Welcome to the Solid State

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Electrical forms of matter:

1700s	conductors & insulators
1900s	superconductors (& semimetals & semiconductors)
Since 2005	topological insulators . . . & topological superconductors & semimetals . . . more?

Tentative Definition

A *topological insulator* is a material that is insulating in the bulk but conducts on its surface.

More accurately, there are two key defining features:

- the physics of the material is time-reversal invariant, and
- these surface states are "topologically protected" (i.e., small modifications of the system do not destroy the surface conduction.

Mathematically attractive aspects:

- The surface is a *defect* between regions governed by different physics
- The Bloch electrons propagating on the surface satisfy a *massless Dirac equation*!

This subject supports two different approaches, just like condensed matter theory does generally. We will learn about both approaches as developed in physics and math.

Physics	Our Topic	Math	Text
single-body	band theory	twisted equivariant K-theory	Freed & Moore
many-body	TFTs as effective actions	invertible fully-extended TFTs	Freed, Kapustin

There are lots of open questions here, on the math side too!

- It's just amazing to use topology to predict new kinds of materials!
- Topological insulators and superconductors should lead to new technology, via spintronics, thermoelectrics, etc.
- The (potential) big application: these materials suggest how to realize Majorana fermions and an approach to topological quantum computing.

You will not be expected to know almost any physics. Just some math that is commonplace around here.
Our seminar will split up into two independent halves.

Topological Band Theory:	Intro - Owen
	Physics - Alessandro
	TEM, I - ?
	TEM, II - ?

TEM = "Twisted Equivariant Matter" by Freed & Moore

Topological Field Theory:	Physics, I - Pavel, O, or A
	Physics, II - ?
	SRE, I - ?
	SRE, II - ?

SRE = "Short-range entanglement . . . " by Freed

Perhaps a paper by Kapustin and company

Main goal

Explore life at the boundary of math and physics

- Learn enough of the basic context to look at survey articles by physicists (see website)
- See how first-rate mathematicians recognize & extract compelling problems from such a context (Freed, Moore, Kapustin will be our models here)
- Point out interesting lines of research

This is the blind leading the blind. So let's enjoy the journey!

Definition

Solid-state physics aims to understand the behavior of solids, such as response to heat or electromagnetic fields. Theorists aim to explain this behavior via quantum mechanics & quantum field theory.

Bear in mind:

Every theoretical description of a physical situation is (at best!) an approximation. It is justified if it works pretty well, at something. (See, e.g., the Drude and Sommerfeld models.)

Let's size up the problem:

- radius of an atom ≈ 1 Å $\quad (= 10^{-10}m)$
- number of atoms per $cm^3 \approx 10^{22}$

That is a lot of electrons, protons, and neutrons! There's no way one can simply solve the Schrödinger equation for such a system.

The nuclei are much heavier than the electrons:

$$\frac{m_p}{m_e} \approx 1836.$$

So to simplify:

1. We will pretend the nuclei are *static*, and hence not treat them via quantum mechanics.
2. We will also only consider solids in which the nuclei are arranged in a crystal: their positions are invariant under the action of a full lattice $\Lambda \subset \mathbb{R}^3$.
3. Only electrons will be treated quantum mechanically.

- For one electron, the Hilbert space is

$$\mathcal{H}_1 = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2.$$

- For N electrons, the Hilbert space is

$$\mathcal{H}_N = \Lambda^N(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2) \subset \bigotimes^N L^2(\mathbb{R}^3) \otimes \mathbb{C}^2,$$

thanks to the Pauli exclusion principle (i.e., the spin-statistics connection).

The Schrödinger equation is

$$i\hbar \frac{\partial \Psi}{\partial t} = H_N \Psi.$$

Here the Hamiltonian has the form

$$H_N = \underbrace{\sum_{i=1}^{N} -\frac{\hbar^2}{2m_e}\nabla_{(i)}^2}_{\text{“kinetic energy”}} + \underbrace{\sum_{\ell \in \Lambda} \frac{Ze^2}{|x_{(i)} - \ell|}}_{\text{electron-nuclei}} + \underbrace{\frac{1}{2}\sum_{i \neq j} \frac{e^2}{x_{(i)} - x_{(j)}}}_{\text{electron-electron}} + \cdots$$

where Z is the atomic number of the nucleus. The dots indicate other terms like spin-orbit coupling or external electromagnetic fields. (These will briefly appear in Alessandro's talk.)

