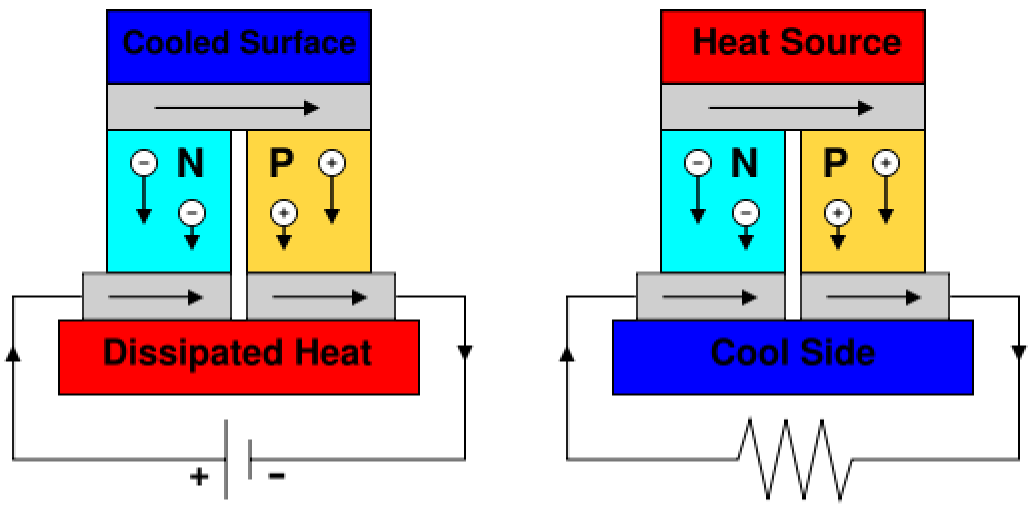
Technische Universität Graz

24. Transport

Jan. 16, 2020

Thermoelectric effects

Peltier effect: driving a through a bimetallic junction causes heating or cooling.



Cooling takes place when the electrons make a transition from low entropy to high entropy at the junction.

Bismuth chalcogenides Bi_2Te_3 and Bi_2Se_3

http://en.wikipedia.org/wiki/Peltier_effect#Peltier_effect

Hall effect

$$f(\vec{k},\vec{r}) \approx f_0(\vec{k},\vec{r}) - \frac{\tau(\vec{k})}{\hbar}\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}}\mu + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k}) \times \vec{B} \right).$$

$$\nabla_{\vec{k}}E(\vec{k}) \cdot \left(\nabla_{\vec{k}}E(\vec{k}) \times \vec{B} \right) = 0$$

$$\nabla_r T = 0$$

$$R_{lmn} = \frac{\nabla_r \tilde{\mu}_l}{e j_m B_n}$$

Nerst effect

$$\vec{j}_{elec} = 0, \quad \nabla T, \quad \vec{B}$$

$$N_{lmn} = \frac{\nabla_r \tilde{\mu}_l}{e \nabla T_m B_n}$$

Ettingshausen effect

$$\nabla_r \tilde{\mu} = 0, \quad \nabla T, \quad \vec{B}$$

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

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

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.

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).

Thermoelectric effects

$$f(\vec{k},\vec{r}) \approx f_0(\vec{k},\vec{r}) - \frac{\tau(\vec{k})}{\hbar}\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k}) \cdot \left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k}) \times \vec{B}\right)$$

Electrical current: $\vec{j}_{elec} = \frac{-e}{4\pi^3}\int v(\vec{k}) f(\vec{k}) d^3k$

Particle current: $\vec{j}_n = \frac{1}{4\pi^3}\int v(\vec{k}) f(\vec{k}) d^3k$

Energy current: $\vec{j}_E = \frac{1}{4\pi^3}\int v(\vec{k}) E(\vec{k}) f(\vec{k}) d^3k$

Heat current: $\vec{j}_Q = \frac{1}{4\pi^3}\int v(\vec{k}) \left(E(\vec{k}) - \mu\right) f(\vec{k}) d^3k$

Thermoelectric effects

Electrical conductivity: $\sigma_{mn} = \frac{j_{em}}{E_n}$ $\quad \nabla T = 0, \vec{B} = 0$

Thermal conductivity: $\kappa_{mn} = \frac{-j_{Qm}}{\nabla T_n}$ $\quad \vec{B} = 0$

Peltier coefficient: $\Pi_{mn} = \frac{j_{Qm}}{j_{en}}$ $\quad \nabla T = 0, \vec{B} = 0$

Thermopower (Seebeck effect): $S_{mn} = \frac{-\nabla \tilde{\mu}_m}{\nabla T_n}$ $\quad \vec{j}_e = 0, \vec{B} = 0$

