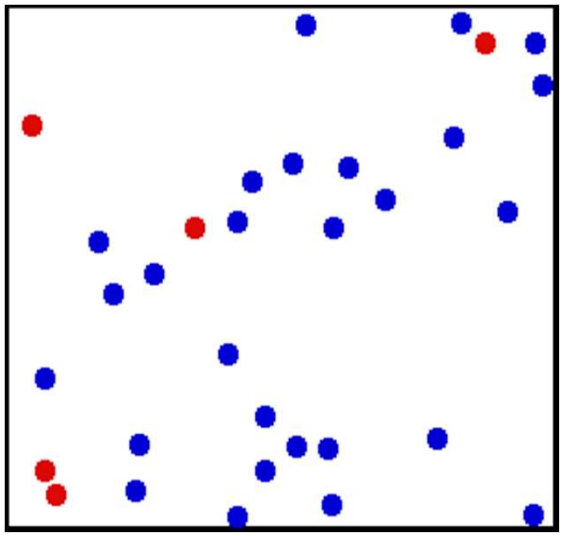
Electrons

kinetic theory

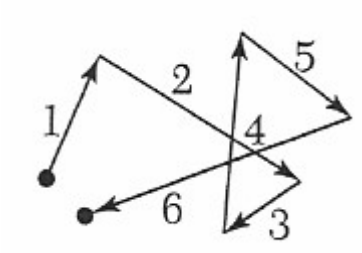
describe electrons as a gas of particles

$v_F = 10^8$ cm/s.



The average time between scattering events τ_{sc} can be calculated by Fermi's golden rule

mean free path: $\boldsymbol{l} = v_F \tau_{sc} \sim 1$ nm - 1 cm



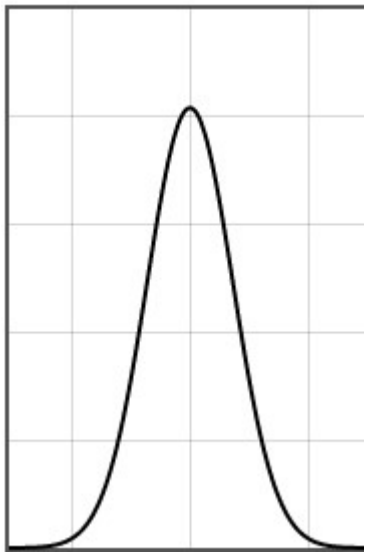
Diffusion equation/ heat equation

$$\frac{dn}{dt} = -D\nabla^2 n$$

Diffusion constant

Fick's law $\vec{j} = -D\nabla n$

Continuity equation $\frac{dn}{dt} = \nabla \cdot \vec{j}$

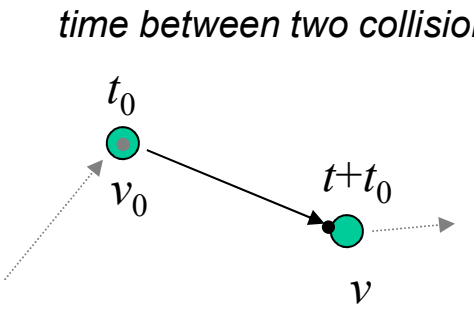


$$n = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-r^2}{4Dt}\right)$$

Diffusive transport

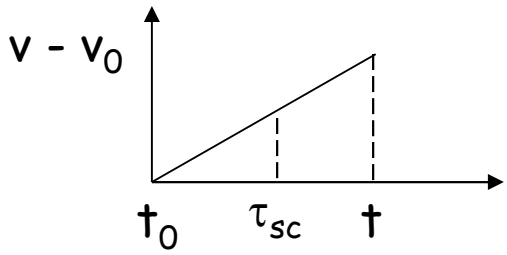
$$\vec{F} = -e\vec{E} = m^* \vec{a} = m^* \frac{d\vec{v}}{dt}$$

$$\vec{v} = \vec{v}_0 - \frac{e\vec{E}}{m^*}(t - t_0)$$



$\langle v_0 \rangle = 0$ $\quad\quad$ $\langle t - t_0 \rangle = \tau_{sc} <$ average time between scattering events

