Fermions and Topological Phases

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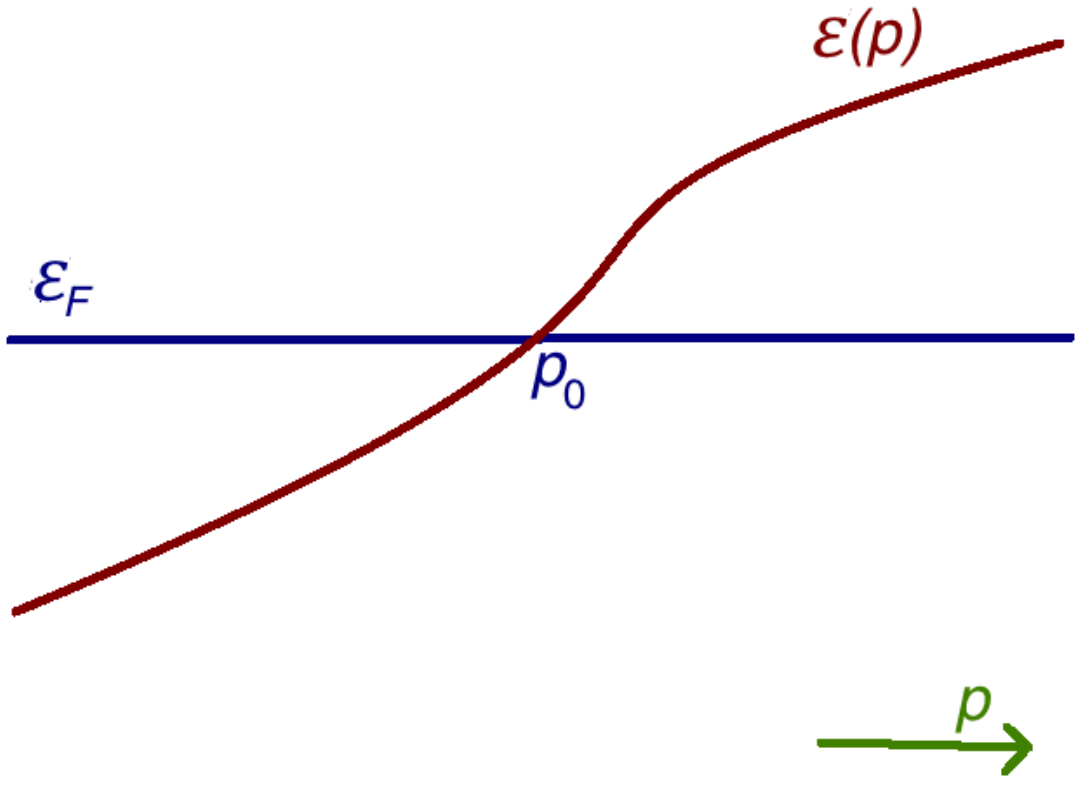
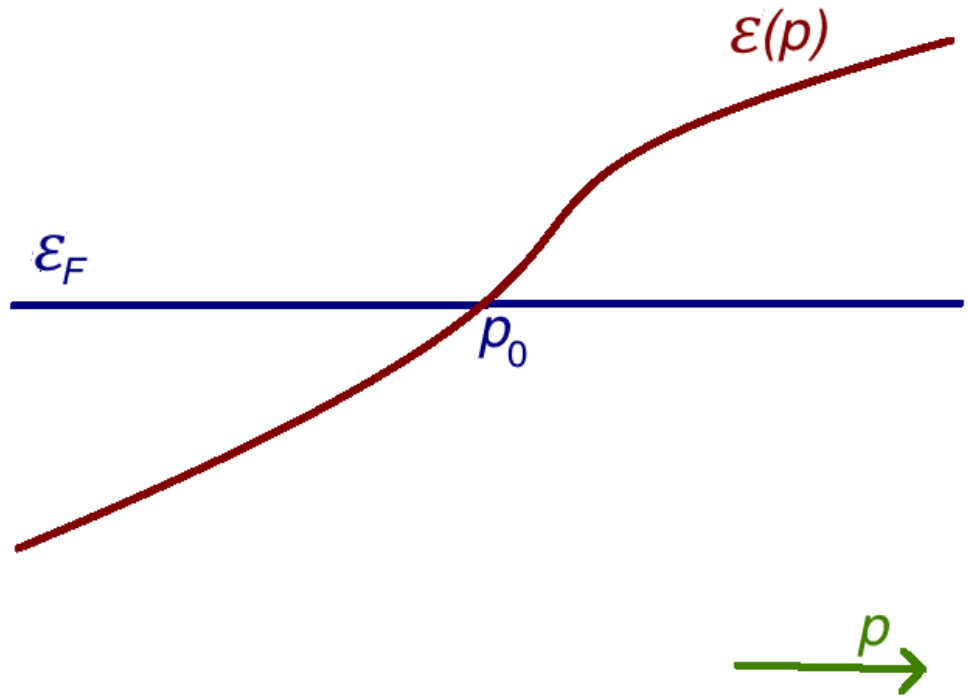
My lectures will be mostly on phases of matter that can be understood in terms of noninteracting electrons and topological band theory. Thus I will be covering topics similar to what you have heard about from Charlie Kane. I hope there will be some value added in my explanations but I cannot promise anything. I will also say a little on the fractional quantum Hall effect.

We will start by asking under what conditions we should expect to find a relativistic dispersion relation for electrons in a crystal. In one dimension the answer is familiar. Writing $\varepsilon(p)$ for the single-particle energy ε as a function of momentum p, generically $\varepsilon(p)$ crosses the fermi energy ε_F with a nonzero slope at some $p = p_0$





Then linearizing the dispersion relation around $p = p_0$, we get

$$\varepsilon = \varepsilon(p_0) + v(p - p_0) + \mathcal{O}((p - p_0)^2), \quad v = \left.\frac{\partial \varepsilon}{\partial p}\right|_{p=p_0}.$$

Apart from the additive constant $\varepsilon(p_0)$ and the shift $p \to p - p_0$, this is a relativistic dispersion relation, analogous to $\varepsilon = cp$, with the speed of light c replaced by v. For $v > 0$ ($v < 0$), the gapless mode that lives near $p = p_0$ travels to the right (left).

The corresponding continuum model describing the modes near $p = p_0$ is

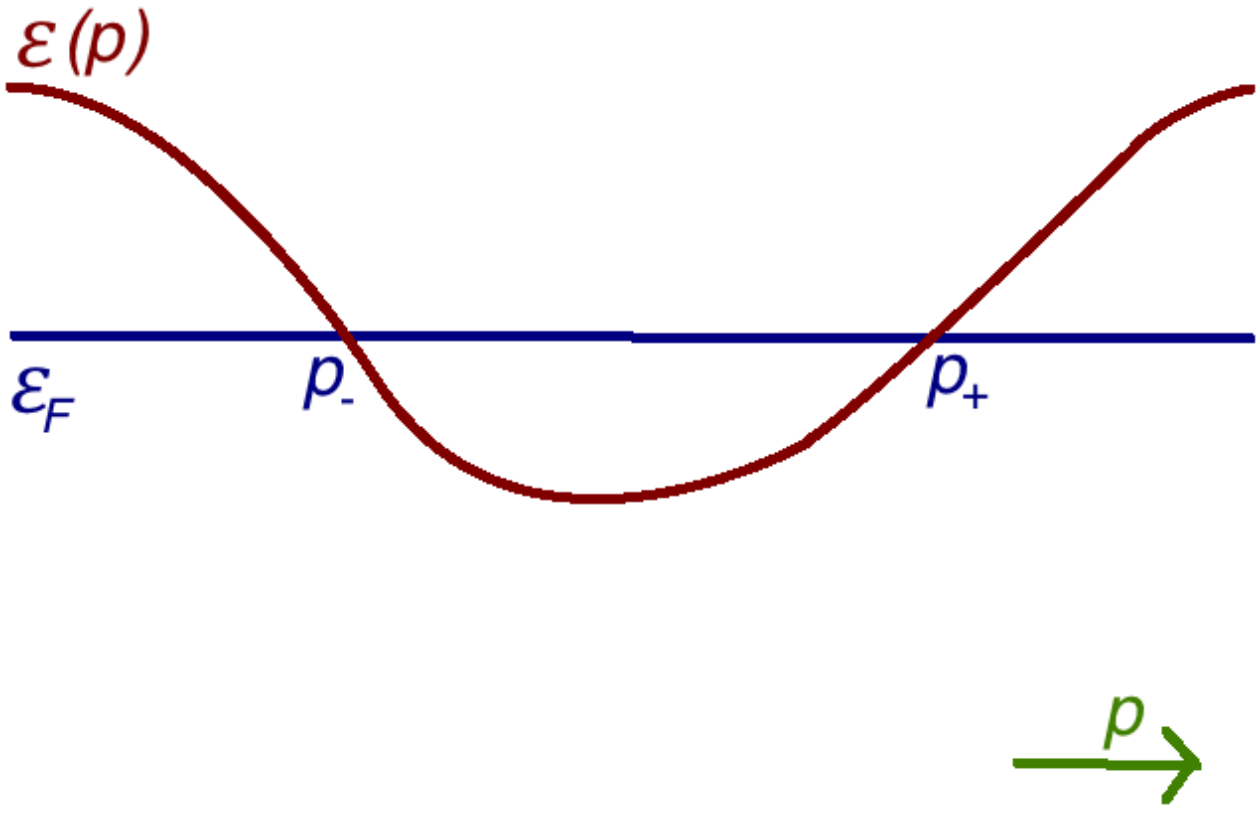
$$H = v \int_{-\infty}^{\infty} \mathrm{d}x \; \psi^* \left(-i \frac{\partial}{\partial x} \right) \psi.$$

This is a relativistic action for a 1d chiral fermion, except that v appears instead of c and $-i\partial/\partial x$ represents $p - p_0$ instead of p. Also we have omitted from H the "constant" $\varepsilon(p_0)$ per particle:

$$\varepsilon(p_0) \int_{-\infty}^{\infty} \mathrm{d}x \, \psi^* \psi.$$

This 1d example also gives an easy first example of how global conditions in topology constrain the possible low energy field theory that we can get – and how these constraints often mirror familiar facts about relativistic field theory and "anomalies." We have to remember that in the context of a crystal, the momentum p is a periodic variable.

Because $\varepsilon(p)$ is periodic, It follows that for every time $\varepsilon(p)$ crosses the fermi energy ε_F from below, there is another time that it crosses ε_F from above



So actually there are equally many gapless left-moving and right-moving fermion modes.

