

Modern Physics (PHY 3305) Lecture Notes

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

SteveSekula, 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=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,

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

- for the $n=2$ band,

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

- for the $n=3$ band,

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

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