$$\vec{v}_d = \frac{-e\vec{E}\tau_{sc}}{m^*} = \frac{-e\vec{E}\ell}{m^* v_F}$$



drift velocity: $\vec{v}_d = -\mu\vec{E}$

Ohm's law: $\vec{j} = -ne\vec{v}_d = ne\mu\vec{E} = \sigma\vec{E}$

Matthiessen's rule

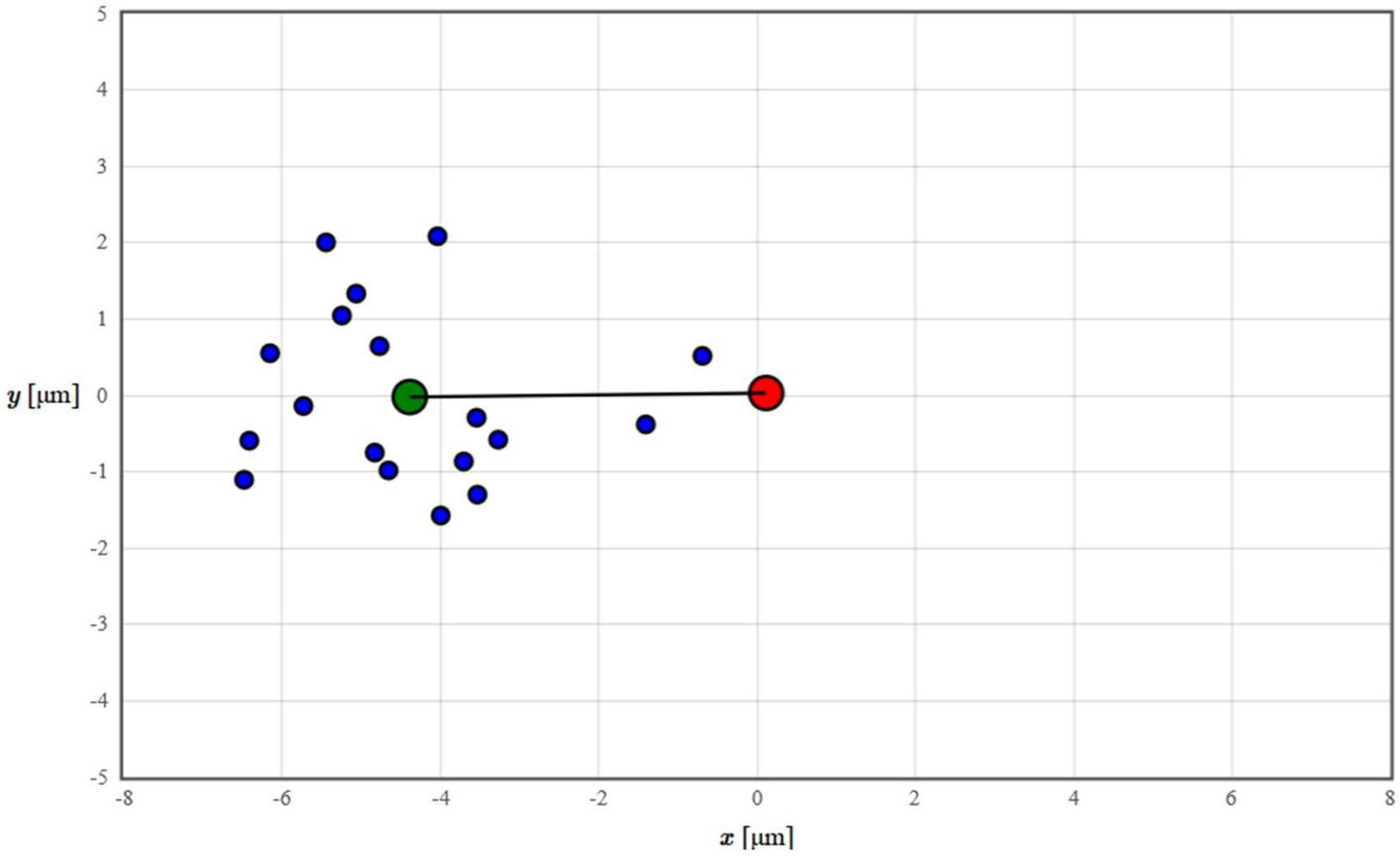
$$\frac{1}{\tau_{sc}} = \frac{1}{\tau_{sc,lattice}} + \frac{1}{\tau_{sc,impurity}}$$

mostly temperature independent

phonons, temperature dependent

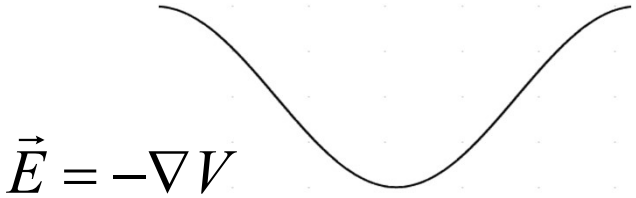
$$\frac{1}{\mu} = \frac{1}{\mu_{lattice}} + \frac{1}{\mu_{impurity}}$$