In relativistic terminology, the right-moving and left-moving modes are said to have positive and negative chirality. The motivation for this terminology is that the massless 2d Dirac equation is

$$\left(\gamma^0 \frac{\partial}{\partial t} + \gamma^1 \frac{\partial}{\partial x}\right) \psi = 0$$

where

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$$

are Dirac matrices. In Hamiltonian form, the Dirac equation is

$$i\frac{\partial \psi}{\partial t} = -i\bar{\gamma}\frac{\partial \psi}{\partial x},$$

where

$$\bar{\gamma} = \gamma^0\gamma^1$$

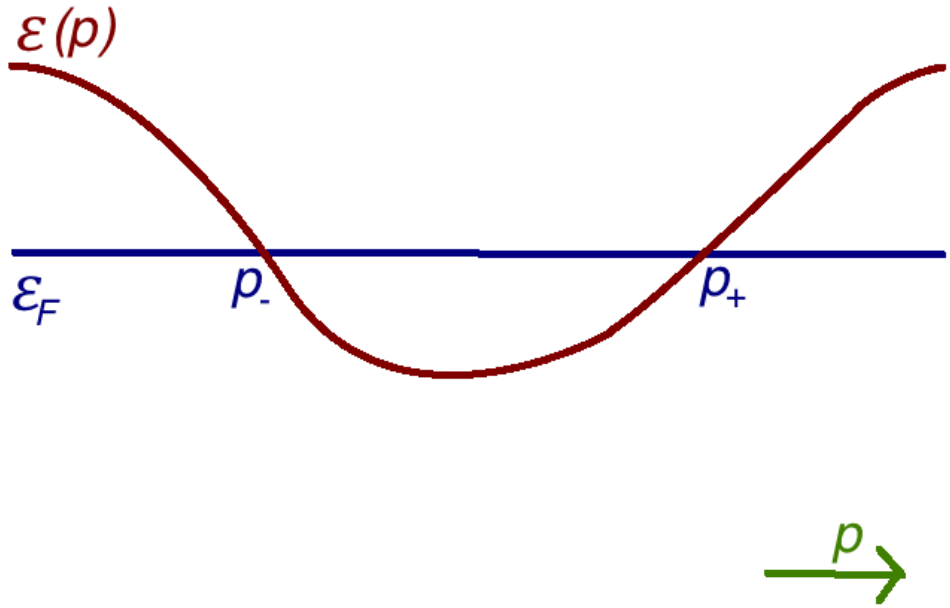
(whose analog in $3+1$ dimensions is usually called γ_5) is the "chirality operator." So a fermion state of positive or negative chirality is right-moving or left-moving.

Thus a more realistic Hamiltonian for the gapless charged modes will be something like

$$H = -v_- \int_{-\infty}^{\infty} \mathrm{d}x \; \psi_-^* \left(-i \frac{\partial}{\partial x} \right) \psi_- + v_+ \int_{-\infty}^{\infty} \mathrm{d}x \; \psi_+^* \left(-i \frac{\partial}{\partial x} \right) \psi_+ .$$

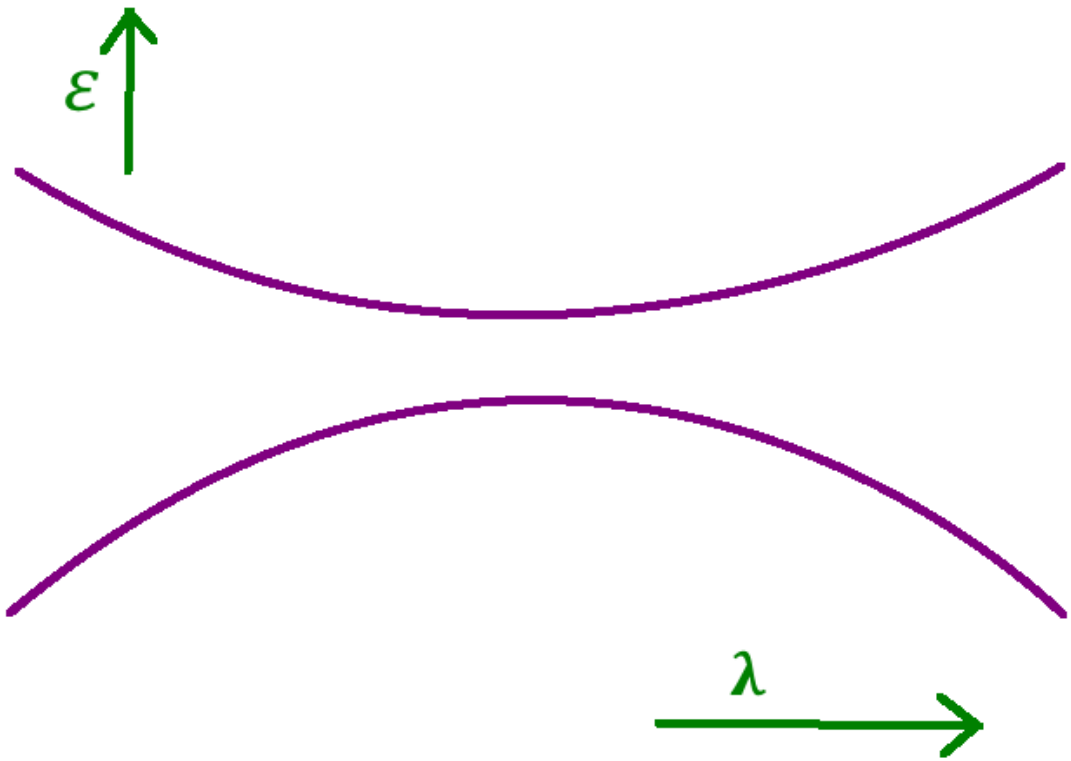
If one is familiar with quantum gauge theories and anomalies, one will recognize that this topological fact – which is a 1d analog of the 3d Nielson-Ninomiya theorem that we get to presently – has saved us from trouble. A purely 2d theory with, say, n_+ right-moving gapless electron modes and n_- left-moving ones is "anomalous," meaning that it is not gauge-invariant and does not conserve electric charge – unless $n_+ = n_-$.

We can actually see the potential anomaly if we re-examine this picture,



but now imagine turning on an electric field. When we turn on an electric field with a sign such that $\mathrm{d}p/\mathrm{d}t > 0$ for each electron, the electrons will all "flow" to the right in the picture. This creates electrons at $p = p_+$ and holes at $p = p_-$, so the charge carried by the $p = p_+$ mode or by the $p = p_-$ mode is not conserved, although the total charge is conserved, of course. Thus charge conservation depends on having both types of mode equally.

There is more one could say in 1 dimension, but instead we are going to go on to 3 dimensions. As a preliminary, recall that quantum mechanical energy levels repel, which means that if $H(\lambda)$ is a generic 1-parameter family of Hamiltonians, parametrized by λ, and with no particular symmetry, then generically its energy levels do not cross as a function of λ:



But how much do levels repel each other? Generically, how many parameters do we have to adjust to make 2 energy levels coincide?

The answer to this question is that we have to adjust 3 real parameters, because a generic 2×2 Hermitian matrix depends on 4 real parameters

$$H = \begin{pmatrix} a & b \\ \bar{b} & c \end{pmatrix},$$

but a 2×2 Hermitian matrix whose energy levels are equal depends on only 1 real parameter

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

To put this differently, any 2×2 Hermitian matrix is

$$H = a + \vec{b} \cdot \vec{\sigma}$$

where $\vec{\sigma}$ are the Pauli matrices. The condition for H to have equal eigenvalues is $\vec{b} = 0$, and this is three real conditions.

In three dimensions, a band Hamiltonian $H(p_1, p_2, p_3)$ depends on three real parameters, so it is natural for two bands to cross at some isolated value $p = p_*$. Near $p = p_*$, and looking only at the two bands in question, the Hamiltonian looks something like

$$H = a(p) + \vec{b}(p) \cdot \vec{\sigma},$$

where $\vec{b}(p) = 0$ at $p = p_*$. Expanding near $p = p_*$,

$$b_i(p) = \sum_j a_{ij}(p - p_*)_j + \mathcal{O}((p - p_*)^2), \quad a_{ij} = \left.\frac{\partial b_i}{\partial p_j}\right|_{p=p_*}.$$

Thus ignoring higher order terms, the band splitting is described near $p = p_*$ by

$$H' = \sum_{i,j} \sigma_i a_{ij}(p - p_*)_j.$$

Apart from a shift $p \to p - p_*$, this is essentially a chiral Dirac Hamiltonian in $3+1$ dimensions. Let us review this fact. The massless Dirac equation in $3+1$ dimensions is

$$\sum_{\mu=0}^{3} \gamma^\mu \partial_\mu \psi = 0, \quad \{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}.$$

In Hamiltonian form, this equation is

$$i\frac{\partial \psi}{\partial t} = -i \sum_k \gamma^0 \gamma^k \frac{\partial \psi}{\partial x^k}.$$

To represent the four gamma matrices, we need 4×4 matrices. However, the matrix

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$$

is Lorentz-invariant. It obeys $\gamma_5^2 = 1$, so its eigenvalues are ± 1. We can place on ψ a "chirality condition" $\gamma_5 \psi = \pm\psi$, reducing to a 2×2 Dirac Hamiltonian. (But then, because of the factor of i in the definition of γ_5, and in contrast to what happens in $1+1$ dimensions, the adjoint of ψ obeys the opposite chirality condition.)

Once we reduce to a 2×2 Dirac Hamiltonian with $\gamma_5 \psi = \pm \psi$, the matrices $\gamma^0 \gamma^i$ that appear in the Dirac Hamiltonian are 2×2 hermitian matrices and we can take them to be, up to sign, the Pauli sigma matrices

$$\sigma^i = \pm \gamma^0 \gamma^i .$$

The point is that, if $\gamma_5 \psi = \pm \psi$, then *in acting on* ψ,

$$\sigma^i \sigma^j = \delta^{ij} + i \epsilon^{ijk} \sigma^k .$$

(It is most simple to just prove this for $i = 1, j = 2$ from the explicit identity $\gamma^0 \gamma^1 \gamma^0 \gamma^2 = i \gamma^0 \gamma^3 \gamma_5$.)

So the Dirac Hamiltonian

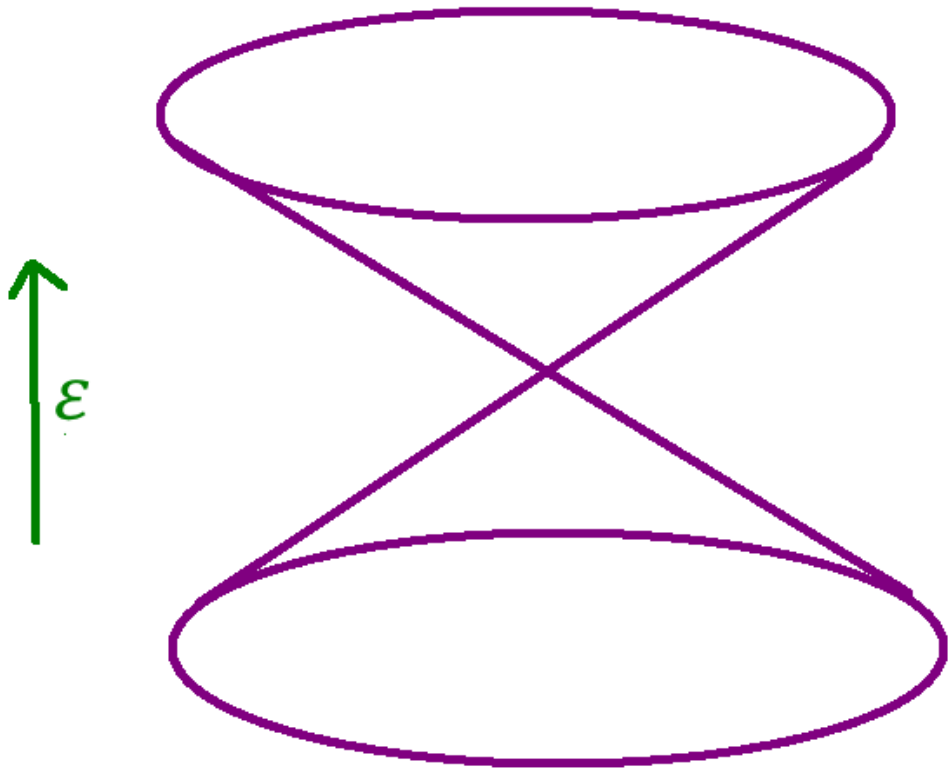
$$H = -i \sum_k \gamma^0 \gamma^k \frac{\partial}{\partial x^k}$$

becomes for a chiral fermion

$$H = \mp ic \sum_k \sigma^k \frac{\partial}{\partial x^k} = \pm c \vec{\sigma} \cdot \vec{p}.$$

(I have restored c, the speed of light.) As a matter of terminology, a charged Dirac fermion of definite chirality with a definite value of γ_5 is called a Weyl fermion. The physical meaning of the eigenvalue of γ_5 is that it determines the fermion "helicity" (spin around the direction of motion). Note that "fixed helicity" only makes sense for a *massless* fermion (which is never at rest) and indeed in the derivation we started with the massless Dirac equation. The corresponding *antiparticle* (hole instead of electron) has opposite helicity, somewhat as it has opposite charge.