Crazy but good idea:

Treat electrons as *independent* but each experiences the same potential function V, which is invariant under Λ.

The function V replaces the electron-electron term with an "average electron charge distribution." There are very effective choices known for some materials.

Now $H = \sum_i H_{(i)}$, where each $H_{(i)}$ is identical. Hence we can find eigenstates separately for each electron i, and then take into account the Pauli exclusion principle. (This is a much easier problem.)

Result

It works really well for many solids!

See any book on solid state physics, like Ashcroft-Mermin or Alloul.

Justification:

Landau's "Fermi liquid theory" gives insight into why this approach often works. To be honest, we're working with essentially independent *quasi-particles*, rather than bare electrons. (There is a modern explanation via Wilsonian arguments.)

We now have our work cut out for us: solve the Schrödinger equation with a Λ-periodic potential.

Bloch's Theorem

The eigenstates of such a Hamiltonian can be chosen to have the form

$$\psi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} u_{n,\mathbf{k}}(\mathbf{x}),$$

where $u_{n,\mathbf{k}}$ is invariant under Λ. Equivalently, the eigenstates can be chosen such that each eigenstate ψ has a *wavevector* $\mathbf{k}$ such that

$$\psi(\mathbf{x} + \ell) = e^{i\mathbf{k}\cdot\ell}\psi(\mathbf{x})$$

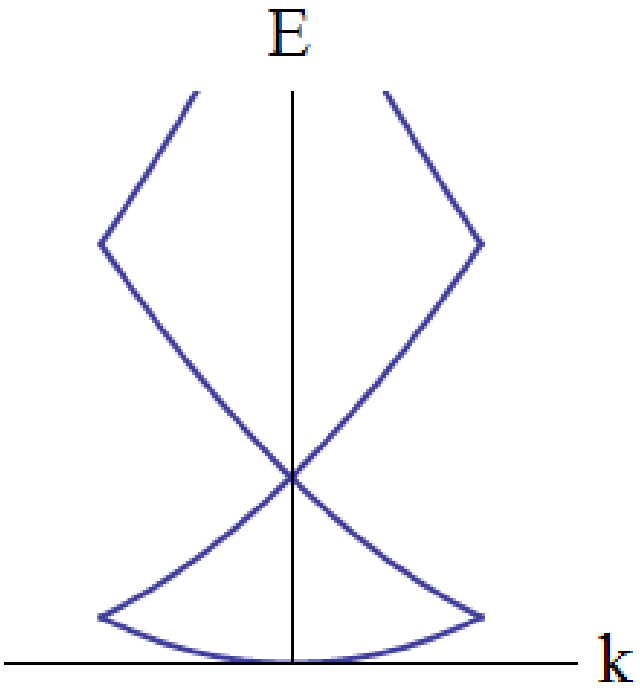
for every $\ell \in \Lambda$.

In short, an eigenstate is a plane-wave times a Λ-periodic function. We call $\mathbf{k}$ the *crystal momentum* of the state.

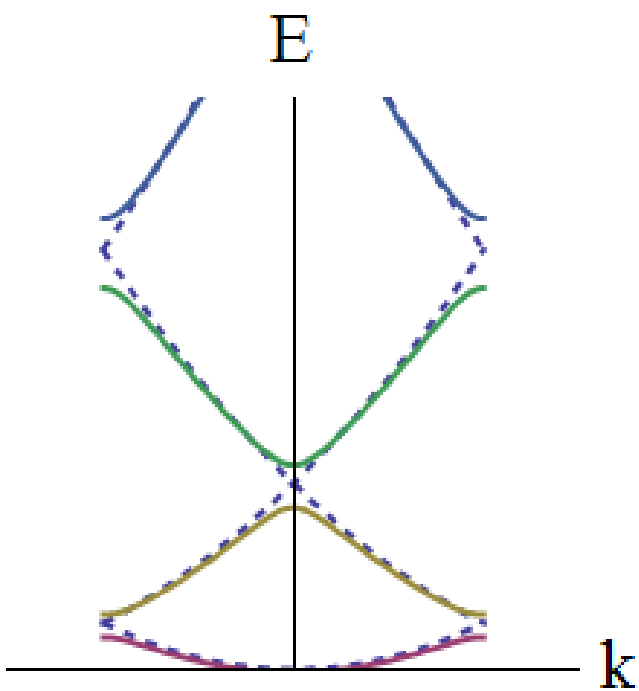
- The proof is simple. Translation by $\ell \in \Lambda$ commutes with H, so we can pick eigenstates for both Λ and H simultaneously.
- The values of crystal momentum $\mathbf{k}$ live in a fundamental domain of the dual lattice $\Lambda^\vee$. (In physics the Voronoi cell is called a Brillouin zone.)
- It is even better to view our problem as parametrized by the *Brillouin torus*, $T_\Lambda = \mathbb{R}^n/\Lambda^\vee$.
- For each value $\mathbf{k} \in T_\Lambda$, there is its *Bloch Hamiltonian* $H(k)$ given by solving for the $u_{n,\mathbf{k}}$. The spectrum is discrete because we are solving on the torus $\mathbb{R}^n/\Lambda$, since the u terms are periodic.