Drift and Diffusion



http://lampx.tugraz.at/~hadley/ss2/transport/drude.php

Einstein relation



$$\vec{E} = -\nabla V$$

$$n = A\exp\left(\frac{-eV}{k_B T}\right)$$ Boltzmann factor

In equilibrium, drift = diffusion

$$-en\mu\vec{E} + eD\nabla n = 0$$

$$\nabla n = -\frac{e}{k_B T} A\exp\left(\frac{-eV_{pot}}{k_B T}\right)\nabla V = -\frac{ne}{k_B T}\nabla V = \frac{ne\vec{E}}{k_B T}$$

$$-en\mu\vec{E} + eD\frac{ne\vec{E}}{k_B T} = 0$$

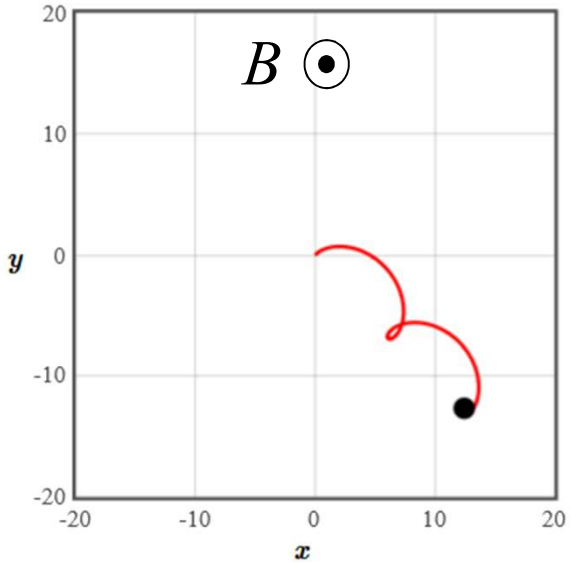
$$\boxed{D = \frac{\mu k_B T}{e}}$$

Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen

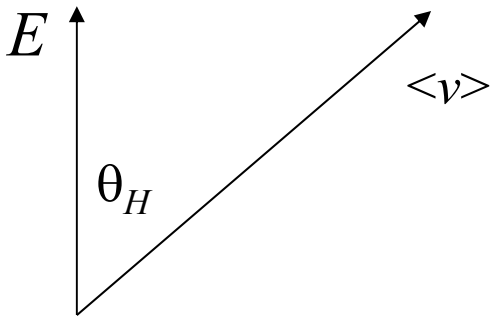
Crossed *E* and *B* fields

Ballistic transport

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v} \times \vec{B}\right)$$



Diffusive transport



Hall angle: $\theta_H = \tan^{-1}\left(-\frac{eB_z\tau_{sc}}{m}\right)$

Magnetic field (diffusive regime)

$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{\vec{v}_d}{\tau_{\text{sc}}} \qquad -\frac{e\tau_{\text{sc}}}{m}\vec{E} = \vec{v}_d$$

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v} \times \vec{B}\right) = m\frac{\vec{v}_d}{\tau_{\text{sc}}}$$

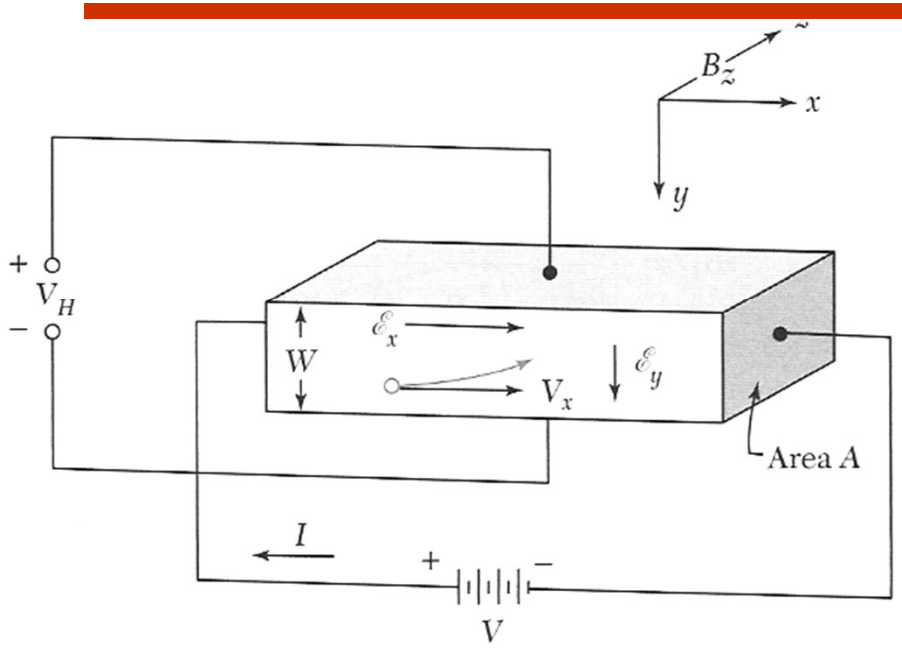
If B is in the z-direction, the three components of the force are