This chiral Dirac Hamiltonian describes two bands with $\varepsilon(p) = \pm|p|$:



The chiral Dirac Hamiltonian basically coincides with the generic Hamiltonian that we found for a 2×2 band crossing

$$H = \sum_{k,j} \sigma_k a_{kj} p_j$$

with the replacement $cp_k \to \sum_j a_{kj} p_j$. This means, of course, that the fermion modes near $p = p_*$ do not propagate at velocity c but much more slowly, and also that they do not necessarily propagate isotropically in the standard Euclidean metric on $\mathbb{R}^3$, but in general the natural metric governing these modes is

$$||p||^2 = \sum_i \left(\sum_j a_{ij} p_j \right)^2 ,$$

i.e. the effective metric is

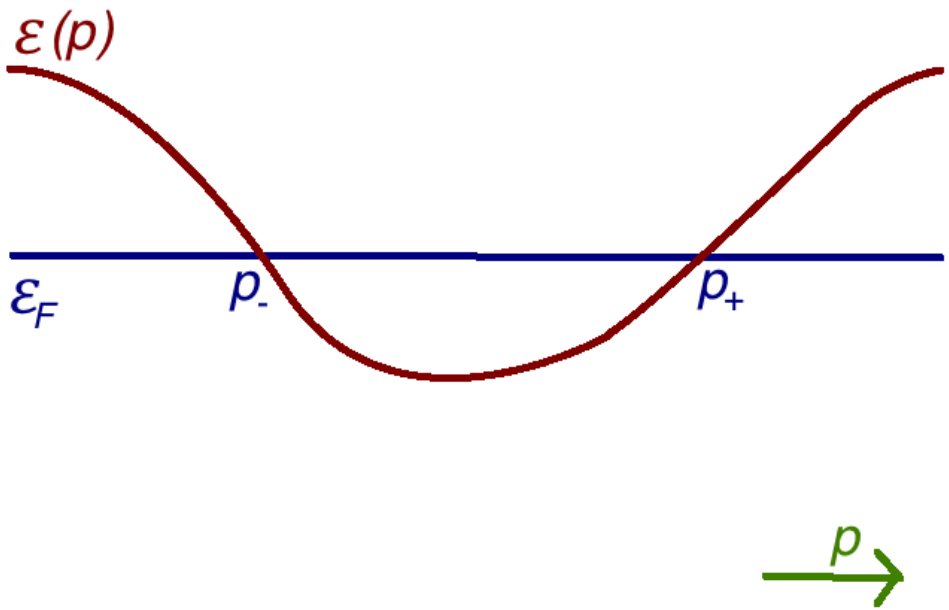
$$G^{ij} = \sum_k a^i{}_k a^j{}_k .$$

Finally, and very importantly, the *chirality* of the gapless electron mode is given by

$$\mathrm{sign}\,\det\left(a_{ij}\right) = \mathrm{sign}\,\det\left(\frac{\partial b_i}{\partial p_j}\right)\Bigg|_{p=p_*}.$$

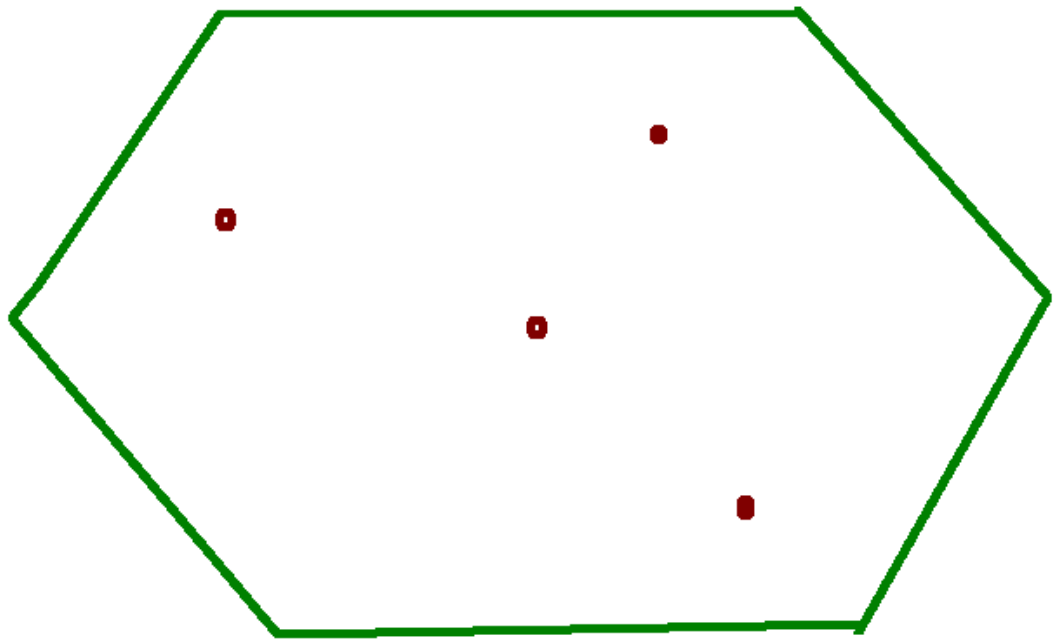
A gap crossing in which this determinant is positive (or negative) corresponds to a relativistic massless chiral fermion (or Weyl fermion) with $\gamma_5 = +1$ (or $\gamma_5 = -1$).

Now, however, we should remember something about relativistic quantum field theory in $3+1$ dimensions: A theory of a $U(1)$ gauge field (of electromagnetism) coupled to a massless chiral charged fermion of one chirality, with no counterpart of the opposite chirality, is anomalous (inconsistent). In $1+1$ dimensions, we avoided such a contradiction because of a simple topological fact that $\varepsilon(p)$ passes downward through the fermi energy as often as it passes upwards:



There is an analogous topological theorem that saves the day in $3+1$ dimensions. It is called the Nielsen-Ninomiya theorem (1981), which originally was motivated to explain some difficulties that had been found in constructing lattice gauge theories for fermions.

In formulating this theorem, we assume that the band Hamiltonian $H(p)$ is gapped except at finitely many isolated points in the Brillouin zone.



We will attach an integer to each of these bad points, and show that these integers add up to 0.

To get started, we assume there are only two bands. Also, by simply subtracting a c-number function of p from $H(p)$, we can make $H(p)$ traceless, without changing the band crossings. So

$$H(p) = \vec{b}(p) \cdot \vec{\sigma}$$

for some vector-valued function $\vec{b}(p)$. Now away from the bad points, $\vec{b}(p) \neq 0$ and so we can define a unit vector

$$\vec{n}(p) = \frac{\vec{b}}{|\vec{b}|}.$$

The mapping $p \to \vec{n}(p)$ is defined away from the bad points. We want to understand its topological properties.

Let us consider just one of the bad points, say at $p = p_*$, and let S be a small sphere around this bad point.

The map $p \to \vec{n}(p)$ is defined everywhere on S. This is a mapping from one two-sphere – namely S – to another two-sphere – parametrized by the unit vector $\vec{n}$. A continuous mapping from one sphere S^n to another sphere of the same dimension always has a "winding number" or "wrapping number," the net number of times the first sphere wraps around the second. This reflects the fact that

$$\pi_n(S^n) \cong \mathbb{Z}.$$

Before developing any general theory, let us see what the winding number is in the case of the relativistic Dirac Hamiltonian

$$H = \pm\vec{\sigma} \cdot \vec{p},$$

where the sign is the fermion chirality. For this Hamiltonian, $\vec{b} = \pm\vec{p}$, and hence $\vec{n} = \pm\vec{p}/|\vec{p}|$. The bad point is $\vec{p} = 0$, and we can take the sphere S that surrounds the bad point to be the unit sphere $|\vec{p}| = 1$. Thus the map from S to the $\vec{n}$-sphere is just

$$\vec{n} = \pm\vec{p}.$$

This is the identity map, of winding number 1, in the case of $+$ chirality, and it is minus the identity map, which winds around in reverse, with winding number -1, in the case of $-$ chirality.

The Nielsen-Ninomiya theorem is the statement that the sum of the winding numbers at the bad points is always 0. Generically (in the absence of lattice symmetries that would lead to a more special behavior) a bad point of winding number bigger than 1 in absolute value will split into several bad points of winding number ± 1. So generically, the bad points all have winding numbers ± 1, corresponding to gapless Weyl fermions of one chirality or the other. In this case, the vanishing of the sum of the winding numbers means that there are equally many gapless modes of positive or negative chirality, as a relativistic field theorist would expect for anomaly cancellation.

How does one prove that the sum of the winding numbers is 0? One rather down-to-earth explanation is as follows. The winding number for a map from S to the two-sphere $|\vec{n}| = 1$ can be expressed as an integral formula:

$$w(S) = \frac{1}{4\pi} \int \mathrm{d}^2 p \; \epsilon^{\mu\nu} \vec{n} \cdot \partial_\mu \vec{n} \times \partial_\nu \vec{n}.$$

An equivalent way to write the same formula is

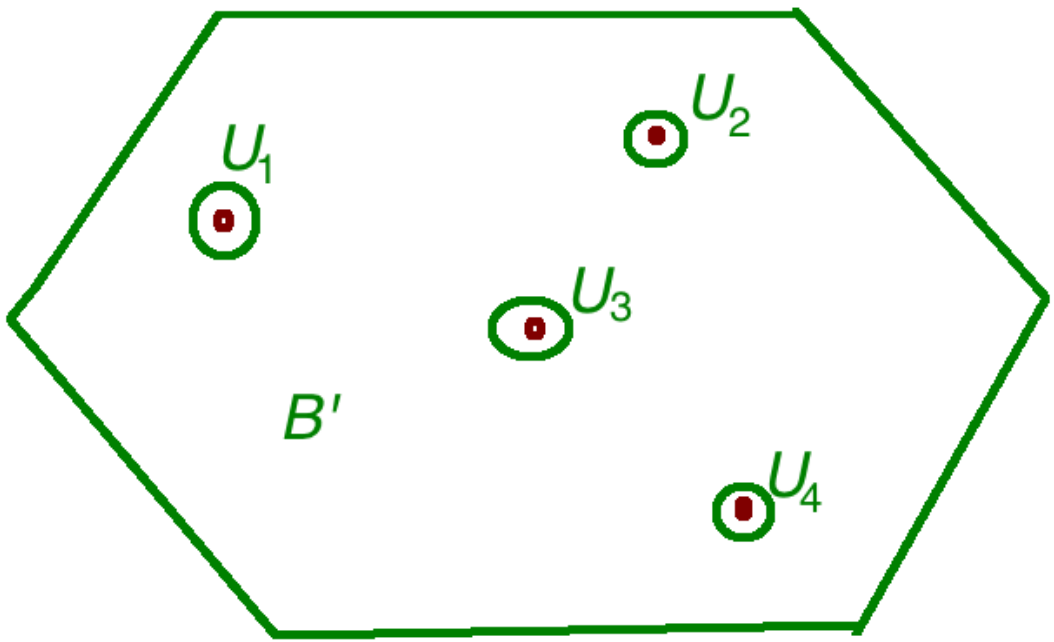
$$w(S) = \frac{1}{4\pi} \int_S \mathrm{d}^2 p \; \epsilon^{\mu\nu} \; \epsilon^{abc} n_a \frac{\partial n_b}{\partial p^\mu} \frac{\partial n_c}{\partial p^\nu}.$$

Now

$$0 = \partial_\lambda \left(\epsilon^{\lambda\mu\nu} \vec{n} \cdot \partial_\mu \vec{n} \times \partial_\nu \vec{n} \right),$$

since the right hand side is $\epsilon^{\lambda\mu\nu} \partial_\lambda \vec{n} \cdot \partial_\mu \vec{n} \times \partial_\nu \vec{n}$, which vanishes because it is the triple cross product of three vectors $\partial_\lambda \vec{n}$, $\partial_\mu \vec{n}$, and $\partial_\nu \vec{n}$ that are all normal to the sphere $|\vec{n}| = 1$.

