2}\right]. \end{aligned} \tag{347}$$

From the last formula it is easy to differentiate F to obtain the pair field:

$$\psi(\boldsymbol{k}) = \tanh \frac{\beta E_{\boldsymbol{k}}}{2} \frac{\partial E_{\boldsymbol{k}}}{\partial \bar{\Delta}(\boldsymbol{k})} = \frac{\Delta(\boldsymbol{k})}{2E_{\boldsymbol{k}}} \tanh \frac{\beta E_{\boldsymbol{k}}}{2}. \tag{348}$$

Finally we can insert this into the gap equation to obtain the self-consistent condition:

$$\Delta(\boldsymbol{k}) = \frac{1}{V} \sum_{\boldsymbol{k}'} U(\boldsymbol{k} - \boldsymbol{k}') \frac{\Delta(\boldsymbol{k}')}{2E_{\boldsymbol{k}'}} \tanh \frac{\beta E_{\boldsymbol{k}'}}{2}. \tag{349}$$

We can do lots of fun stuff with this ⌣. First let us take the infinite volume limit,

$$\Delta(\boldsymbol{k}) = \int \frac{d^d \boldsymbol{k}'}{(2\pi)^d} U(\boldsymbol{k} - \boldsymbol{k}') \frac{\Delta(\boldsymbol{k}')}{2E_{\boldsymbol{k}'}} \tanh \frac{\beta E_{\boldsymbol{k}'}}{2}. \tag{350}$$

Now let us specialize to some simple situation. We make the very reasonable approximation of weak interactions, so that the gap Δ is small. Then the denominator $E_{\boldsymbol{k}'}$ is almost vanishing near the Fermi surface of the pure system, i.e. when $\epsilon_{\boldsymbol{k}} = 0$. In that case this region will dominate the integral. Let us further suppose that $\Delta(\boldsymbol{k})$ is approximately constant for these momenta, i.e. we have s-wave pairing, and we may as well also take $U(\boldsymbol{k})$ approximately constant over the same region. Then the integrand becomes a function of $\boldsymbol{k}'$ only through the energy $\epsilon \equiv \epsilon_{\boldsymbol{k}'}$, so we can trade the momentum integral for one over energy. We have

$$\Delta = \int_{-\omega_0}^{\omega_0} d\epsilon \, \mathcal{N}(\epsilon) U \frac{\Delta}{2\sqrt{\epsilon^2 + |\Delta|^2}} \tanh \frac{\beta \sqrt{\epsilon^2 + |\Delta|^2}}{2}. \tag{351}$$

Here $\mathcal{N}(\epsilon)$ is the density of states (per spin) as a function of energy, and we included a cut-off ω_0 around the Fermi energy which reflects the approximations. We can eliminate a factor of Δ from the above equation, which is valid in the superconducting phase where it is non-zero. Furthermore, since for small Δ the system is dominated by small ϵ, we can approximate $\mathcal{N}(\epsilon) \approx \mathcal{N}(0)$.

Then the gap equation becomes

(352)
$$\mathcal{N}(0)U\int_0^{\omega_0} d\epsilon\,\frac{\tanh\frac{\beta\sqrt{\epsilon^2+|\Delta|^2}}{2}}{\sqrt{\epsilon^2+|\Delta|^2}}=1.$$

This equation determines the gap as a function of temperature and interaction strength. For example, at zero temperature, the tanh becomes unity and the zero temperature gap $\Delta_0=\Delta(T=0)$ obeys the equation

(353)
$$\mathcal{N}(0)U\int_0^{\omega_0} d\epsilon\,\frac{1}{\sqrt{\epsilon^2+|\Delta_0|^2}}=1.$$

The integral can be carried out to give

(354)
$$\ln\frac{\omega_0+\sqrt{|\Delta_0|^2+\omega_0^2}}{|\Delta_0|}=\frac{1}{\mathcal{N}(0)U},$$

which yields

(355)
$$|\Delta_0|\sim 2\omega_0 e^{-\frac{1}{\mathcal{N}(0)U}},\qquad \text{for } \mathcal{N}(0)U\ll 1.$$

Finally the non-perturbative nature of the superconducting instability is apparent: the zero temperature gap as a function of the interaction has an essential singularity.