$$-e\left(E_x + v_{dy}B_z\right) = m\frac{v_{dx}}{\tau_{\text{sc}}}$$

$$-e\left(E_y - v_{dx}B_z\right) = m\frac{v_{dy}}{\tau_{\text{sc}}}$$

$$-e\left(E_z\right) = m\frac{v_{dz}}{\tau_{\text{sc}}}$$

The Hall Effect (diffusive regime)



$$v_{d,x} = -\frac{eE_x\tau_{sc}}{m} - \frac{eB_z}{m}\tau_{sc}v_{d,y}$$

$$v_{d,y} = -\frac{eE_y\tau_{sc}}{m} + \frac{eB_z}{m}\tau_{sc}v_{d,x}$$

$$v_{d,z} = -\frac{eE_z\tau_{sc}}{m}$$

If $v_{d,y} = 0$,

$E_y = v_{d,x}B_z = V_H/W = R_H j_x B_z$ $\quad$ V_H = Hall voltage, R_H = Hall Constant

$j_x = -\, nev_{d,x}$

$$R_H = E_y/j_x B_z = -\,1/ne$$

Metal	Method	Experimental R_H, in 10^{-24} CGS units	Assumed carriers per atom	Calculated $-1/nec$, in 10^{-24} CGS units
Li	conv.	−1.89	1 electron	−1.48
Na	helicon	−2.619	1 electron	−2.603
	conv.	−2.3		
K	helicon	−4.946	1 electron	−4.944
	conv.	−4.7		
Rb	conv.	−5.6	1 electron	−6.04
Cu	conv.	−0.6	1 electron	−0.82
Ag	conv.	−1.0	1 electron	−1.19
Au	conv.	−0.8	1 electron	−1.18
Be	conv.	+2.7	—	—
Mg	conv.	−0.92	—	—
Al	helicon	+1.136	1 hole	+1.135
In	helicon	+1.774	1 hole	+1.780
As	conv.	+50.	—	—
Sb	conv.	−22.	—	—
Bi	conv.	−6000.	—	—

Annalen der Physik, vol. 265, pp. 343–347, 1886

IX. *Ueber das Auftreten electromotorischer Kräfte in Metallplatten, welche von einem Wärmestrome durchflossen werden und sich im magnetischen Felde befinden;*

von A. v. Ettingshausen und stud. W. Nernst.

(Aus d. Anz. d. k. Acad. d. Wiss. in Wien, mitgetheilt von den Herren Verf.)

Bei Gelegenheit der Beobachtung des Hall'schen Phänomens im Wismuth wurden wir durch gewisse Unregelmässigkeiten veranlasst, folgenden Versuch anzustellen.

Eine rechteckige Wismuthplatte, etwa 5 cm lang, 4 cm breit, 2 mm dick, mit zwei an den längeren Seiten einander gegenüber liegenden Electroden versehen, ist in das Feld eines Electromagnets gebracht, sodass die Kraftlinien die Ebene der Platte senkrecht schneiden; dieselbe wird durch federnde Kupferbleche getragen, in welche sie an den kürzeren Seiten eingeklemmt ist, jedoch geschützt vor directer metallischer Berührung mit dem Kupfer durch zwischengelegte Glimmerblätter.

http://dx.doi.org/10.1002/andp.18862651010

Boltzmann Group

Albert von Ettingshausen, Prof. at TU Graz.

Nernst was a student of Boltzmann and von Ettingshausen. He won the 1920 Nobel prize in Chemistry.

(Standing, from the left) Walther Nernst, Heinrich Streintz, Svante Arrhenius, Hiecke, (sitting, from the left) Aulinger, Albert von Ettingshausen, Ludwig Boltzmann, Ignacij Klemencic, Hausmanninger (1887).