For each bad point p_α, let U_α be a small open ball around p_α whose boundary is a sphere S_α. Let B be the full Brillouin zone, and let B' be what we get by removing from B all of the U_α. Thus the boundary of B' is $\partial B' = \cup_\alpha U_\alpha$.



Then from Stokes's theorem,

$$\begin{aligned} 0 &= \frac{1}{4\pi} \int_{B'} \mathrm{d}^3 p \; \partial_\lambda \left(\epsilon^{\lambda\mu\nu} (n \cdot \partial_\mu n \times \partial_\nu n) \right) \\ &= \sum_\alpha \frac{1}{4\pi} \int_{S_\alpha} \mathrm{d}^2 p \; \epsilon^{\mu\nu} \; \vec{n} \cdot \partial_\mu \vec{n} \times \partial_\nu \vec{n} \\ &= \sum_\alpha w(S_\alpha). \end{aligned}$$

Thus the sum of the winding numbers at bad points is 0, as promised.

If one is familiar with differential forms, one can express this argument more briefly as follows. Let us write $S_{\vec{n}}$ for the two-sphere $\vec{n} = 1$ and let η be its volume form. It is a closed form whose integral is 1:

$$0 = \mathrm{d}\eta, \qquad \int_{S_{\vec{n}}} \eta = 1.$$

Given a map $\varphi : S \to S_{\vec{n}}$, the corresponding winding number is

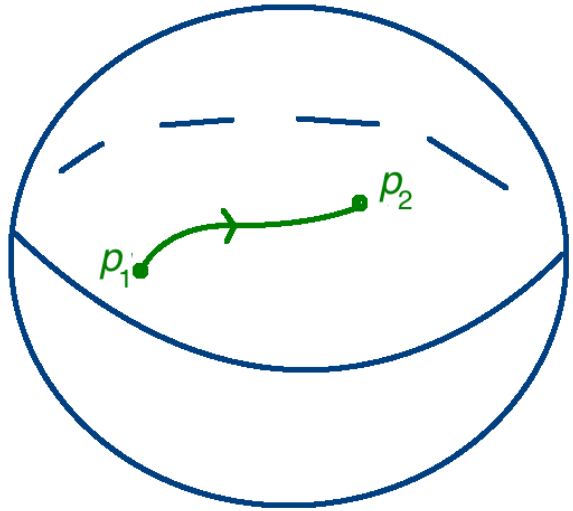
$$w(S) = \int_S \varphi^*(\eta).$$

So

$$0 = \int_{B'} \varphi^*(\mathrm{d}\eta) = \int_{B'} \mathrm{d}\varphi^*(\eta) = \sum_\alpha \int_{S_\alpha} \varphi^*(\eta) = \sum_\alpha w(S_\alpha).$$

There is another way to describe this, which involves the *Berry connection*, and more fundamentally the line bundle on which the Berry connection is a connection. For each value of p away from the bad points, the Hamiltonian $H(p)$ has one negative eigenvalue, so the space of filled fermion states of momentum p is a 1-dimensional complex vector space that I will call $\mathcal{L}_p$. A vector in $\mathcal{L}_p$ is a wave function ψ_p that obeys $H(p)\psi_p = -\psi_p$. We can ask for ψ_p to be normalized, $\langle \psi_p, \psi_p \rangle = 1$, but there is no natural way to fix the *phase* of ψ_p.

However, suppose that we vary p continuously by a path $p = p(s)$ from, say, p_1 to p_2:

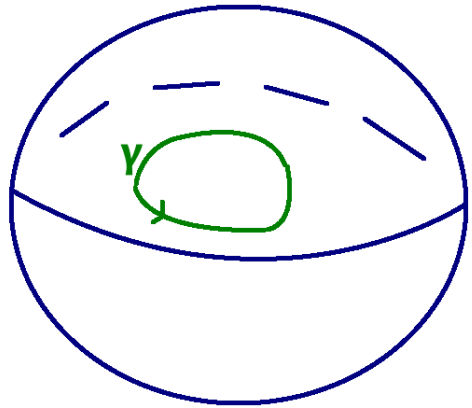


(You can think of this as a path that lies in a sphere $|p - p_*| = \epsilon$ around a bad point p_*.) If we make any arbitrary choice of the phase of ψ_p at $p = p_1$, then we can parallel transport the phase of ψ_p along the given path by requiring that at all p along the path

$$\langle \psi_p, \frac{\mathrm{d}}{\mathrm{d}s} \psi_p \rangle = 0.$$

(The real part of this equation ensures that $\langle \psi_p, \psi_p \rangle$ is constant along the path, and the imaginary part of the equation determines how the phase of ψ_p depends on the parameter s.)

Having a rule of parallel transport of the phase of ψ_p along any path amounts to defining a *connection* on B' (more exactly on the line bundle $\mathcal{L} \to B'$ whose sections we are parallel transporting). A *connection* on a complex line bundle $\mathcal{L}$ is the same as an abelian gauge field, which we will call $\mathcal{A}$. Parallel transport around a closed loop γ



using the Berry connection does not bring us back to the starting point. That is, the Berry connection is not flat; it has a curvature $\mathcal{F} = \mathrm{d}\mathcal{A}$. This curvature, divided by 2π represents (modulo torsion) the *first Chern class* of the line bundle $\mathcal{L} \to B'$:

$$c_1(\mathcal{L}) \longleftrightarrow \frac{\mathcal{F}}{2\pi}.$$

If p_α is one of the bad points at which two bands cross and S_α is a small sphere around p_α then the flux of $\mathcal{F}/2\pi$ over the sphere S_α is the winding number, as defined earlier:

$$w_\alpha(S) = \int_{S_\alpha} \frac{\mathcal{F}}{2\pi}.$$

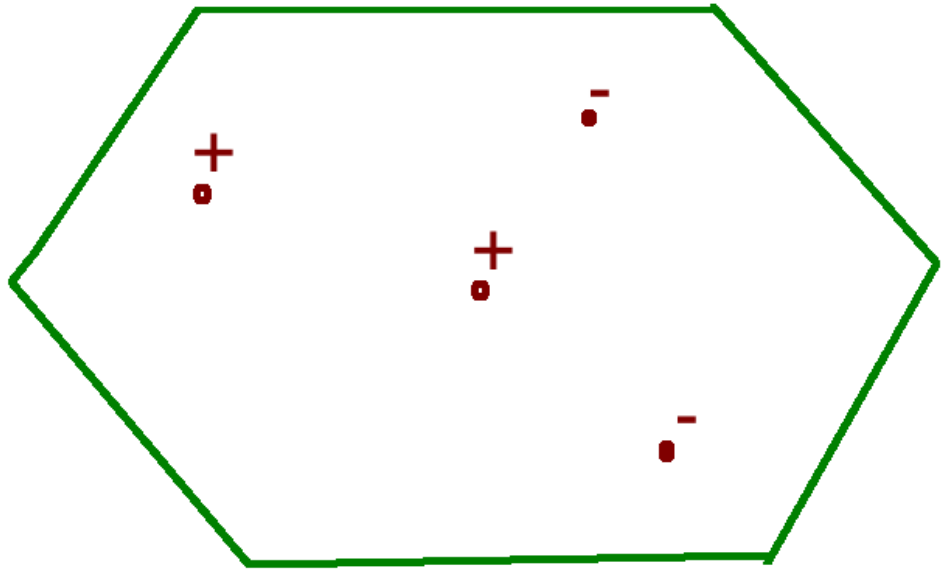
The Bianchi identity for any abelian gauge field $\mathcal{A}$ tells us that

$$\mathrm{d}\mathcal{F} = 0.$$

So once again we get the Nielsen-Ninomiya theorem

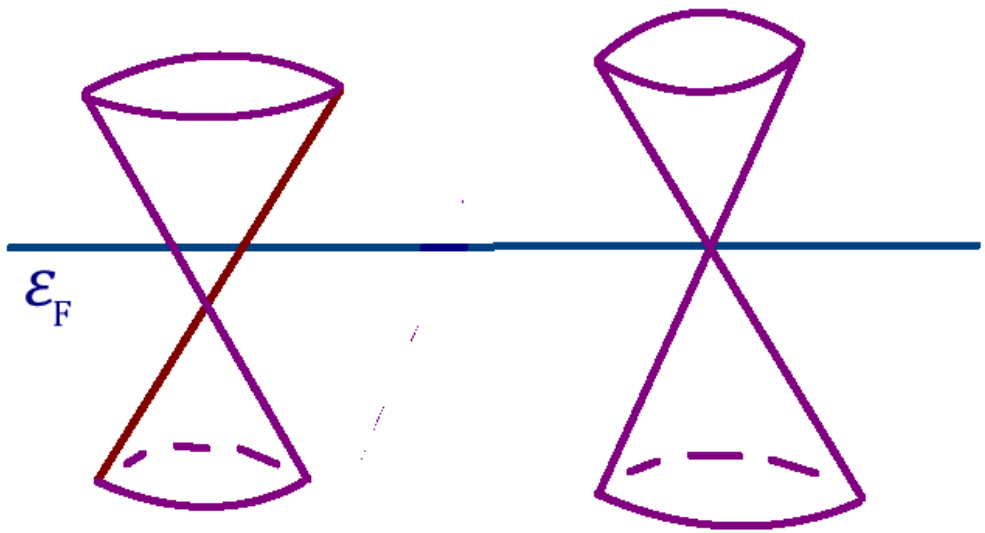
$$0 = \int_{B'} \frac{\mathrm{d}\mathcal{F}}{2\pi} = \sum_\alpha \int_{S_\alpha} \frac{\mathcal{F}}{2\pi} = \sum_\alpha w(S_\alpha).$$

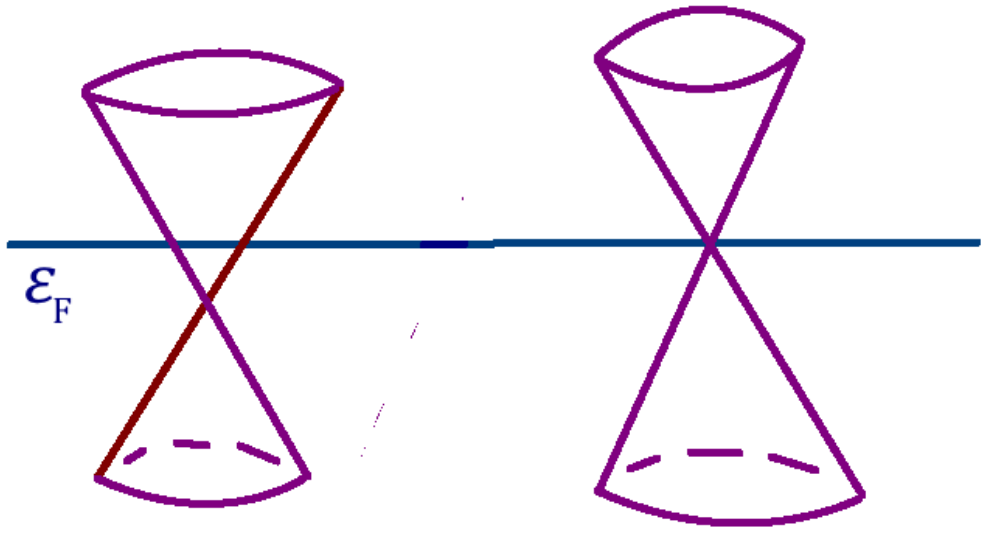
So a more precise picture of the bad points in the Brillouin zone for a generic two-band system looks like this:



A bad point labeled by $+$ or $-$ supports a gapless Weyl fermion of positive or negative chirality; the Nielsen-Ninomiya theorem says that there are equally many $+$ and $-$ points.