Lecture 17 (1h 15mins)
March 13th, 2018

We can also determine the critical temperature T_c, at which $\Delta(T_c)=0$, by asking for the solution of Eq. (352) for $|\Delta|=0$:

(356)
$$\mathcal{N}(0)U\int_0^{\omega_0} d\epsilon\,\frac{\tanh\frac{\beta_c\epsilon}{2}}{\epsilon}=1.$$

We can define a new variable $x=\beta_c\epsilon/2$, which gives

(357)
$$\mathcal{N}(0)U\int_0^{\beta_c\omega_0/2} dx\,\frac{\tanh x}{x}=1.$$

This determines T_c, which for weak interactions will be low, so $\beta_c\omega_0\gg 1$, and

we can use asymptotics to approximate the integral:

(358)
$$\int_0^{\beta_c\omega_0/2} dx\,\frac{\tanh x}{x} \approx \ln(1.13\beta\omega_0),$$

which finally gives

(359)
$$k_B T_c \approx 1.13\omega_0 e^{-\frac{1}{N(0)U}}.$$

Note that both the gap and the critical temperature depend on the cut-off ω_0, which is a rather phenomenological parameter. However, their ratio is independent of them, which gives a famous result from BCS theory:

(360)
$$\Delta_0 = 1.764 k_B T_c.$$

8.4 *Phenomenology of superconductivity*

This is mainly intended as a class on techniques and theory of quantum matter. But I can hardly tell you about BCS theory without visiting a few of the phenomena of superconductivity, and how to understand them.

Ginzburg-Landau theory

Most of the most striking phenomena actually arise not from BCS theory, but from an earlier approach known as Ginzburg-Landau (GL) theory. GL theory was not originally derived microscopically, but just postulated, like the Landau theory of phase transitions. Later it was derived from BCS theory. The key ingredient is to recognize that superconductivity is described by an *order parameter* which carries "charge 2" under the electromagnetic U(1) gauge symmetry. This is nothing but the gap function or pair field. Physically it can be thought of as the Bose condensate wavefunction of Cooper pairs.

GL theory proceeds by assuming that the free energy of the system can be written as a local functional of the order parameter and its derivatives, which can further be expanded in a series in the order parameter. Requiring gauge invariance and including the magneto-static energy one obtains the celebrated GL free energy:

(361)
$$F = \int d^3\boldsymbol{x}\,\left[\frac{1}{2m*}\left|\left(\frac{\hbar}{i}\boldsymbol{\nabla} + \frac{2e}{c}\boldsymbol{A}\right)\psi\right|^2 + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{|\boldsymbol{B}|^2}{8\pi}\right].$$

GL theory includes the concept of a complex order parameter taken from quantum physics of condensates, but is otherwise a classical theory. This free energy can be derived from our path integral approach by expanding the

effective action, Eq. (320), in a series in Δ, keeping only the zero Matsubara frequency $\bar{\omega}_n = 0$ corresponding to the time-averaged gap, and expanding also in $\boldsymbol{q}$, the "center of mass" momentum of the pairs. When we assume Δ is independent of τ, we obtain the action equal to βF, since the imaginary time integral can be carried out explicitly.

The power of GL theory is its simplicity. We can easily use it to study phenomena in the superconducting state. For example, it is easy to see the Meissner effect: a SC expels magnetic field from its interior. To see this, we take $\alpha < 0$, for which the minimum free energy state has a non-zero $|\psi| = \sqrt{-\alpha/\beta}$. We can write

$$\psi = \sqrt{n_s^*} e^{i\theta}, \tag{362}$$

where θ is a phase that becomes well-defined in the SCing state.

Meissner effect

Taking the derivative of the free energy with respect to the vector potential gives the current,

$$\begin{aligned} \boldsymbol{j} &= \frac{\hbar e}{i m^*} \left(\psi^* \boldsymbol{\nabla}\psi - \boldsymbol{\nabla}\psi^* \psi\right) + \frac{(2e)^2}{m^* c} \boldsymbol{A}|\psi|^2 \\ &= \frac{2e\hbar n_s^*}{m^*} \left(\boldsymbol{\nabla}\theta + \frac{2e}{\hbar c}\boldsymbol{A}\right). \end{aligned} \tag{363}$$

