Modern Physics (PHY 3305) Lecture Notes

Solid-State Physics: Conduction and Insulation (Ch. 10.5-10.6)

Steve Sekula, 25 March 2010 (created 25 March 2010)

Review

no tags

- We had a participatory discussion about model-building how to construct a 1-D model of a solid from things we already know (Coulomb potential, finite square well, etc.)
- We had a participatory discussion about what wave functions look like in such a solid
- We then talked about energy and how it's distributed in a solid: bands and gaps
- We closed with a review of kinds of solids:
 - Covalent Solids
 - strongest class, shared electron located squarely between neighboring atoms. Bad conductors, high melting points, materially hard (e.g. diamond)
 - Ionic Solids
 - next strongest class, where ions with partially filled valence energy levels (shells) seize electrons from one another to mutually fill their levels. Also bad conductors, materially hard, high melting points. Table salt (*NaCl*) is a good example (brittle).
 - Metallic Solids
 - Electrons are left over after bonding occurs, and these electrons are essentially free to roam about the solid. This leads to an amorphous distribution of attraction in the material electrons are no locked between atoms, and the bonds are weaker. These are malleable (soft), good conductors, lower melting points.
 - Molecular Solids
 - Noble elements form molecules with no electrons leftover. However, they can bond to one another through weak electric dipole moments that are fleeting as charge distributions alter in the solid. Ethanol is an example. They are very soft, and form at low temperatures. If there is a more permanent dipole moment (as in water), the bonds are stronger. This more strong

molecular bond explains why water has a comparatively high melting point.

Use the *PhET* simulation on 2 and N-well systems to review what happens when atoms come together:

http://phet.colorado.edu/simulations /sims.php?sim=Double_Wells_and_Covalent_Bonds http://phet.colorado.edu/simulations/sims.php?sim=Band_Structure

An N atom system

Discuss what happens when N atoms (N is large) come together. Still treat the problem as a 1-D periodic lattice. Consider a single electron, and then expand this discussion to what happens when there is 1 conduction electron per atom.

For a completely free electron, the momentum of an electron in a given energy state with corresponding wave number k is given by $p = \hbar^2 k^2/2m$. What determines momentum for an electron in a periodic lattice?

Bands and Gaps Revisited

Bands in an N-atom system contain so many very closely spaced energy levels as to be easily treated as a CONTINUUM of energy states. What do the probability densities at the top of one band and the bottom of the next band look like?

(See Band demonstration in *PhET* simulation).

For large N, they approach this case:

(Draw a periodic 1-D lattice of ions and sketch the probability density as a function of location of ions for the top and bottom of the band)

The probability densities have the following dependence on the lattice spacing, *a* (the distance between ion cores). At the top of one band (say, the n=1 band), there is maximum kinetic energy for that band and the probability density has nodes at the ion cores (minimum potential energy). At the bottom of the next band (n=2), there is maximum potential energy and the probability density has nodes between the ion cores.

They are periodic, and the periodicity gives us a relationship between the

wavelength and the spacing of the lattice:

• for the n=1 band,

$$a = \frac{1\lambda}{2}$$

$$a=rac{2\lambda}{2}$$

■ for the n=3 band,

$$a=rac{3\lambda}{2}$$

So the relationship at the top of a band and the bottom of the next band is given by:

$$a=n\lambda/2$$

or when

$$k=2\pi/\lambda=\pi n/a$$

The gaps are marked by places where the periodicity is the same but where the kinetic and potential energy have sharply different contributions to the total energy. However, in both cases the kinetic energy is nearly the same for electrons in the two levels,

$$KE = \hbar^2 k^2/2m.$$

Thus, we can conclude that:

• The jump between bands (the band gap) n and n+1 occurs when:

$$k = n\pi/a.$$

The top of a band has n anti-nodes per atom. If there are N atoms overall, then this state has nN anti-nodes. The top of band n+1 will have (n+1)N anti-nodes. Thus, the number of states from the top of one band to the top

of the next is N.

• Each band consists of N states

Because N is so large, each band is essentially a CONTINUUM of energies. The spreading of energies within a band depends on how much wave functions of adjacent states overlaps, and thus:

• the thickness of each band depends not on the number of atoms but their spacing, which in turn determines how waves are distributed between the lattice points.

We can then see how this picture can be summarized using all of these pieces.

- 1. The kinetic energy of an electron in an ideal square well is $p = \hbar^2 k^2/2m$, so kinetic energy has a quadratic dependence on the wave number (inverse wave length) of the electron.
- 2. In one large well of width L, all of the energy of an electron in the well is kinetic (since there U = 0), and we can write the total energy of electrons in the different states as a parabola, with the allowed wavelengths marked as points in k-space. (Draw a parabola, with the y axis being total energy and the x-axis being $k/(\pi/L)$, which is just *n*, and show the parabolic behavior.
- 3. In a lattice, the wave functions of each state look like distorted versions of the ideal square well, so their kinetic energies can be described still by $p = \hbar^2 k^2/2m$.
- 4. However, when $k = n\pi/a$, there will occur a "gap" between the band of allowed energies since here the potential energy increases for the same kinetic energy at the next level up. Show the slide of the distorted parabola, indicating the jumps (gaps) due to this fixing of wave number but rapid change in potential energy (increasing potential energy).

Discussion about filled/partially filled bands

We've talked about the properties of states, but haven't really considered what happens when you then stick a whole bunch of valence electrons into the system. If we have 1 valence electron per atom, then we have N valence electrons that can occupy all of these states.