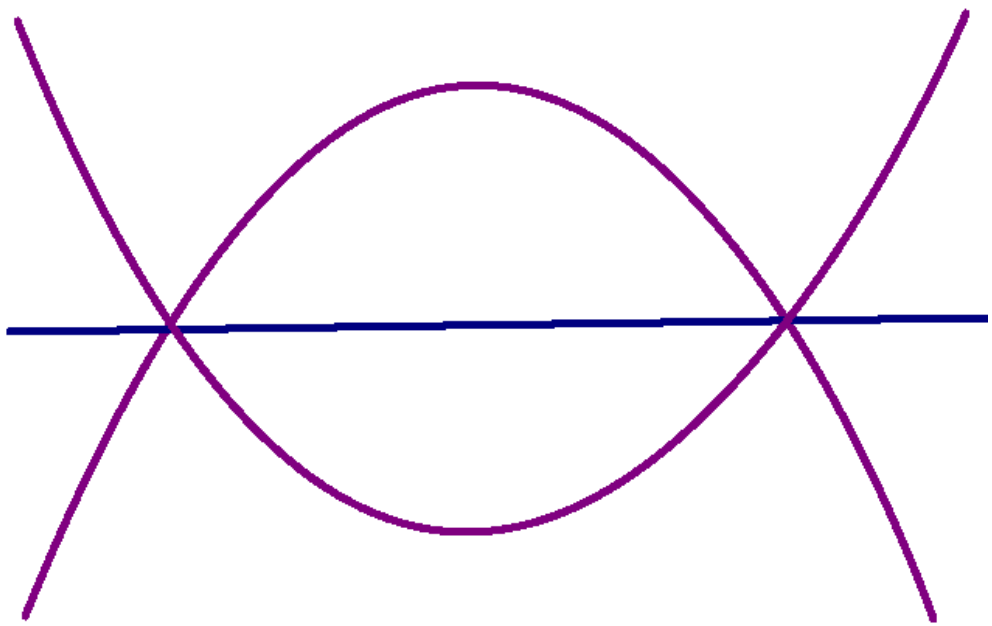
This is all very well, but if we want this to lead to striking effects in condensed matter physics, it won't do to have the band crossing at a random energy; we are really only interested in a band crossing that is at, or very near, the fermi energy ε_F. Thus we want the picture to look like the one on the right and not the one on the left:



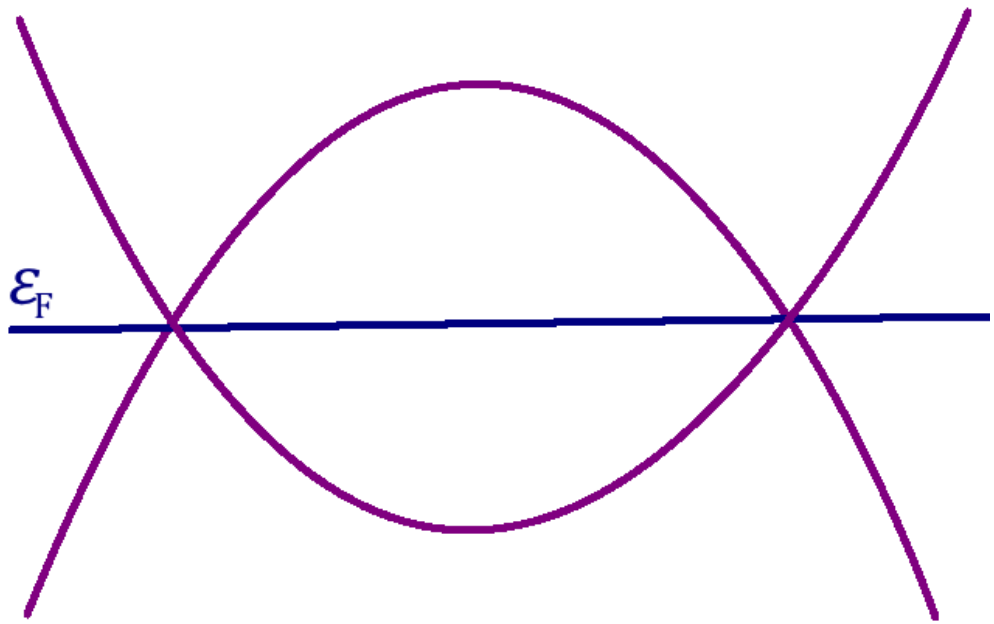


Ideally, we want *all* band crossings to be at or very near ε_F. If instead we have one of each type, we will get a "normal metal" (because of the band crossing that is below or above ε_F) and its effects will probably swamp the more subtle "semi-metal" effects due to the band crossing which is at ε_F. (Also I am not certain that band theory is a good enough theory so that the details of what happens far away from ε_F are meaningful.)

How can we arrange that *all* band crossings occur at ε_F? Well, first of all, how can we arrange so that they are all at the same energy? In the context of condensed matter physics, the way to do this is to find a material that has discrete spatial symmetries (or spatial symmetries combined with time-reversal symmetry) that permute all of the bad points. Some of these symmetries have to be orientation-reversing, since they have to exchange $+$ and $-$ points. The picture will then look more like this:

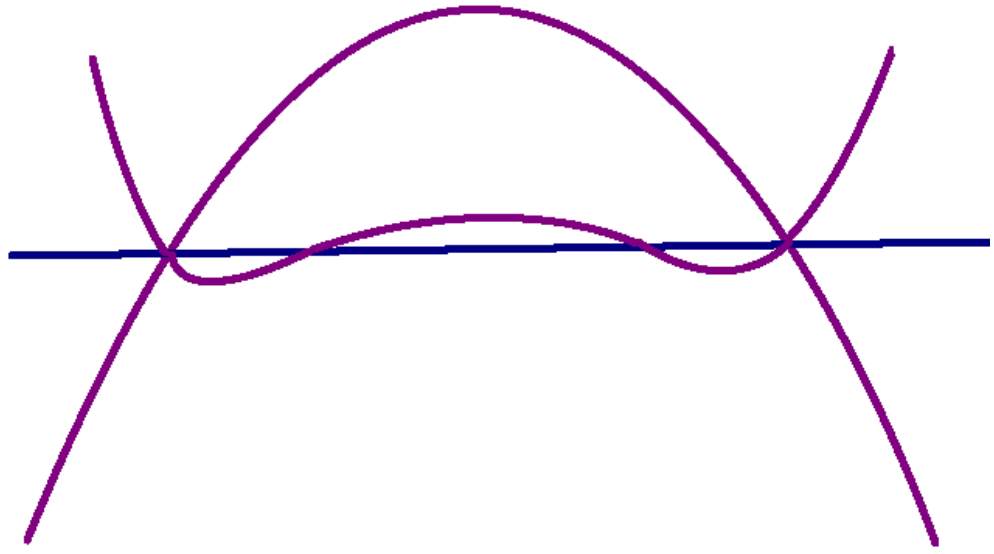


But how can we arrange so that the energy at which the band crossings occur is precisely ε_F? Here we run into one of the beautiful things in this subject. We can get that for free, because the number of electrons per unit cell is an integer. For example, if there is precisely one electron per unit cell that is supposed to be filling the two bands in our model, the fermi energy will be where we want it:



There are a lot of famous examples, the oldest being graphene (in two dimensions) and some contemporary ones that we are hearing about this week. To be more exact, it is natural to have the band crossings at ε_F in the sense that, given a band Hamiltonian like the one we have assumed, any nearby band Hamiltonian with the same symmetries leads to the same picture. But this result is not forced by the universality class; a large enough deformation preserving the discrete symmetries will give an ordinary metal.

To show this, here I have tried to draw a picture with the same left-right symmetry, but with a crucial wiggle in $\varepsilon(p)$:

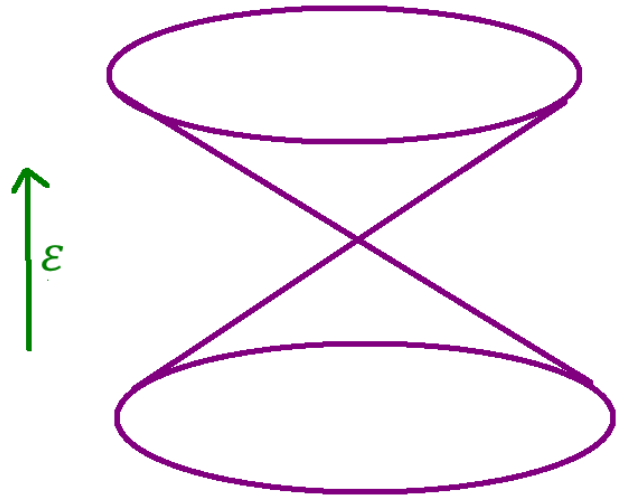


With this band structure, ε_F will be above the energy of the band crossings, leading to a fairly normal metal.

When I said, "the band crossings will be at the fermi level if 1 electron state per unit cell is occupying these bands," you may have wondered about the following question: Is spin being included in this counting? Actually, our discussion has been so general that it makes sense with or without spin. But there are two somewhat different cases.

In one case, spin-orbit couplings are important. It is not a good approximation to consider spin to be decoupled from orbital motion. The bands we have been drawing are the exact bands, taking spin and spin-dependent forces into account.