Hall effect: $R_{lmn} = \frac{E_l}{j_{em} B_n}$ $\quad \nabla T = 0, j_{el} = 0$

Nerst effect: $N_{lmn} = \frac{E_l}{B_m \nabla T_n}$ $\quad j_{elec} = 0$

Student Projects

- **Transport**
  - Thermoelectric effects
  - Crystal momentum
  - Boltzmann equation
  - Relaxation time approximation
  - Current densities
  - Electrochemical potential
  - Electrical conductivity
  - Thermoelectric currents
  - Seebeck effect
  - Free-electron model
    - Electrical conductivity
    - Electrical contribution to the thermal conductivity
    - Wiedemann–Franz law
  - Transport in 1-D crystals
    - Current of Bloch waves in 1-D

Calculate some transport property for a free electron gas or for a semiconductor.

Numerically calculate a transport property for a one dimensional material.

Hall effect

Bloch waves in 1-D

Consider an electron moving in a periodic potential $V(x)$. The period of the potential is a, $V(x+a)=V(x)$. The Schrödinger equation for this case is,

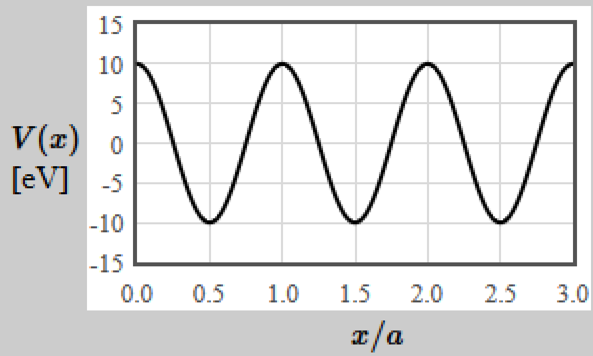
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi. \tag{1}$$

Quantum mechanically, the electron moves as a wave through the potential. Due to the diffraction of these waves, there are bands of energies where the electron is allowed to propagate through the potential and bands of energies where no propagating solutions are possible. The Bloch theorem states that the propagating states have the form,

$$\psi=e^{ikx}u_k(x). \tag{2}$$

where k is the wavenumber and $u_k(x)$ is a periodic function with periodicity a.

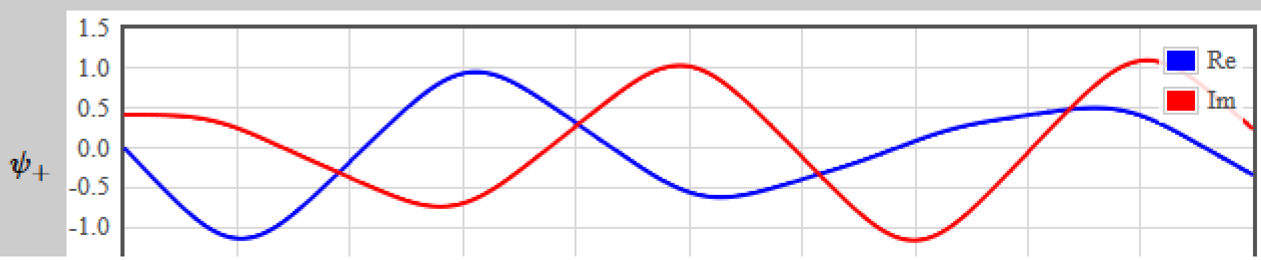
There is a left moving Bloch wave $\psi_-=e^{-ikx}u_{k-}$ and a right moving Bloch wave $\psi_+=e^{ikx}u_{k+}$ for every energy. The following form calculates the Bloch waves for a potential $V(x)$ that is specified in the interval between 0 and a. A discussion of the calculation can be found below the form.