(I hope you see the possibility for K-theoretic thinking there: understanding eigenvalues of endomorphisms of vector bundles . . .)

We can plot the spectrum over the fundamental domain.



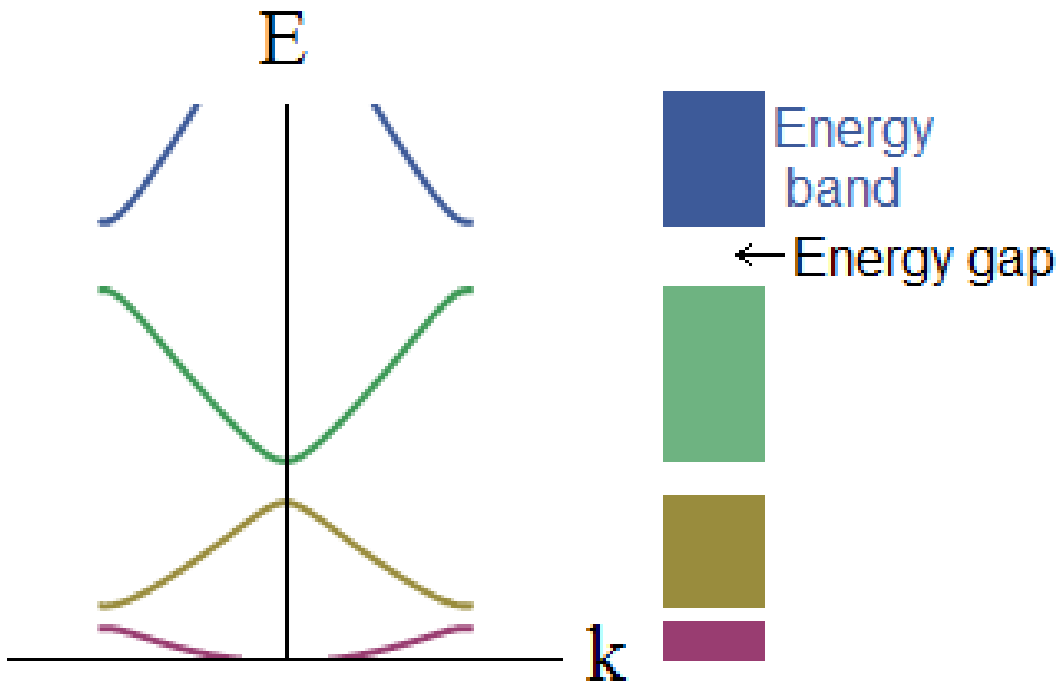
free



(weak) potential

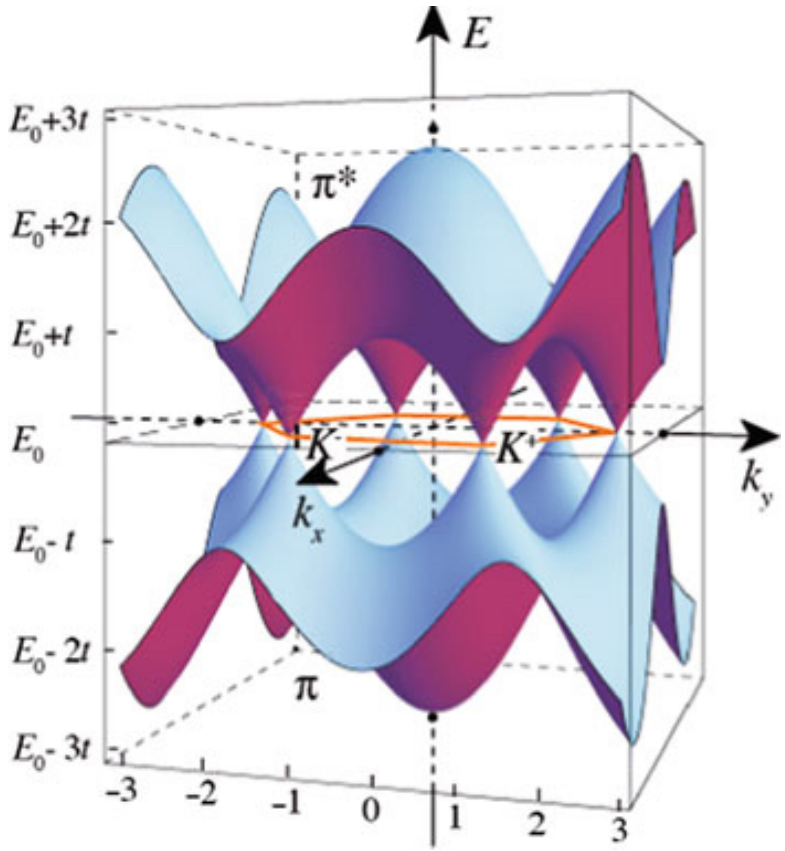