In the second case, spin-dependent forces are small and in the first approximation one ignores them and considers orbital motion only. In such a case, our two bands

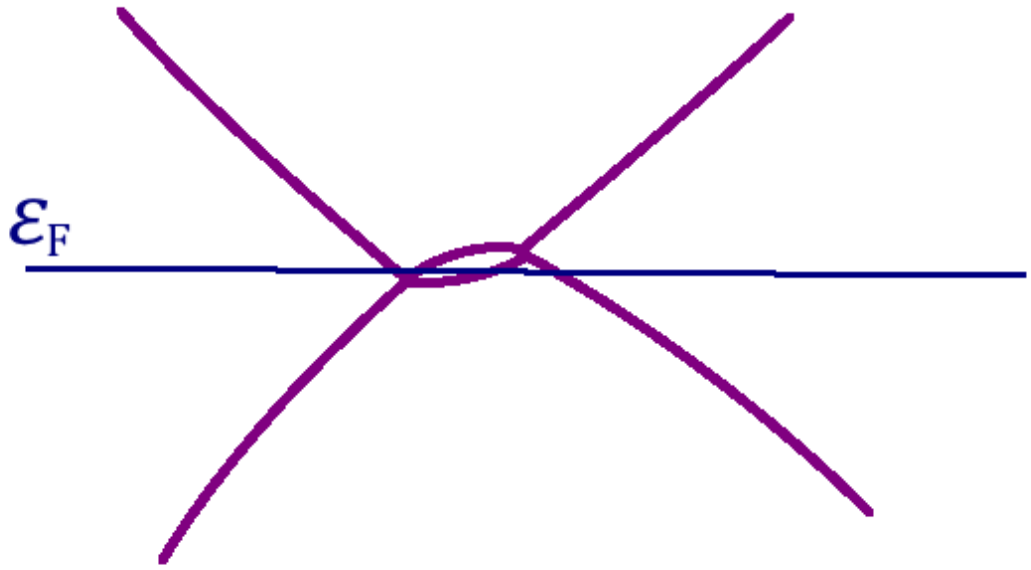


are orbital bands. When we include spin, in first approximation we simply double the picture, so that now there are four bands – two copies of what has been drawn. In this approximation, we get 2 chiral Weyl fermions, and they have the same chirality because (if the spin is decoupled from orbital motion) the spin up and spin down electrons have the same band Hamiltonian and so the same chirality.

However, there always are spin-orbit forces in nature and generically the two pairs of bands will be split. The exact problem is a four-band problem. Assuming the density of electrons is such that 2 of the 4 bands are supposed to be filled, the crossings we care about (as they may be at or very near the Fermi energy) are those between the second and third bands, in order of increasing energy.

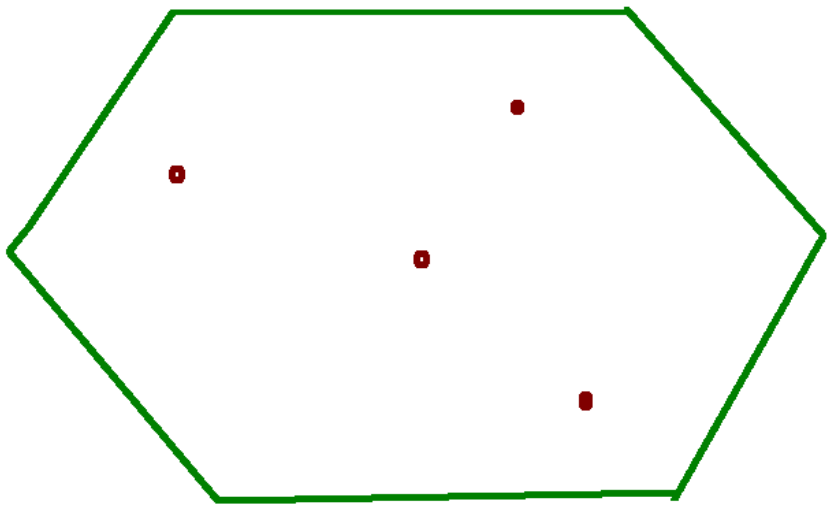
We have not yet analyzed problems with more than 2 bands, so the following statement involves jumping ahead slightly. A more general form of the Nielsen-Ninomiya theorem that we come to in a moment ensures that there will still be two Weyl crossings between the second and third bands (with the same chirality as before) but generically (for weak spin-orbit couplings) at slightly different energies and momenta. The fermi energy cannot equal the energy of each of these crossings, and generically it does not equal either of them, but it will be close.

A very crude picture of two Weyl crossings neither of which is quite at the fermi energy is here:

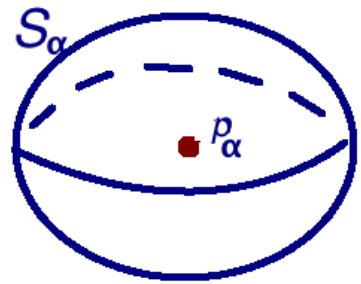


Naively this leads to a normal metal with a very small density of charge carriers, but I believe that condensed matter physicists know that in such a case the fermi liquid is subject to various instabilities.

Now let us discuss the generalization of the Nielsen-Ninomiya theorem for an N band system. We assume that the density of electrons is such that k bands should be filled, for some integer $k < N$. We let $\mathcal{H}_p$ be the full N-dimensional space of states at momentum p. At any value of p such that the k^{th} band (in order of increasing energy) does not meet the $k + 1^{th}$, $\mathcal{H}_p$ has a well-defined subspace $\mathcal{H}'_p$ spanned by the k lowest states. The definition of $\mathcal{H}'_p$ does not make sense at points at which the k^{th} band meets the $k + 1^{th}$. Just as before, to make this happen we have to adjust three parameters, so there will be finitely many bad points in the Brillouin zone at which $\mathcal{H}'_p$ is not defined:



Wherever $\mathcal{H}'_p$ is well-defined, it defines a k-dimensional subspace of $\mathcal{H}_p \cong \mathbb{C}^N$. The space of all k-dimensional subspaces of $\mathbb{C}^N$ is called the Grassmannian $\mathrm{Gr}(k, N)$. If p_α is an isolated point on which $\mathcal{H}'_p$ is not defined, then $\mathcal{H}'_p$ is defined on a small sphere S_α around p_α



Because

$$\pi_2(\mathrm{Gr}(k, N)) \cong \mathbb{Z},$$

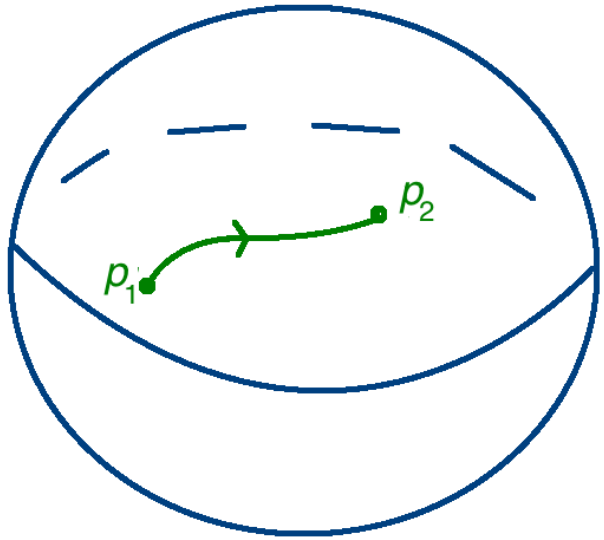
we can attach an integer-valued winding number $w(S_\alpha)$ to each p_α.

Any of the explanations that we gave before for the case of two bands can be adapted to prove the Nielsen-Ninomiya theorem

$$\sum_{\alpha} w_\alpha = 0.$$

For example, let us consider the explanation based on the Berry connection. Letting B' be as before the "good part" of the Brillouin zone with small neighborhoods of bad points removed, we have a rank k complex vector bundle $\mathcal{H}' \to B'$ whose fiber at $p \in B'$ is $\mathcal{H}'_p$. This is just the bundle spanned by the k lowest bands. On this bundle, there is a Berry connection, which is now a $U(k)$ gauge field.

It is defined as follows. To parallel transport $\psi(p) \in \mathcal{H}'_p$ along a path $\gamma \subset B'$,



we require that

$$\langle \psi' | \frac{\mathrm{d}}{\mathrm{d}s} | \psi \rangle = 0, \quad \text{for all} \;\; \psi' \in \mathcal{H}'_p.$$

In other words, $\mathrm{d}\psi/\mathrm{d}s$ is required to be orthogonal to $\mathcal{H}'_p$, for all s. This gives a connection or $U(k)$ gauge field $\mathcal{A}$ on $\mathcal{H}' \to B'$. It has a curvature $\mathcal{F} = \mathrm{d}\mathcal{A} + \mathcal{A} \wedge \mathcal{A}$. The winding number $w(S_\alpha)$ is

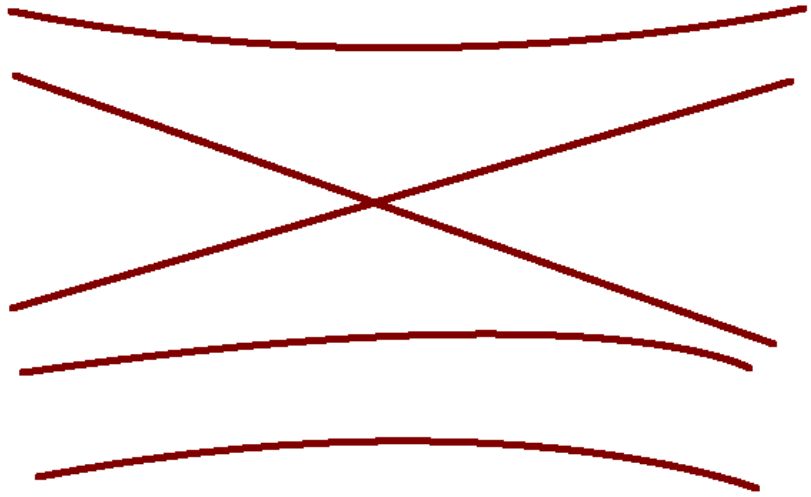
$$w(S_\alpha) = \int_{S_\alpha} c_1(\mathcal{H}') = \int_{S_\alpha} \frac{\mathrm{Tr}\mathcal{F}}{2\pi}.$$

Using the Bianchi identity $\mathrm{d}\mathrm{Tr}\,\mathcal{F} = 0$, we get, with the help of Stokes's theorem

$$0 = \int_{B'} \mathrm{d}\frac{\mathrm{Tr}\,\mathcal{F}}{2\pi} = \sum_{\alpha} \int_{S_\alpha} \frac{\mathrm{Tr}\,\mathcal{F}}{2\pi} = \sum_{\alpha} w(S_\alpha).$$

As you can see, the proof using the Berry connection is the same as it was for two bands, except that we have to put a trace everywhere.

Generically, the winding number at a bad point is ± 1, just as in the two band case. The generic behavior at a crossing of winding number ± 1 is the familiar Weyl crossing between the k^{th} and $k+1^{th}$ bands.



So the points with winding number ± 1 give chiral Weyl fermions, and the Nielsen-Ninomiya theorem says that there are equally many of these of positive or negative chirality.

None of this relied on discrete symmetries, though much of it becomes richer if one does consider materials with discrete symmetries. But what if we want to get massless Dirac fermions in 2 space dimensions rather than 3? This will not work without discrete symmetries because generically there would be no band crossings as we vary the 2 parameters of a 2-dimensional Brillouin zone.

In $2+1$ dimensions, there are only three γ matrices $\gamma^0, \gamma^1, \gamma^2$, and they can be given a 2-dimensional representation. So a Dirac fermion in $2+1$ dimensions has only 2 components and the massless Dirac Hamiltonian is

$$H = \sigma_1 p_1 + \sigma_2 p_2.$$

(To derive this from the relativistic Dirac equation $\gamma^\mu \partial_\mu \psi = 0$ is similar to what we did in 3 space dimensions.) The energy levels are $\pm|p|$, and there is a level crossing at $p = 0$. We know that such a level crossing is nongeneric in 2 space dimensions, and concretely it is possible to perturb the Dirac Hamiltonian by adding a mass term:

$$H = \sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 m.$$

The massive Dirac Hamiltonian has nondegenerate energy levels $\pm\sqrt{p^2 + m^2}$.