- What is the Fermi Energy?
- At T=0 (or at temperatures lower then the Fermi temperature, which corresponds to the Fermi energy), how will N electrons fill the available states in a crystal lattice?
- What are some scenarios for what the highest-energy bands will look like (those below which all energy states in lower bands are filled)?

Conduction and Insulation

The classical picture of conduction is as follows:

Valence electrons are free to move about the solid (the conductor). However, they may suffer collisions with positive ions. This picture was introduced to explain why you can apply a voltage across a conductor (an electric field) but the electrons coming out the other end of the conductor don't have energies (velocities) corresponding to accelerating the same electrons in vacuum. They very quickly reach terminal velocity in the conductor and cease to accelerate. Collisions are a retarding force.

DISCUSSION:

Without the application of an electric field, what do the velocities of electrons in a lattice look like, on average? Consider our 1-D lattice, where electrons can move left or right. What will the velocity of a single electron look like? What above a whole bunch of electrons?

GUIDE: any electron can move left or right. There's a 50/50 change a given electron is doing that at a moment in time. Thus, with equal number of electrons going left and right, there is zero net velocity and no current.

What happens when you apply an electric field?

Consider the effect of an electric field on an electron moving right or left, if the field is applied to the left (remember that F = qE and q = -e for an electron, where $e = 1.6 \times 10^{-19}$ C.

The relationship between current density (number of electrons/per unit area per unit time) and the applied electric field is given by:

$$j = \sigma E$$

where σ is the *CONDUCTIVITY* of the material, and is related to the number of charge carriers, their mass, and the time between collisions with ions. The reciprocal of conductivity is resistivity:

$$\sigma=1/
ho$$

Classically, conductivity decreases as the collision time decreases. That is, when collisions are frequent one expects more resistance to motion. One way to decrease collision time is to increase temperature, which increases the vibration of the ions from their lattice points and thus puts more ions in the path of a moving electron more often.

But in metals, measured collision times are MUCH larger than one expects from a theory in which an electron can collide with any ion. So metals and their conductivity cannot be explained by the classical theory.

DISCUSSION:

What insights may be gained into conductivity from our 1-D crystal lattice? Think instead of the electron as a wave.

GUIDE:

- When the lattice is perfect and the ions completely still (T=0), the electron wave has a single wavelength when in a given state, and thus a fixed momentum. Such a situation is akin to a free particle, where the electron simply barrels from one end of the lattice to the other without changing its momentum.
- What could cause the momentum of the electron wave to change as a function of distance?

• ideas:

- imperfections in the lattice, such as a different kind of atom at some location in the crystal (contamination)
- missing atoms from lattice sites. This changes a in that location, and thus λ and p. When a increases, what happens to p?
- thermal motion: changes the *a* between atoms as they vibrate about their equilibrium points. This changes *a* and thus *p*.

The quantum description provides deep insight into what conduction actually is. It is, in fact, observed that conductivity decreases with T - it actually varies linearly, suggesting that ionic motion, not merely the presence of ions, is the key to this effect.

DISCUSSION:

Which effects do you think are most important? For instance at room temperature?

GUIDE:

- Thermal effects dominate until T gets very small, so at room temperature these effects usually dominate conductivity.
- At low T, lattice irregularities are the problem. These effects are largely independent of temperature, and so become significant only at low T. Their resistance is thus also a fixed contribution to the total resistance of the material.

What Defines a Conductor?

Piece together our discussion of conductivity (electrons moving left or right either with or without an electric field applied) and our discussion of filling states in a crystal lattice with electrons to discuss conductivity quantum mechanically.

DISCUSSION:

How can we picture conduction quantum mechanically? Consider the metal as just one large finite square well, with no bands and gaps. What then is the relationship between conduction and energy levels?

- What is the energy of an electron in a state n with wave number k?
 That's just its kinetic energy, in an ideal square well, so we expect an electron to have E = KE = ħ²k²/2m in the well.
- What does the momentum look like for electrons in each state when NO electric field is applied?
 - There can be two electrons per energy level, and on average one will have momentum +k and the other -k.
- From this, we can sketch total energy vs. wave number for a solid with no electric field applied (show slide)

- What will happen to the electrons (and how they fill states) when the electric field is applied in the -x direction?
 - Consider what happens to an electron with +k and one with -k if a small electric field is applied. Assume the effect of that electric field will be to increase the momentum of the electrons by an amount $+\epsilon$.
 - Electrons with wave number +k will increase to $k + \varepsilon$, and those with -k will also increase to $-k + \varepsilon$. The effect will be to shift electrons with negative momentum out of higher energy states into lower energy states, while those with positive momentum will go from lower energy states to high energy states. The net effect is illustrated on the slides.

So conduction is this effect. There is a state just above the Fermi energy where a +k electron can go under the application of an electric field. This causes a reshuffling of electrons, with a net increase in the total energy of the system. However, this is quantum mechanics: if the field is not strong enough to promote an electron up to a higher level, then there is no place for another electron to fill, and in that case nobody goes anywhere and there is no conduction.

Gaps and their Role in Determining Conductivity

So who gets to be a conductor, and who gets to be an insulator?

DISCUSSION:

- Consider instead the more realistic 1-D lattice situation, replacing the ideal square well with our bands and gaps.
- Which solids get to be conductors? Which get to be insulators? Discuss.

Next Time

- More discussion about conduction
- Discussions about semi-conduction
- Future directions: superconductivity