Sorry I am probably using cgs units with the factors of c here. By using the Maxwell equation

$$\boldsymbol{\nabla} \times \boldsymbol{B} = \frac{4\pi}{c} \boldsymbol{j}, \tag{364}$$

we can take the curl of this equation to obtain

$$\nabla^2 \boldsymbol{B} = \frac{16\pi e^2 n_s^*}{m^* c^2} \boldsymbol{B} = \frac{4\pi e^2 n_s}{m c^2} \boldsymbol{B} \equiv \frac{1}{\lambda^2} \boldsymbol{B}, \tag{365}$$

taking $m^* = 2m$, $n_s^* = n_s/2$, where m and n_s are the electron mass and density, respectively (really the latter is the density of superconducting electrons). This is the Helmholtz equation, and it implies magnetic fields are screened and decay exponentially towards the interior of a superconductor with screening length λ. This length is called the "London penetration depth".

The expulsion of flux from a superconductor is ultimately thermodynamic in origin. To see this, return to the GL energy and just choose the gauge $\theta = 0$ (this is ok if there are no topological defects), and ψ constant. The free energy

is

(366)
$$F = \int d^3\boldsymbol{x} \left[\frac{4e^2 n_s^*}{2m^* c^2} |\boldsymbol{A}|^2 + \frac{|\boldsymbol{B}|^2}{8\pi} + \text{const.} \right].$$

A non-zero field in the superconductor requires a gradient of the vector potential, e.g. $A_x = B_z y$, so that $|\boldsymbol{A}|$ gets arbitrarily large in a large sample. This means the energy of a superconductor with a non-zero field grows faster than the volume of the sample! That is obviously too high in energy, and if a material is forced to accomodate an internal field, it will simply destroy the superconductivity to do so. For sufficiently small fields, however, the superconductivity wins and the field is expelled.

Vortices

Another basic phenomena in superconductors is the existence of *vortices*. This is a topological defect in which the phase is not constant but winds non-trivially:

(367)
$$\oint_{\mathcal{C}} \boldsymbol{\nabla}\theta \cdot d\boldsymbol{r} = 2\pi n_w,$$

where n_w is an integer winding number, and the contour $\mathcal{C}$ encloses the "vortex core". In a three-dimensional superconductor vortices are curves that can be extended or form loops. In two dimensions they are point objects.

The existence of supercurrents: currents which flow without dissipation (by name the defining property of superconductivity) is closely related to the existence of vortices. One can think of a persistent superflow through an annulus as a large vortex whose core has been "pinned" in the hole inside the annulus. The winding of the phase around this hole gives the current stability. For the current to decay vortices must escape from the hole to the outside of the annulus, one at a time, which costs considerable free energy and is almost impossible at low temperatures. See Sec.6 of the 217a notes for a more detailed explanation.

Manifestations of the gap

Generally, phenomena which are related to quasi-particles (electrons, holes) are not described by GL theory, and require the BCS formulation. The basic phenomena are captured by the BdG equations, which show that quasiparticles have a gap, like in a semi-conductor, and are mixtures of electrons and holes. The gap is visible in a number of measurements:

- **Tunneling:** tunneling from a metal into a superconductor, across a barrier, is suppressed by the gap. Only once a voltage equal to Δ is applied is enough energy supplied for an electron to tunnel in or out of the superconductor. The I-V curve of a N-SC tunnel junction reflects this.

- **Optics:** The optical conductivity of a superconductor shows a gap for frequencies between zero and 2Δ. This is like a semiconductor. The difference from a semiconductor is that the superconductor has a delta function peak at zero frequency reflecting the superfluid density.
- **Thermal conductivity:** The condensate, being a single state, has zero entropy, and so carries no heat. Since the quasiparticles have a gap, the thermal conductivity in a superconductor is strongly suppressed, $\kappa \sim e^{-\Delta/k_B T}$. It is interesting that a superconductor is a perfect conductor of electricity and a very bad conductor of heat. It is different for a superfluid (why?).
- **Thermodynamics:** Most thermodynamic quantities are exponentially dependent on temperature at low T, due to the gap. This includes the specific heat, the penetration depth, etc. Note that this exponential dependence is *not* true in a gapless superconductor, where the momentum dependence of $\Delta(\boldsymbol{k})$ includes some zeros at the Fermi surface. The most famous example is the d-wave superconductivity of the cuprates.

8.5 *Topological superconductivity*

We'll finish by linking the subject of superconductivity back to topology. Modern theory of topological superconductivity focuses on the BdG quasiparticles, and asks if they might have topological invariants and boundary modes similar to those of normal electrons. The most interesting aspect of topological superconductors is their ability to host *Majorana fermions*.