On the left we have $E(k) = k^2$ for the free particle. On the right, a weak periodic potential affects the values at the boundary.

Projecting out the momentum direction, we see gaps emerge.



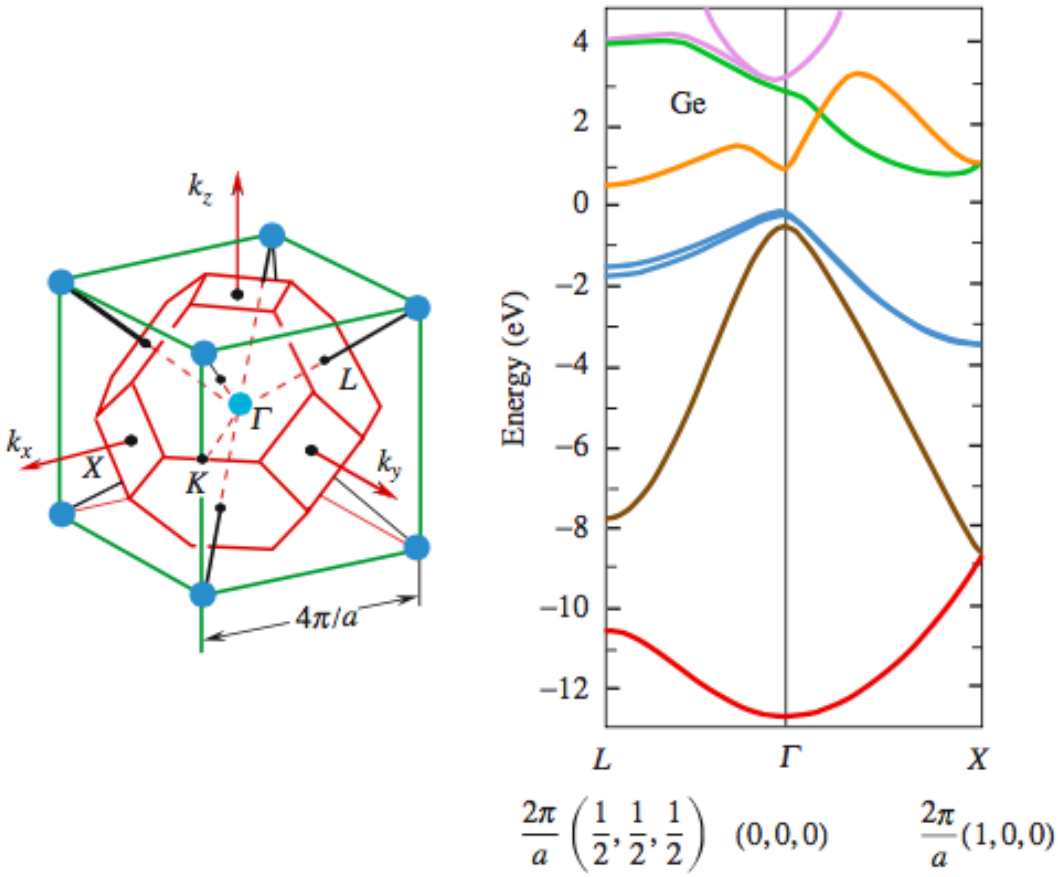
This behavior is "generic" for periodic potentials. (Thanks to mysterious blogger for these pictures.)