Thermal conductivity

$$\vec{j}_U = \bar{E}\vec{j}$$

Average particle energy

$$u = \bar{E}n$$

internal energy density

$$\vec{j}_U = -\bar{E}D\nabla n = -D\nabla u$$

$$\vec{j}_U = -D\frac{du}{dT}\nabla T = -Dc_v\nabla T$$

$$\vec{j}_U = -K\nabla T$$

Thermal conductivity

$$K = Dc_v$$

$$K \to 0 \quad \text{as} \quad T \to 0$$

Wiedemann - Franz law

$$\frac{K}{\sigma} = \frac{Dc_v}{ne\mu}$$

Einstein relation: $$D = \frac{\mu k_B T}{e}$$

Dulong - Petit: $$c_v = 3nk_B$$

$$\frac{K}{\sigma} = \frac{3k_B^2}{e^2} T$$

Wiedemann Franz law $$L = \frac{K_{el}}{\sigma T} = 2.32 \times 10^{-8} \quad \mathrm{W\,\Omega/K^2}$$

Lorentz number

Lorenz number

$$L = \frac{K_{el}}{\sigma T} = 2.32 \times 10^{-8} \qquad \mathrm{W\,\Omega/K^2}$$

Table 5 Experimental Lorenz numbers

	$L \times 10^8$ watt-ohm/deg^2			$L \times 10^8$ watt-ohm/deg^2	
Metal	0°C	100°C	Metal	0°C	100°C
Ag	2.31	2.37	Pb	2.47	2.56
Au	2.35	2.40	Pt	2.51	2.60
Cd	2.42	2.43	Su	2.52	2.49
Cu	2.23	2.33	W	3.04	3.20
Mo	2.61	2.79	Zn	2.31	2.33

At low temperatures the classical predictions for the thermal and electrical conductivities are too high but their ratio is correct. Only the electrons within $k_B T$ of the Fermi surface contribute.

CIF file

Consider the material described by this CIF file.

(a) What is the Bravais lattice of this material?

(b) How many atoms are there in the basis of this crystal?

(c) What are the primitive lattice vectors of this crystal?

(d) What is the volume of the primitive unit cell and what is the volume of the conventional unit cell?

(e) How many elements are there in the point group of this crystal?

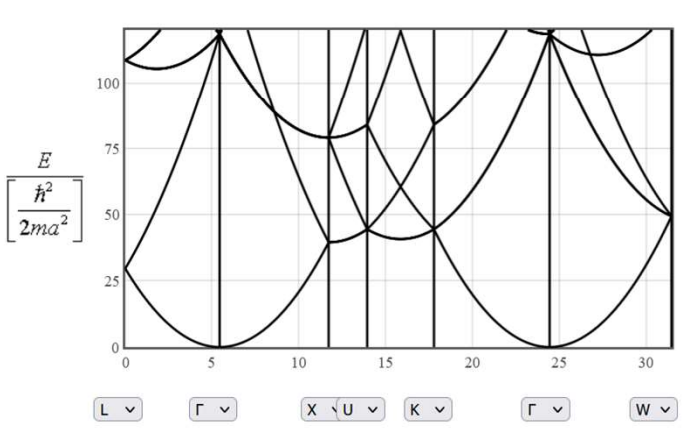
(f) How many optical branches are there in the phonon dispersion of this crystal? Are the transverse branches degenerate in the [100] direction?

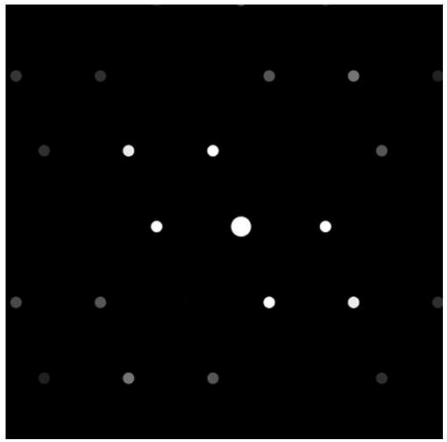
(g) What are the primitive reciprocal lattice vectors?