Majorana chain

A very nice example was provided by Kitaev. It is a one-dimensionless chain of spin-less (or fully spin-polarized) fermions in the presence of BCS pairing:

(368)
$$H = \sum_j \left[-w(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) - \mu(c_j^\dagger c_j - \frac{1}{2}) + \Delta^* c_j c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger \right].$$

Note that if we Fourier transform the pairing term we have

$$\sum_j \Delta c_{j+1}^\dagger c_j^\dagger = \sum_k \Delta e^{ik} c_k^\dagger c_{-k}^\dagger = \sum_k \frac{\Delta}{2} \left(e^{ik} c_k^\dagger c_{-k}^\dagger + e^{-ik} c_{-k}^\dagger c_k^\dagger \right)$$

(369)
$$= \sum_k \Delta i \sin k \, c_k^\dagger c_{-k}^\dagger.$$

So we can identify the gap function $\Delta_k = i\Delta \sin k$ which is odd in momentum. This is odd-parity pairing. It fits with our prior discussion since the spin state of the pair is symmetric, which makes it a triplet pair. A singlet is not possible for spin-polarized electrons. Kitaev's model is simple because it involves only nearest-neighbor pairing in real space, but this is not essential.

Let us fully rewrite the Hamiltonian in momentum space, in order to diagonalize it. We have

(370)
$$H = \sum_k \left[-(2w\cos k + \mu)\, c_k^\dagger c_k - i\Delta \sin k\, c_k^\dagger c_{-k}^\dagger + i\Delta^* \sin k\, c_{-k} c_k \right].$$

We can define the Nambu field

(371)
$$\psi_k = \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}.$$

Then we have

(372)
$$H = \frac{1}{2} \sum_k \psi_k^\dagger \begin{pmatrix} -2w\cos k - \mu & -2i\Delta \sin k \\ 2i\Delta^* \sin k & 2w\cos k + \mu \end{pmatrix} \psi_k \equiv \frac{1}{2} \sum_k \psi_k^\dagger\, \mathcal{H}(k)\, \psi_k.$$

The BdG Hamiltonian matrix $\mathcal{H}(k)$ has the property of particle-hole symmetry:

(373)
$$\sigma^x \mathcal{H}(k) \sigma^x = -\mathcal{H}^*(-k).$$

This is actually required of any BdG Hamiltonian and is really a property of the rewriting in terms of the Nambu spinor. Note that as a consequence any eigenstate of $\mathcal{H}(k)$ with energy ϵ is accompanied by another eigenstate with the opposite energy of $\mathcal{H}(-k)$. The negative energy states are in fact redundant. Of course, we can see this easily find the eigenvalues of $\mathcal{H}(k)$, which are $\pm\epsilon_k$ with

(374)
$$\epsilon_k = \sqrt{(2w\cos k + \mu)^2 + 4|\Delta|^2 \sin^2 k}.$$

For the system to be gapless, i.e. for there to exist a solution to $\epsilon_k = 0$, we need $\sin k = 0$ so $k = 0, \pi$, and then we also need $2w\cos k + \mu = 0$ which requires $|\mu| = 2|w|$. It seems the chain is gapped except at some special critical points where $|\mu| = 2|w|$. These critical points are not accidental: they turn out to be indicative of a topological distinction between one phase for $|\mu| < 2|w|$ and another for $|\mu| > 2|w|$.

To understand the nature of the phases, it is helpful to introduce *Majorana fermions*. We can define Majorana fermion operators by

(375)
$$\gamma_{2j-1} = c_j + c_j^\dagger, \qquad \gamma_{2j} = -ic_j + ic_j^\dagger.$$

These operators are Hermitian and obey the relations

(376)
$$\gamma_l^\dagger = \gamma_l, \qquad \gamma_l\gamma_m + \gamma_m\gamma_l = 2\delta_{lm}.$$

Majorana fermion operators are weird. It takes two of them to form a single complex fermion, which is a two level system. So in some loose sense a single Majorana operator describes "half" of a two-level system. In terms of these operators, the Hamiltonian becomes

(377)
$$H = \frac{i}{2}\sum_j \left[-\mu\gamma_{2j-1}\gamma_{2j} + (w+\Delta)\gamma_{2j}\gamma_{2j+1} + (-w+\Delta)\gamma_{2j-1}\gamma_{2j+2}\right]$$