These functions are also called dispersion relations. In two dimensions, they can be come quite beautiful.



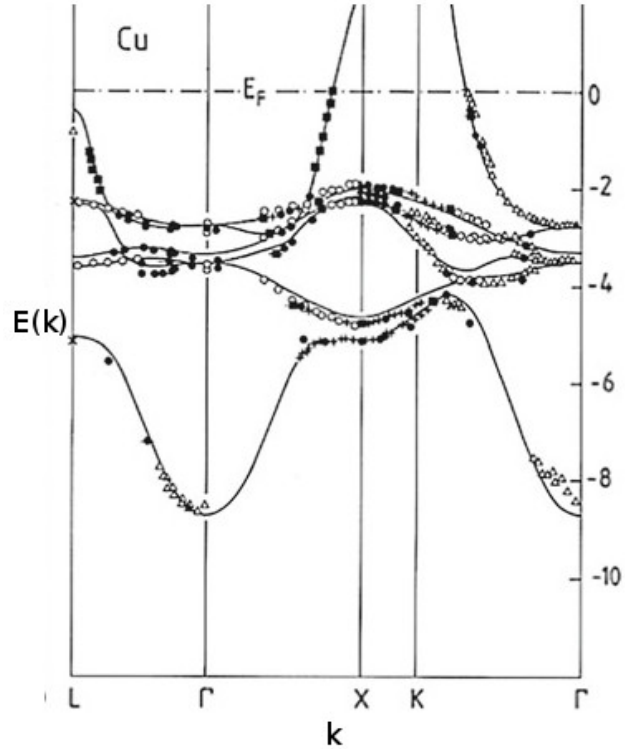
This picture is the band structure graphene, an amazing new material. Notice the six points where the levels touch.

Here is a common type of diagram.



On the left is the Brillouin zone, with special points labelled. On the right are spectra along straight line paths between special points.

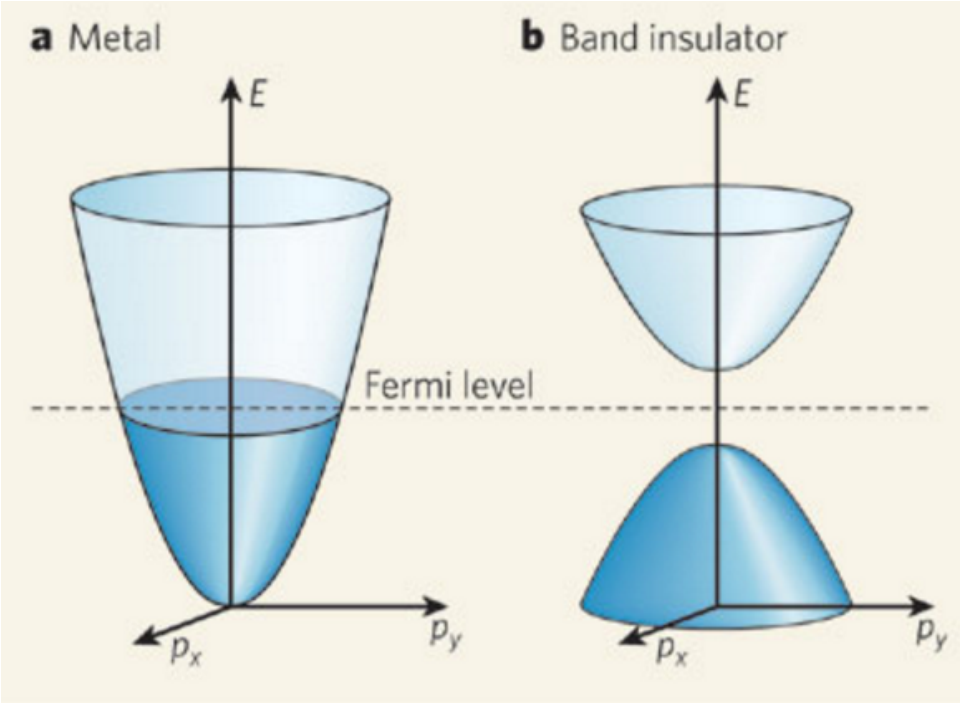
Physicists have developed powerful computational tools for estimating such band structures from atomic spectra and crystal structure.