However, the mass term violates some symmetries. The *reflection* symmetry of

$$H = \sigma_1 p_1 + \sigma_2 p_2$$

is

$$\psi(x_1, x_2) \to \sigma_2 \psi(-x_1, x_2)$$

and the mass term

$$H' = m\sigma_3$$

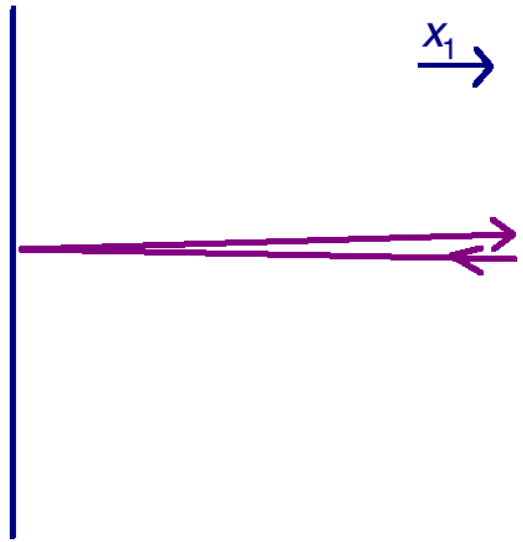
is odd under this. The mass term is similarly odd under time-reversal.

The physical reason that a mass term violates reflection symmetry R and time-reversal symmetry T is as follows. If ψ is a two-component electron field in two dimensions, then one component of ψ is a creation operator and one is an annihilation operator. Hence ψ describes for each value of $\vec{p}$ only a single state of charge 1 (along with a corresponding hole or antiparticle of charge -1). If the ψ particle is massive, we can study it in its rest frame and its one spin state will transform with spin $1/2$ or $-1/2$ under the rotation group. (In 2 space dimensions, the rotation group is just the abelian group $SO(2)$ and has 1-dimensional representations.) Either choice of sign is odd under R or T, so the mass term must violate R and T.

By contrast, if $m = 0$, the fermion cannot be brought to rest and in 2 space dimensions, we cannot define its spin. So the $m = 0$ theory can be R and T conserving.

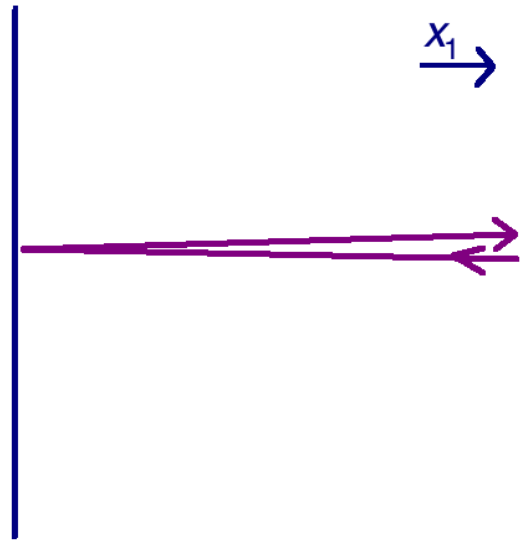
This tells us that in a 2d crystal, it should be possible to find gapless Dirac-like modes as long as the crystal has a suitable R or T symmetry, and the gapless modes occur at an R- or T-invariant value of the momentum. It is not hard to give examples but we don't quite have time right now unfortunately. I will just remark that rather as we discussed for Weyl points in 3 space dimensions, there are two versions, either a material that with spin included has an R or T symmetry that leads to a gapless mode, or a material with small spin-orbit forces that has the appropriate property if spin and spin-orbit forces are ignored – in which case, in the real world, one will get modes with a very small gap but not quite zero. The most famous example of the second type is graphene (often discussed with spin ignored; the spin-dependent effects were analyzed by Kane and Mele as we heard yesterday).

Instead I want to begin our discussion of edge modes. We will do this in 3 space dimensions and we will start by considering a non-chiral massless Dirac fermion ψ. (For now, never mind how to realize this in condensed matter physics.) We suppose that ψ is confined to a half-space (possibly the interior of a crystal) and we ask what kind of boundary condition it should obey when it is reflected from a boundary. For reflection at right angles, as I've tried to sketch here



a simple boundary condition would conserve angular momentum.

By "conserving angular momentum" I mean that if the normal direction to the boundary is the x_1 direction, then the corresponding component J_1 of angular momentum should be conserved.



Since the direction of motion is reversed in the scattering, the helicity has to be reversed. For a Dirac fermion, that is OK, because it has both helicities.

For a Dirac fermion with or without a bare mass obeying the Dirac equation

$$\left(i \sum_{\mu=0}^{3} \gamma^{\mu} \partial_{\mu} - m \right) \psi = 0$$

the angular-momentum conserving and helicity-reversing boundary condition (for a boundary at $x_1 = 0$) is

$$i\gamma_1 \psi|_{x_1=0} = \pm \, \psi|_{x_1=0} \, .$$

Either choice of sign will do. This boundary condition obviously is invariant under rotation around the x_1-axis; the assertion that it is "helicity-reversing" is valid if $m = 0$ or the energy is much greater than m.

But what sort of boundary condition can we have for a massless Weyl fermion, with only one helicity? Obviously, the boundary condition cannot reverse the helicity, and therefore it cannot conserve angular momentum. Any boundary condition will have to pick a preferred direction in the boundary plane. For a chiral Dirac Hamiltonian

$$H = -i\vec{\sigma} \cdot \frac{\partial}{\partial \vec{x}}$$

a good boundary condition at $x_1 = 0$ is

$$M\psi|_{x_1=0} = \psi|_{x_1=0}$$

with

$$M = \sigma_2 \cos\alpha + \sigma_3 \sin\alpha$$

for some angle α.

What makes this a good boundary condition is that it makes $H = -i\vec{\sigma} \cdot \vec{\nabla}$ hermitian. To prove that $H = -i\vec{\sigma} \cdot \vec{\nabla}$ is hermitian,

$$\langle \psi_1, H\psi_2 \rangle = \langle H\psi_1, \psi_2 \rangle$$

one has to integrate by parts. A potential boundary term in this integration by parts vanishes because

$$\{M, \sigma_1\} = 0$$

and our choice $M = \sigma_2 \cos\alpha + \sigma_3 \sin\alpha$ was made to ensure this. In particular, it won't work if we pick $M = \sigma_1$, and that again shows that the boundary condition cannot be invariant under rotation of the $x_2 - x_3$ plane.

The choice of angle α doesn't really matter, since it can be absorbed in a rotation of the $x_2 - x_3$ plane. So let us just take $\alpha = 0$, meaning that the boundary condition is $\sigma_2\psi| = \psi|$.

Now something very interesting happens. Let us try to solve the equation $H\psi = 0$ assuming that $\sigma_2\psi = \psi$ everywhere (not only on the boundary) and also assuming that $\partial\psi/\partial x_2 = 0$. Then

$$H\psi = (\sigma_1\partial_1 + \sigma_2\partial_2 + \sigma_3\partial_3)\,\psi = \sigma_1(\partial_1 - i\partial_3)\psi.$$

(I used $\sigma_3 = -i\sigma_1\sigma_2$ so $\sigma_3\psi = -i\sigma_1\psi$.) So we can solve $H\psi = 0$ with

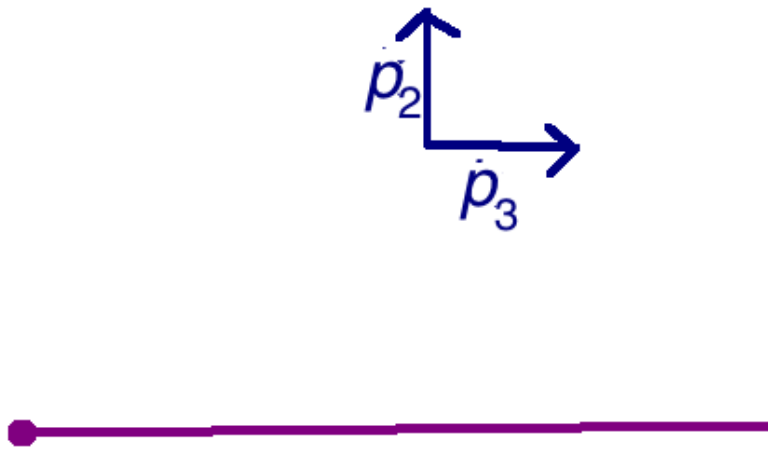
$$\psi = \exp(ikx_3 - kx_1)\psi_0,$$

and this is plane-wave normalizable if

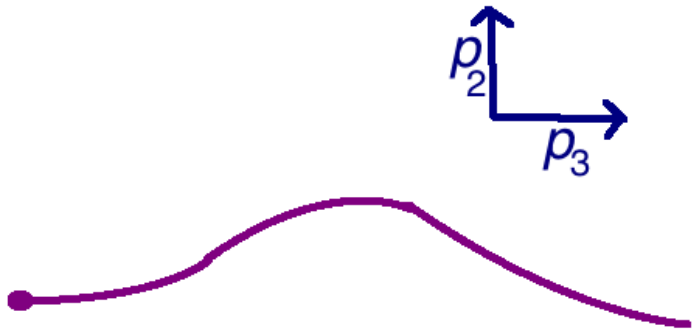
$$k > 0.$$

(ψ_0 is a constant obeying $\sigma_2\psi_0 = \psi_0$.) What is special about these solutions is that they decay exponentially away from the boundary.

So we have found a half-line of states localized near the boundary, and parametrized by $p_3 = k > 0$. In the presence of a boundary at $x_1 = 0$, p_1 is of course not conserved, so the components of the momentum that are conserved are p_2 and p_3. In the $p_2 - p_3$ plane the spectrum of localized states is a ray from the origin in the $+p_3$ direction:



In a condensed matter application, the fact that these boundary-localized states have exactly zero energy is not universal. We could modify the Hamiltonian by all kinds of higher order terms, leading to something more like this:

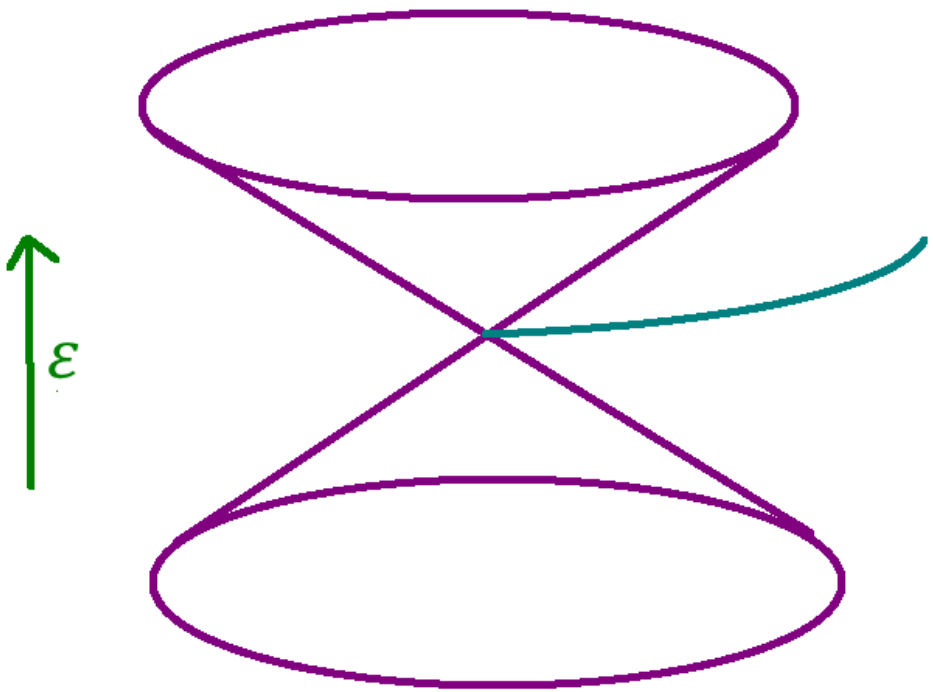


What is universal is that there is a curve – a "Fermi arc" – of boundary-localized states that begins at "zero momentum," i.e. at the projection to the $p_2 - p_3$ plane of the value of $\vec{p}$ at which there was a band crossing in bulk. Indeed, the calculation that we did was universal near the band crossing point.