Here we took Δ real for simplicity. We can get a simple understanding of the two phases by considering special cases within the two phases. In the phase with $|\mu| > 2|\Delta|$, we can take $\Delta = w = 0$. Then we have

(378)
$$H_{\text{triv}} = -\frac{i\mu}{2}\sum_j \gamma_{2j-1}\gamma_{2j} = -\frac{i\mu}{2}\sum_j \left(\gamma_j^\dagger\gamma_j - \frac{1}{2}\right).$$

This is obviously a trivial case. In the ground state all the original fermion states are either occupied or empty.

The other phase is more interesting. We can take $\Delta = w$ and $\mu = 0$. Then we obtain

(379)
$$H_{\text{non-triv}} = iw\sum_j \gamma_{2j}\gamma_{2j+1}.$$

This looks a lot like the previous trivial Hamiltonian, but with one important exception: the "partners" of the Majorana fermions have been switched. The fermions with even index are now paired with the odd index to their right, instead of to their left. We can "solve" Eq. (379) by going back to complex fermion operators, using the new combinations:

(380)
$$\tilde{c}_j = \frac{1}{2}(\gamma_{2j} + i\gamma_{2j+1}), \qquad \tilde{c}_j^\dagger = \frac{1}{2}(\gamma_{2j} - i\gamma_{2j+1}).$$

which gives

(381)
$$H_{\text{non-triv}} = 2w\sum_{j=1}^{N-1}\left(\tilde{c}_j^\dagger\tilde{c}_j - \frac{1}{2}\right).$$

Each of the new fermion modes is just occupied or empty. This looks almost the same as for the trivial phase, but notice that we only obtain $N-1$ com-

plex fermions this way, for a chain of N original sites. This is because there are *unpaired* Majorana fermions at the ends: γ_1 and γ_{2N} do not enter the Hamiltonian. These are often called "Majorana zero modes", although this is not as good a terminology as unpaired Majorana fermions. We can combine them into a new operator $D = i\gamma_1\gamma_{2N}$ which has eigenvalues ± 1 and commutes with $H_{\text{non-triv}}$. This means that the system has a two-fold degeneracy. The degeneracy is unusual in that it is a two-level system which is not localized anywhere in space, but rather is "shared" between the two ends.

Formally, we can introduce one more complex fermion $d, d^\dagger$, and write $D = 2d^\dagger d - 1$, but this fermion is completely non-local. The two degenerate states are connected by the action of d or $d^\dagger$ (or γ_1, γ_{2N}), and hence differ by ± 1 fermion. In fact, for an isolated system of fermions, we can always define a fermion parity operator, $P = (-1)^{N_f}$, where N_f is the total fermion number, and this fermion parity must be conserved since the Hamiltonian is a bosonic operator in which all terms contain an even number of fermion operators. In the Majorana representation, the fermion parity is

(382)
$$P = \prod_{j=1}^{N} (-i\gamma_{2j-1}\gamma_{2j}).$$

We can see that each factor of P is just what appears in H_{triv}, and so P is uniquely fixed in the ground state of the trivial phase. In the non-trivial phase, it is useful to rewrite P by

(383)
$$P = -i\gamma_1 \left(\prod_{j=1}^{N-1} (-i\gamma_{2j}\gamma_{2j+1} \right) \gamma_{2N}.$$

In the ground states of $H_{\text{non-triv}}$, the operators inside the product are all fixed, so P reduces to D. Thus two states of opposite parity are degenerate in this case.

Now we can imagine perturbing away from the special values $\Delta = w$, $\mu = 0$. In general this will introduce coupling between the pairs of Majoranas. However, since there is a large gap, the internal Majoranas (or the corresponding complex fermions) can be integrated out to obtain some effective Hamiltonian containing only the two Majoranas at the ends:

(384)
$$H_{\text{eff}} = -it\gamma_1\gamma_{2N}.$$

Here t is the result of integrating out the internal fermions, but in the limit of a long chain, we expect that t decays exponentially with N. The parameter t describes the splitting ($2|t|$) between the two almost-degenerate parity states. Importantly, it vanishes exponentially with the length of the chain, and so the degeneracy is robust and restored in the thermodynamic limit. One can actually directly obtain the wavefunctions of the Majorana zero modes by

solving the BdG equations with an open end in a semi-infinite system.