The continuous curves are estimates for copper. The dots are experimental measurements. (Thanks to Alloul for these pictures.)

I've suppressed an important issue so far, and I won't say much now.
We want the thermodynamic limit, where we work with a sequence of finite-volume regions of space $\{V_i\}$ and finitely many particles $\{N_i\}$ and take the limit as $i \to \infty$, with $vol(V_i) \to \infty$, $N_i \to \infty$, but $N_i/V_i \to \rho$, a fixed density.
Consider the case of larger and larger "boxes." The pictures of bands just need to be modified by restricting to a lattice of wavevectors, which grows denser and denser.

I bring this up to clarify the role of statistics. The ground-state for finite volume V_i will fill up the first $N_i/2$ energy levels, since the Pauli exclusion principle allows two electrons to occupy each energy level. (Give them different spin vectors.) In the thermodynamic limit, you get a Fermi energy and a Fermi surface.



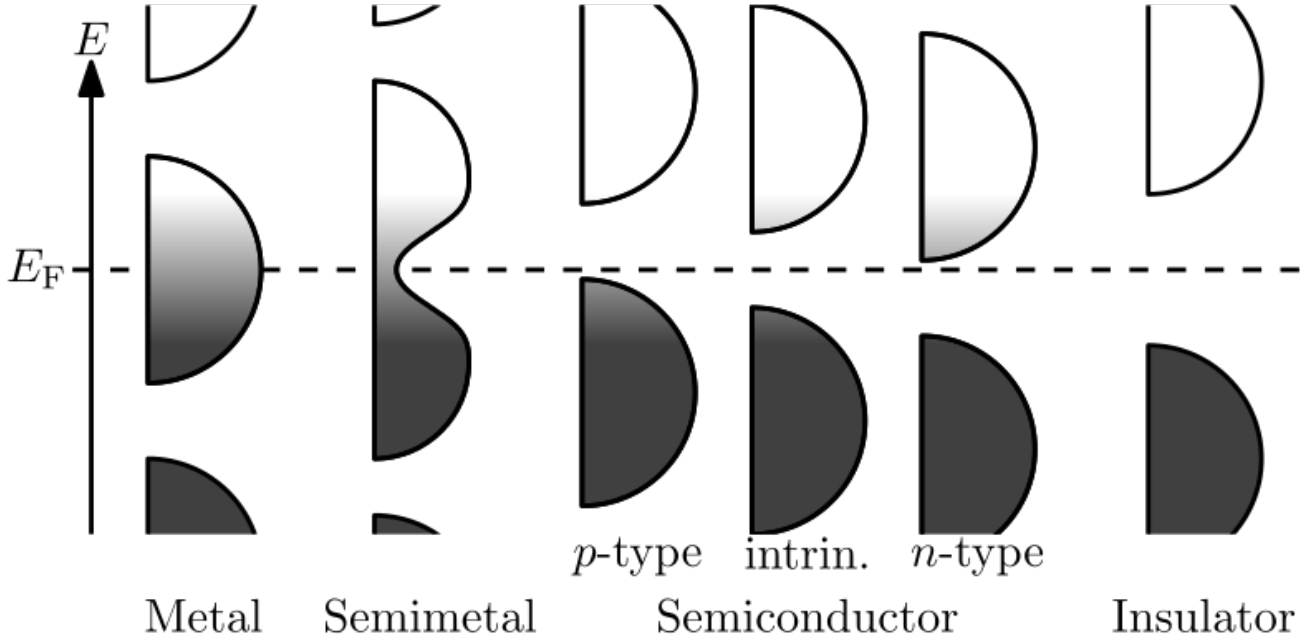
(Thanks to Fuhrer and Adam for this 2D picture.)