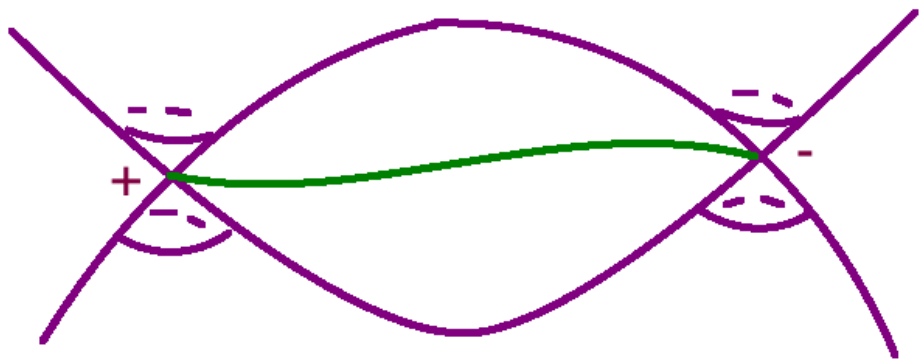
The way that the Fermi arc ends is that the boundary-localized state

$$\psi = \exp(ikx_3 - kx_1)\psi_0$$

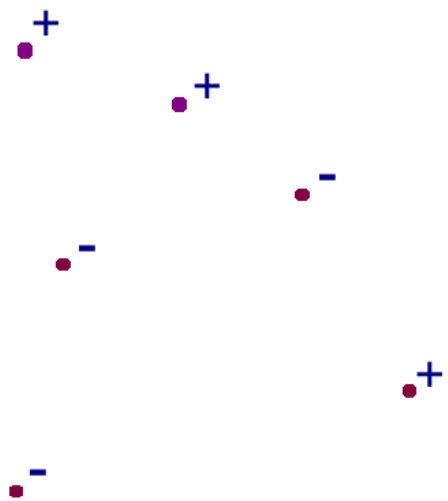
stops being localized near the boundary as $k \to 0$. At $k = 0$, the boundary localized state coincides with the $\vec{p} = 0$ limit of a bulk state. A somewhat helpful but also somewhat misleading picture of the spectrum is this:



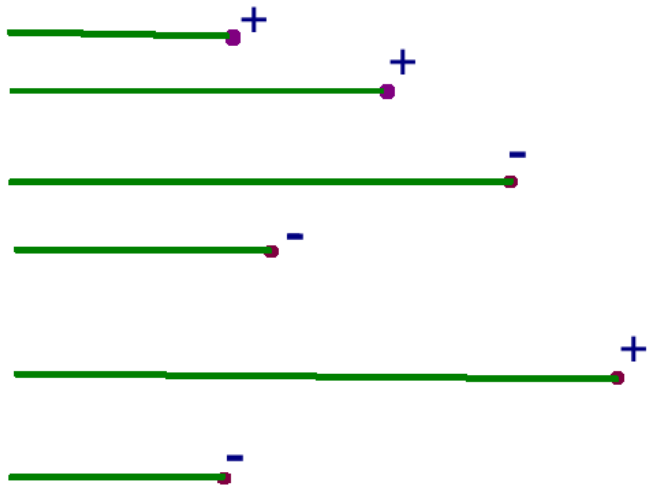
But what happens at the other end of the Fermi arc? It seems that the only way for such an arc of boundary-localized states to end is by ceasing to be normalizable, which happens precisely when they meet continuum states. So the second end of the Fermi arc is another Weyl cone, this one of opposite chirality:



In condensed matter, we know from the Nielsen-Ninomiya theorem that there always are multiple Weyl points in the Brillouin zone, say at momenta $\vec{p}_\alpha$, $\alpha = 1, \ldots, s$:

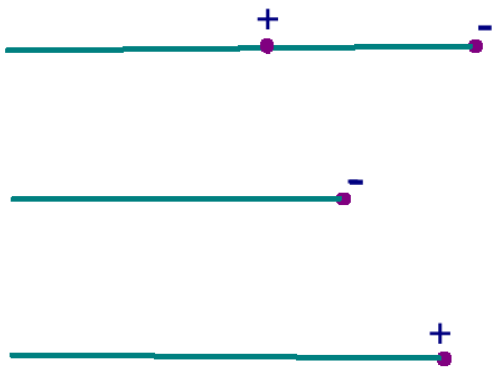


In bulk, because momentum is conserved, gapless modes at different values of $\vec{p}$ do not "mix" with each other and can be treated separately. But when we consider the behavior near a boundary, the "perpendicular" component $p^{\perp}$ of the momentum is not conserved and we should only use $p^{\parallel}$. So we project the bad points to 2 dimensions:



As long as the projections $p_{\alpha}^{\parallel}$ of the Weyl points are all distinct, they will be connected pairwise by Fermi arcs, as I have described.

But if two Weyl points of opposite chirality project to the same point in the boundary momentum space,



then there is no need for either one to connect to a Fermi arc. From a low energy point of view, the two modes of opposite chirality combine to a Dirac fermion with both chiralities, and it can satisfy the Dirac boundary condition (namely $i\gamma_1\psi| = \pm\psi|$) that we mentioned at the beginning. This does not lead to a Fermi arc. Of course, whether two given Weyl points have the same projection on the boundary depends on which boundary face we consider. But the discrete symmetries that make Weyl points interesting can also make it natural, for some crystal facets, that two Weyl points have the same projection.

It is also possible to get boundary-localized modes from Dirac fermions, and since this is important in understanding topological insulators, it is the last topic I will describe today. In the absence of discrete symmetries, and without tuning any parameters, it is not natural in condensed matter physics to get a massless Dirac (as opposed to Weyl) fermion. That is simply because for a four-component fermion field ψ with both chiralities, mass terms are possible, in fact there are two such terms:

$$\left(i \sum_{\mu} \gamma^{\mu} \partial_{\mu} - m - m' \gamma_5 \right) \psi = 0.$$

To get a massless Dirac fermion, we need a reason for $m = m' = 0$. It turns out that it is actually possible to achieve this in the context of a crystal with suitable discrete symmetries, but unfortunately there is not time to explain this today.

The only symmetry that we will assume is time-reversal symmetry, and this is enough to set one of the two parameters to 0 but not both. The Dirac equation becomes

$$\left(i \sum_{\mu} \gamma^{\mu} \partial_{\mu} - m \right) \psi = 0.$$

Generically m is not 0 but of course if we adjust one parameter (for example the chemical composition of an alloy) we can hope to pass through a point with $m = 0$. It turns out that this is the phase transition between an ordinary insulator and a topological one. For now, we consider a sample with boundary and look for a mode localized near the boundary.

We take the boundary at $x_1 = 0$ and the natural Dirac boundary condition $i\gamma_1\psi| = \psi|$. (The sign does not really matter and there is no reason for the boundary condition to jump when m passes through 0.) Let $x_\parallel$ be the coordinates along the boundary and

$$i\gamma \cdot \partial^\parallel = i\sum_{\mu\neq 1} \gamma^\mu \partial_\mu$$

the $2+1$-dimensional Dirac operator along the boundary. We can obey the $3+1$-dimensional Dirac equation with

$$\psi = \exp(mx_1)\psi_\parallel(x_\parallel)$$

where

$$i\gamma_1\psi_\parallel = \psi_\parallel, \quad \gamma \cdot \partial^\parallel \psi_\parallel(x_\parallel) = 0.$$

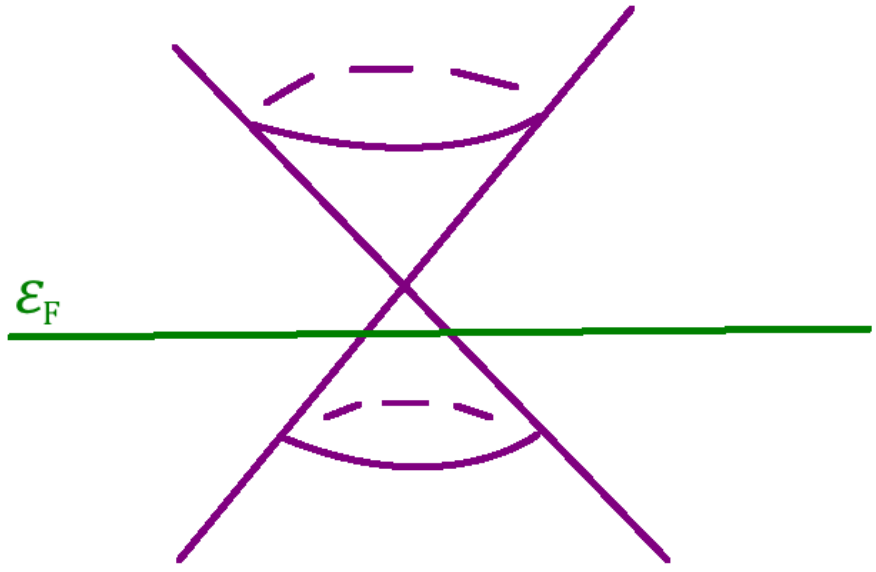
For $m > 0$, this solution is highly unnormalizable. But for $m < 0$, it is plane-wave normalizable and localized along the boundary. We have found one of the main characteristics of the topological insulator phase: the boundary supports a gapless fermion mode.

To be more precise, since $\psi_{\|}$ was constrained to obey the massless $2+1$ dimensional Dirac equation

$$\gamma \cdot \partial^{\|} \psi_{\|}(x_{\|}) = 0,$$

we get a $2+1$ dimensional massless Dirac fermion. (Because of the additional constraint $i\gamma_1 \psi_{\|} = \psi_{\|}$ which removes half the modes, the original 4-component fermion in 3+1 dimensions gives a single 2-component massless Dirac fermion in $2+1$ dimensions.)

Generically in the context of condensed matter physics the fermi energy ε_F does not pass through the Dirac point in the boundary theory



so the boundary of a topological insulator is more like an ordinary metal than the Weyl semimetals that we talked about before.

To summarize the last point, we have learned that in a generic 1-parameter family of T-conserving band theories, there can be a phase transition between a phase with no localized boundary modes and a phase with a massless 2d fermion on the boundary. At the phase transition point, there is a massless 3d Dirac fermion.

For tomorrow, we will start with quantum Hall systems in 2 dimensions – and then eventually make contact with Weyl semi-metals in 3 dimensions.