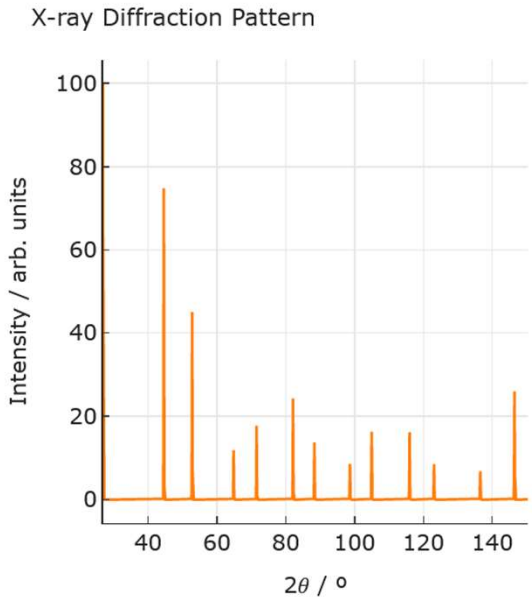
(h) What is the length of the reciprocal lattice vector $\vec{G}_{123}$?

(i) What is the square of the x-ray structure factor of the $\vec{G}_{123}$ reflection?

(j) Sketch the electronic band structure of this crystal using the empty lattice approximation.







x-ray diffraction

The table to the right shows the intensity of diffraction peaks that were measured in an x-ray diffraction experiment on a single crystal. The three components of the scattering vector Δk are given in units of [1/m]. The intensities have been normalized to their largest value.

(a) What are the primitive lattice vectors of this crystal in real space?

(b) What Bravais lattice does this crystal have?

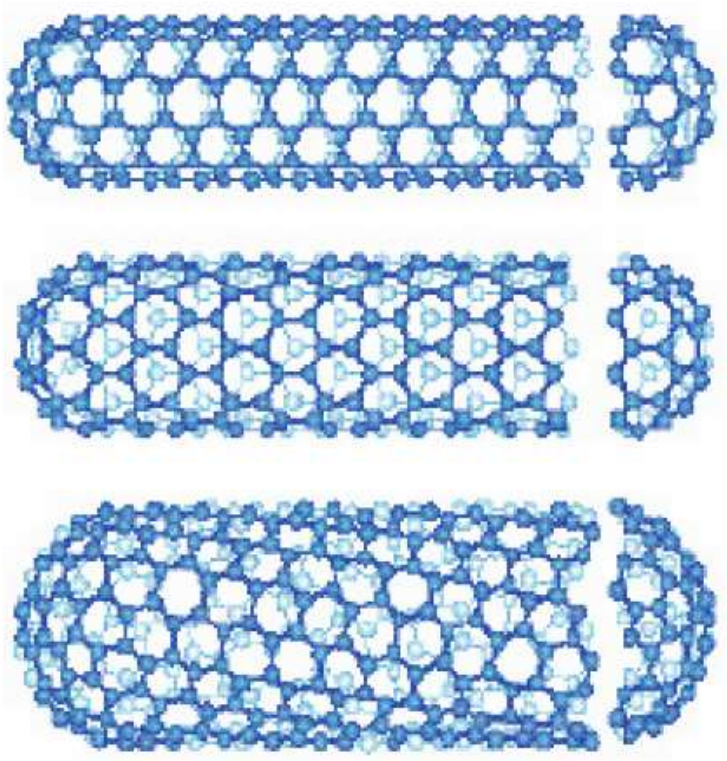
(c) How can you estimate the number of atoms in the basis? How many atoms do you estimate are in the basis of this crystal?

(e) How could you determine what atoms are in the basis and how they are arranged?

(d) Knowing how the atoms are arranged in the basis, how could you determine the point group of this crystal?

Δk_x	Δk_y	Δk_z	Intensity
0	0	0	1
-1.5E10	0	0	0.229
0	-1.5E10	0	0.229
0	0	-1.5E10	0.229
0	0	1.5E10	0.229
0	1.5E10	0	0.229
1.5E10	0	0	0.229
-1.5E10	-1.5E10	0	0.667
-1.5E10	0	-1.5E10	0.667
-1.5E10	0	1.5E10	0.667
-1.5E10	1.5E10	0	0.667
0	-1.5E10	-1.5E10	0.667
0	-1.5E10	1.5E10	0.667
0	1.5E10	-1.5E10	0.667
0	1.5E10	1.5E10	0.667
1.5E10	-1.5E10	0	0.667
1.5E10	0	-1.5E10	0.667
1.5E10	0	1.5E10	0.667
1.5E10	1.5E10	0	0.667
-1.5E10	-1.5E10	-1.5E10	0.192
-1.5E10	-1.5E10	1.5E10	0.192
-1.5E10	1.5E10	-1.5E10	0.192
1.5E10	1.5E10	1.5E10	0.192
1.5E10	-1.5E10	-1.5E10	0.192
1.5E10	-1.5E10	1.5E10	0.192
1.5E10	1.5E10	-1.5E10	0.192
1.5E10	1.5E10	1.5E10	0.192