We can now explain some important terminology:

- an *insulator* is a material whose Fermi level is between two bands (in the "forbidden energies")
- a *conductor* is a material whose Fermi level cuts across a band

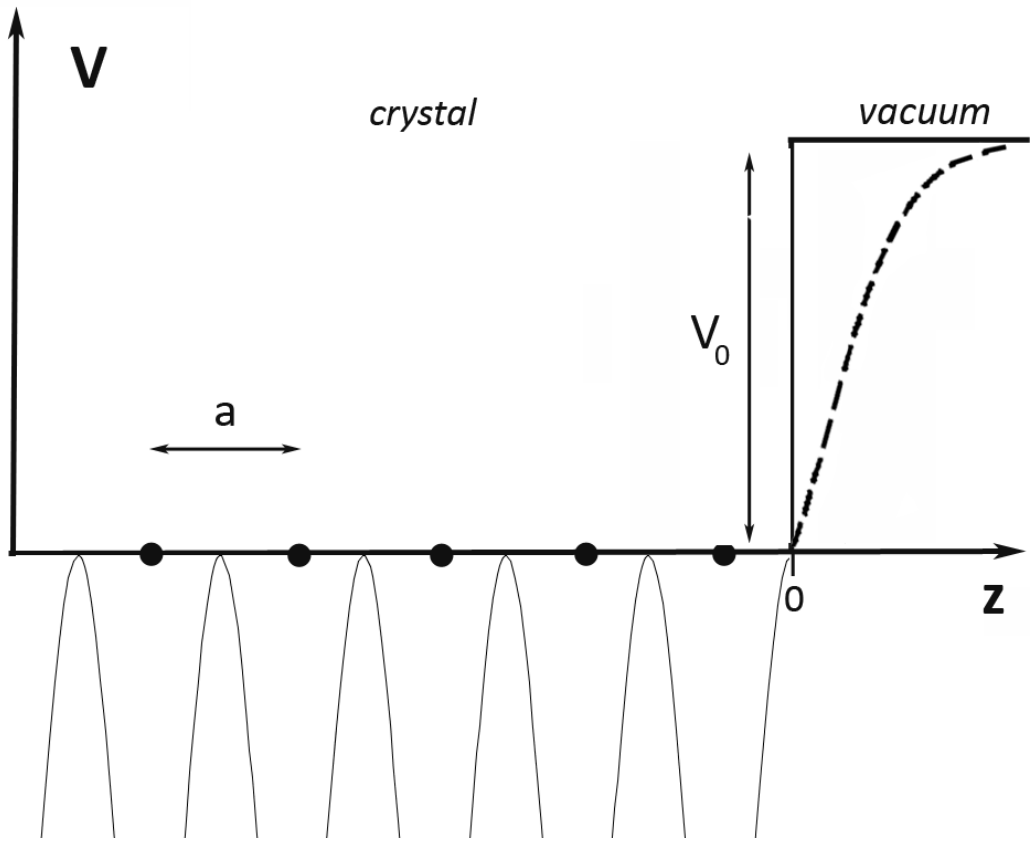
The basic idea is that any perturbations of the system (like heat or an electric field) will kick some electrons into states above the Fermi level, where they will conduct. It takes a lot more energy if you need to jump over an energy gap.

Here's a picture of how the different electrical forms of matter can be distinguished (from Wikipedia).