The above approach focuses on the boundary states of the Majorana chain. We could define a boundary topological invariant which is the parity of the number of unpaired Majorana modes at one edge. This is $+1$ in the trivial phase and -1 in the non-trivial phase. It is possible to also define a bulk invariant, but due to time I will not do this now. Kitaev's original paper explains this very nicely.

Other topological superconductors

Kitaev's topological phase is an example of a topological superconductor with no special symmetries in one dimension. If one imposes more symmetries, for example adding time-reversal symmetry, the structure changes. Dimensionality also plays a role. For global non-unitary symmetries, Schnyder and colleagues, and independently Kitaev, worked out a full classification of topological superconductors (and insulators) at level of quadratic fermion Hamiltonians. This has a beautiful structure, and is now known as the "periodic table" of topological insulators and superconductors (periodic because it has some repeating structure). You might read about it. Even this is not a complete story, and it is known that some topological phases are modified or unified by interactions. We will not get into any more of this here.

Instead of attacking this full classification question, I will give an example of another topological superconductor, this time in two dimensions. This is the spin polarized "p+ip" superconductor, with the gap function

(385)
$$\Delta(\boldsymbol{k}) = \langle c_{\boldsymbol{k}} c_{-\boldsymbol{k}} \rangle = (k_x + ik_y) v(k),$$

where $v(k)$ is some function of the magnitude $k = |\boldsymbol{k}|$ only. This is an odd-parity state as it must be for spin-polarized electrons, and it is intrinsically complex, and so breaks time-reversal symmetry. There is a conjugate state which is physically distinct where the prefactor in Eq. (385) is replaced by $k_x - ik_y$. For such a gap function, the BdG Hamiltonian is

(386)
$$H = \sum_{\boldsymbol{k}} \left[\epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} + v(k)(k_x + ik_y) c^\dagger_{\boldsymbol{k}} c^\dagger_{-\boldsymbol{k}} + \text{h.c.} \right].$$

It is convenient to adopt the Nambu notation (Eq. (371)), and rewrite this as

(387)
$$H = \frac{1}{2} \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} \begin{pmatrix} \epsilon_{\boldsymbol{k}} & v(k)(k_x + ik_y) \\ v(k)(k_x - ik_y) & -\epsilon_{\boldsymbol{k}} \end{pmatrix} \psi_{\boldsymbol{k}}.$$

From this one can extract the BdG energies, which are $\pm E(\boldsymbol{k})$, with

(388)
$$E(\boldsymbol{k}) = \sqrt{\epsilon^2_{\boldsymbol{k}} + |v|^2 |k|^2}.$$

As in Kitaev's chain, we can ask when this is gapless. The second term is zero if and only if $\boldsymbol{k} = 0$, so the energy vanishes only if $\epsilon_{\boldsymbol{k}=\boldsymbol{0}} = 0$. One can take a simple model with $\epsilon_{\boldsymbol{k}} = k^2/(2m) - \mu$, and the transition occurs when $\mu = 0$.

In the vicinity of the transition, we can focus on the critical modes around $\boldsymbol{k} = 0$, and therefore approximate $\epsilon_{\boldsymbol{k}} \approx \epsilon_{\boldsymbol{k}=0} \equiv -\mu$, and also approximate $v(k) \approx v(0) = v$, and the BdG Hamiltonian becomes

(389)
$$H = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} \begin{pmatrix} -\mu & v(k_x + ik_y) \\ v(k_x - ik_y) & \mu \end{pmatrix} \psi_{\boldsymbol{k}} = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} \left[vk_x\tau^x - vk_y\tau^y - \mu\tau^z \right] \psi_{\boldsymbol{k}}.$$

We recognize this as a 2d Dirac Hamiltonian. The parameter μ plays the role of a Dirac mass. We know that such a 2+1d Dirac equation describes an integer quantum Hall transition, with the Hall conductivity changing by one unit as the mass changes.

But wait! The Nambu Hamiltonian is redundant. Only half of the modes are actually physical. Due to this redundancy, there is actually only one branch of excitations, not two, described by Eq. (389). This is a 2d Majorana fermion, and the transition at $\mu = 0$ describes a critical Majorana fermion, not a critical Dirac fermion. This distinction is crucial, and quite interesting. For our simple model, there are two phases.