Carbon nanotubes - rolled up graphene



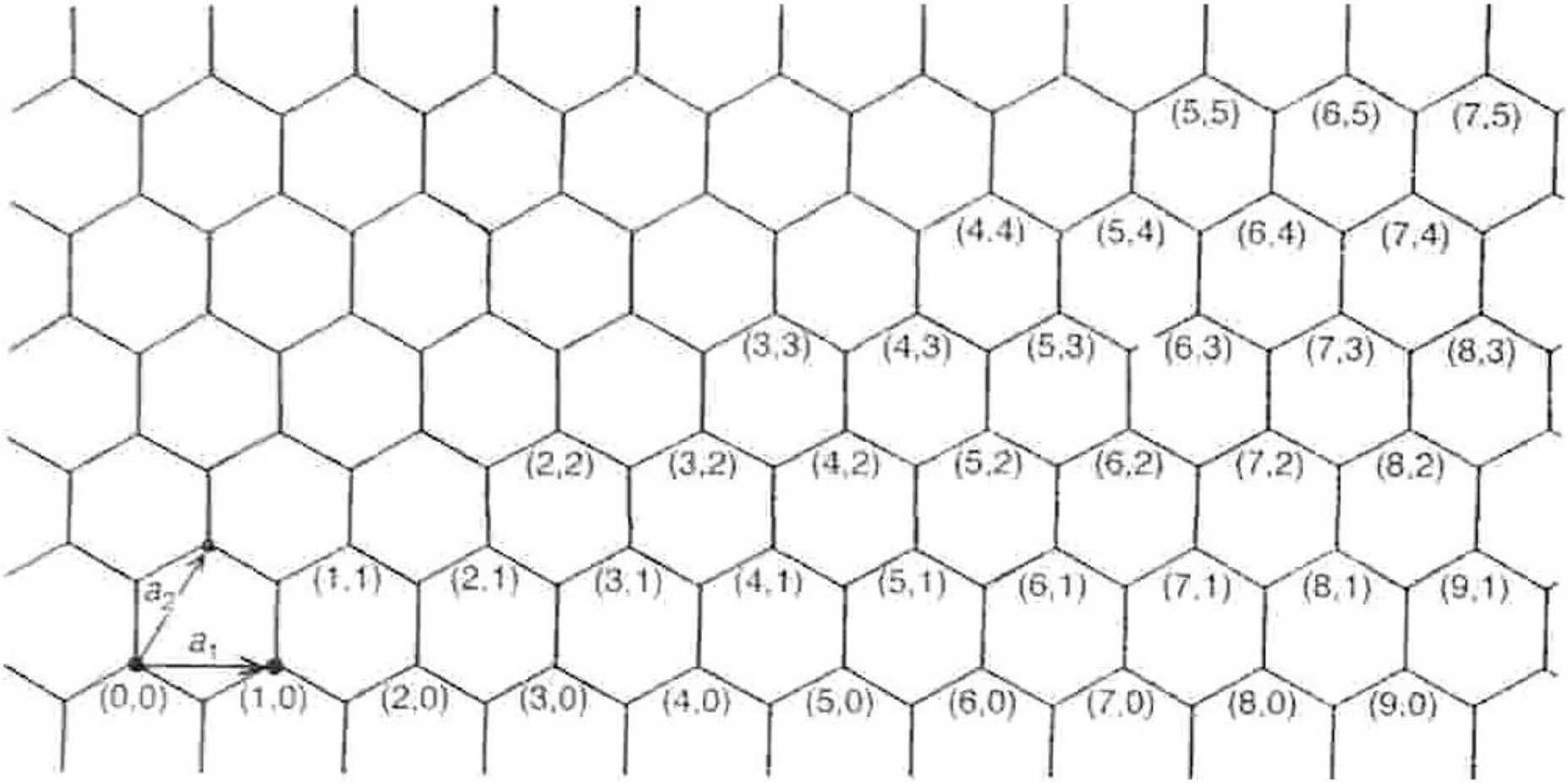
armchair

zig-zag

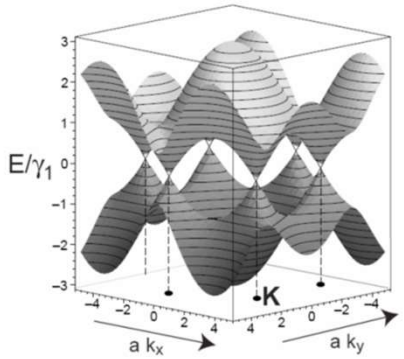
chiral

www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

(*m*,*n*) notation

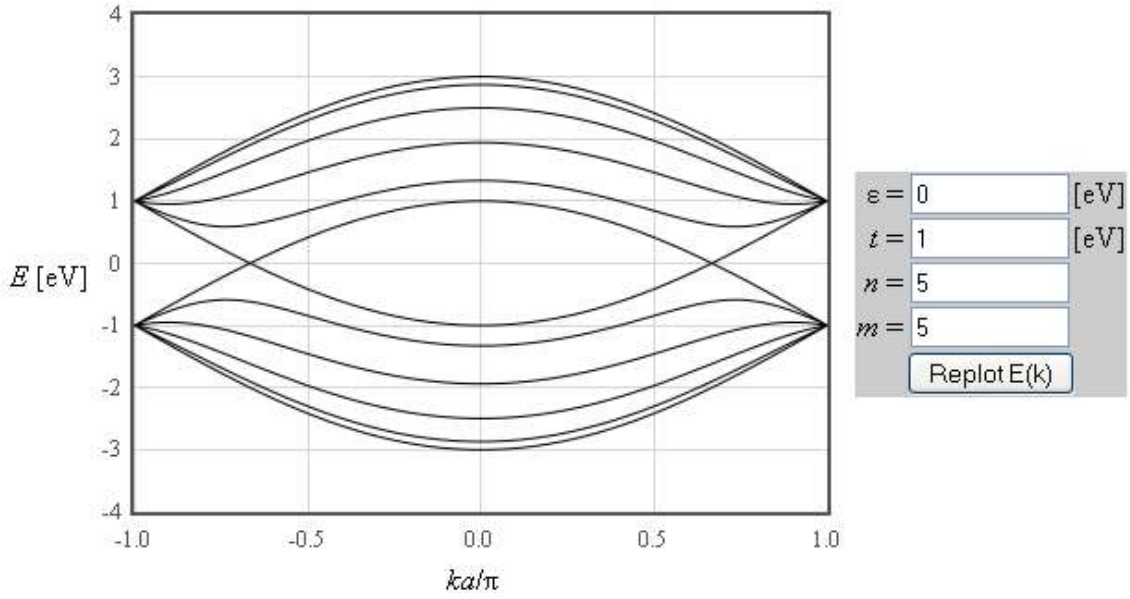


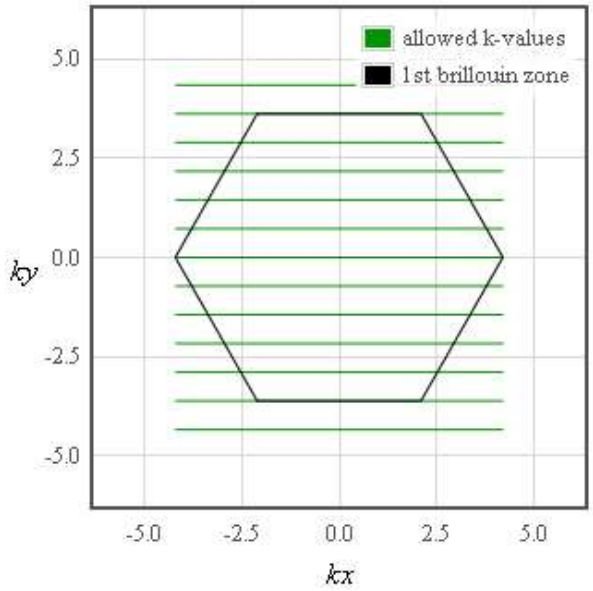
http://www.personal.rdg.ac.uk/~scsharip/tubes.htm



Carbon nanotubes

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$





metallic (5,5) armchair tube

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/CNTs.html

- Band structure calculations: GaN, 6H SiC, GaAs, GaP, Ge, InAs
- Calculated electron density of states
  - Al fcc, Au fcc, Cu fcc, Na bcc, Pt fcc, W bcc, Si diamond, Fe bcc, Ni fcc, Co fcc, Mn bcc, bcc, Gd hcp, Pd fcc, Pd_3Cr, Pd_3Mn, PdCr, PdMn , GaN, 6H SiC, GaAs, GaP, Ge, InAs

Bandstructure of hexagonal gallium nitride (GaN)

The bandstructure calculation for gallium nitride was calculated using the program Quantum Espresso (version 5.2.1) and the pseudopotentials for Ga and N.