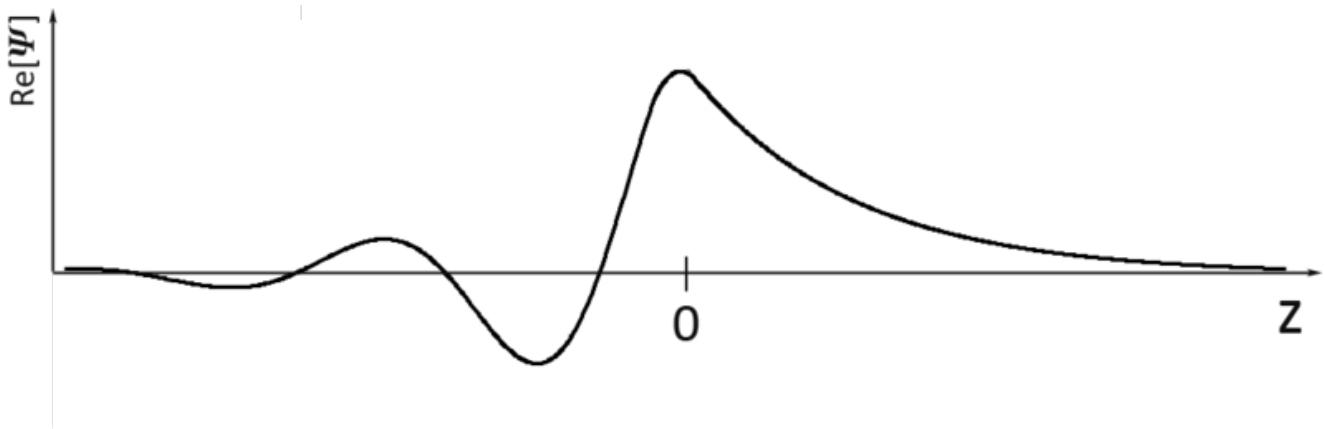


In an insulator, the band below the level is called a "valence band" and above is called a "conduction band."

Ignoring the other limitations of the independent electron approximation, we cannot ignore the fact that crystals do not extend forever. The potential looks something like this:

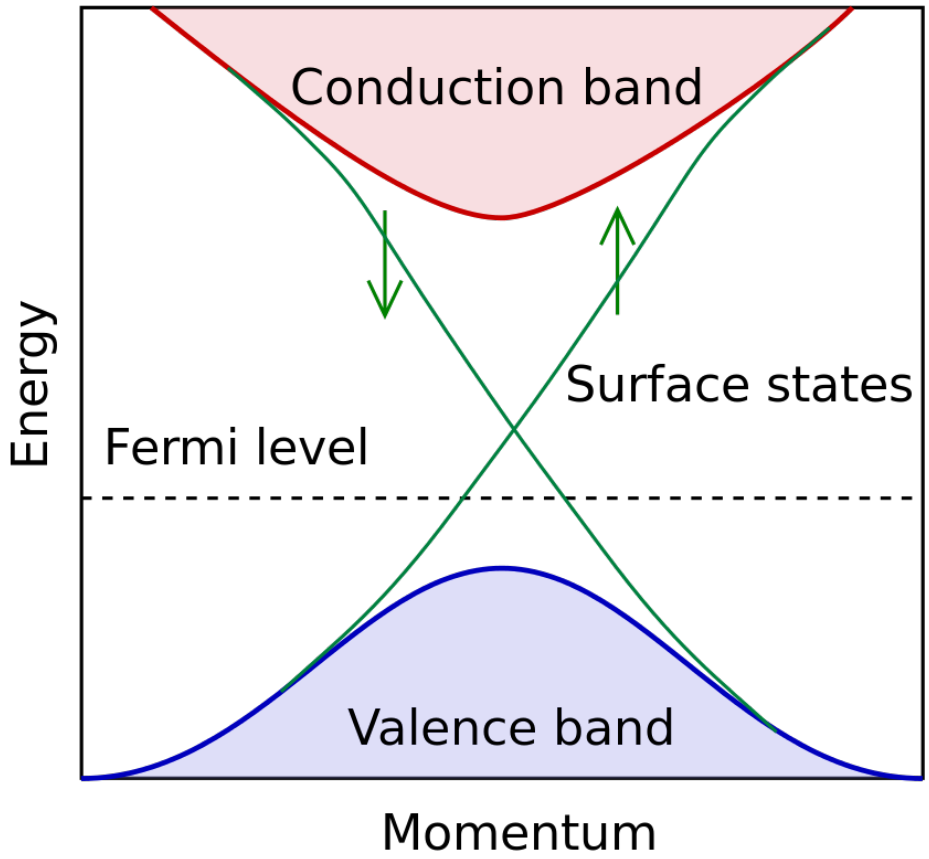


Given the vast number of atoms in just one small piece of matter, it's reasonable to use the Bloch solutions in the interior. Near the boundary, however, these are not a good model.



There are solutions that "localize" along the surface, known as surface states. They may have their own dispersion relations.

Now we can interpret the fundamental band diagram of a topological insulator.



The bands (in green) of the surface states cross the Fermi level and hence are conducting. The bulk is an insulator. (Thanks to Wikipedia.)