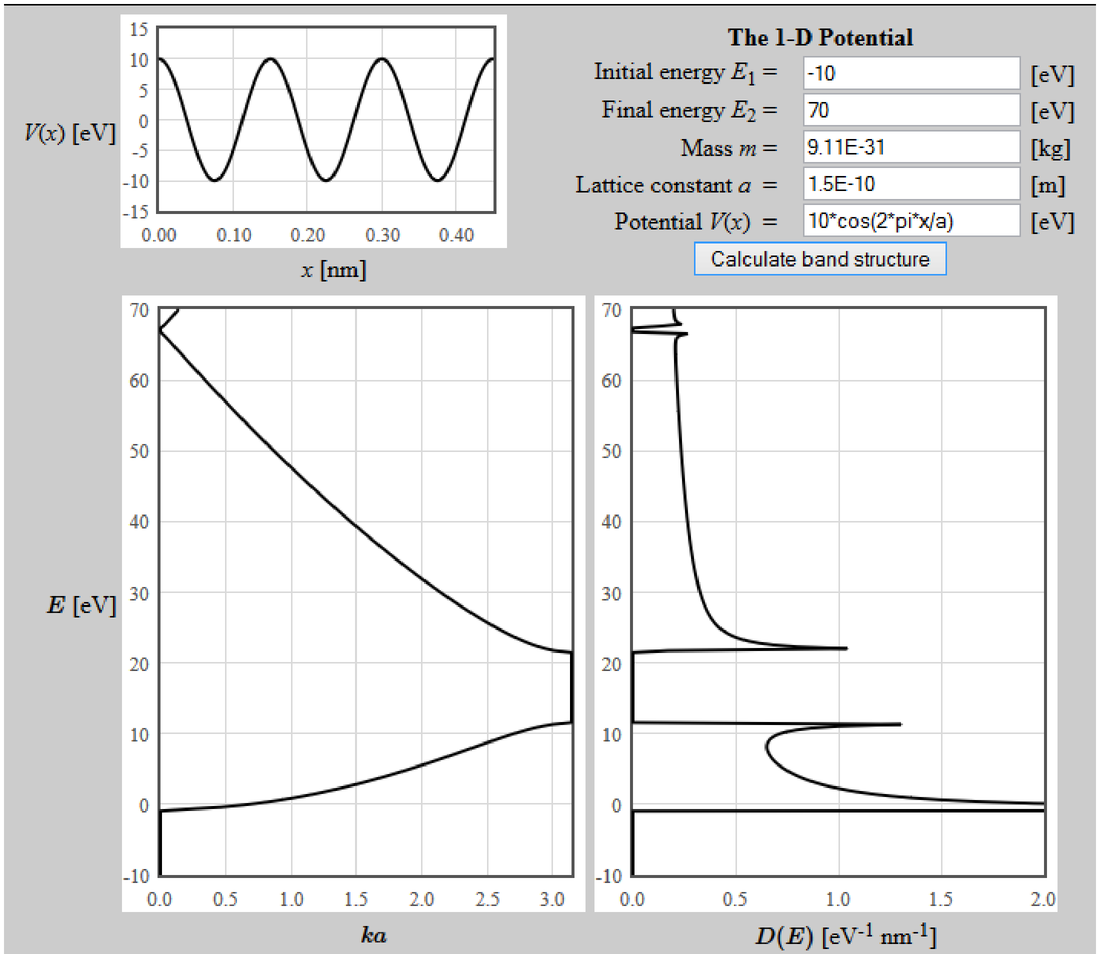
The 1-D Potential

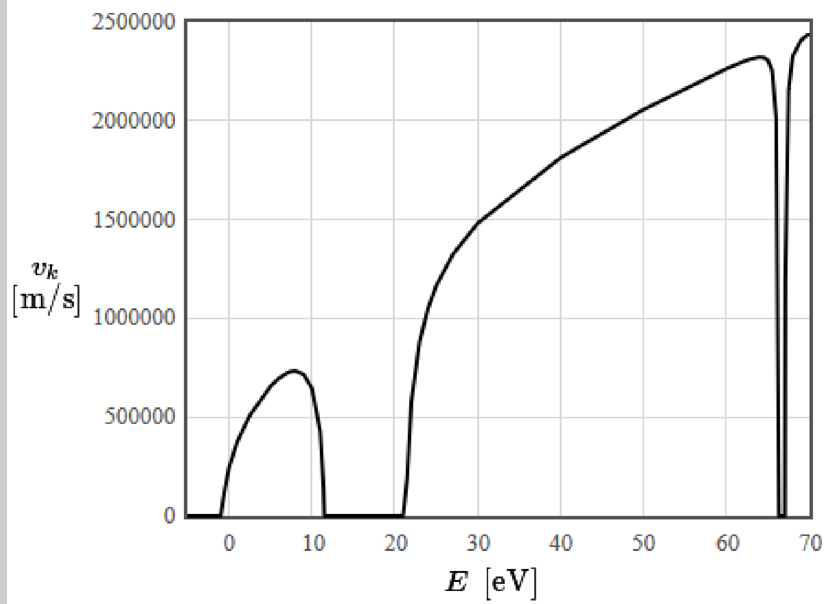
Energy E =	10	[eV]
Mass m =	9.11E-31	[kg]
Lattice constant a =	1.5E-10	[m]
Potential $V(x)$ =	10*cos(2*pi*x/a)	[eV]

Calculate Bloch waves



Velocity of *k*-states





$$v = \frac{1}{\hbar}\frac{dE}{dk}$$

Crystal Physics

Crystal Physics

Crystal physics explains what effects the symmetries of the crystal have on observable quantities.

An Introduction to Crystal Physics Ervin Hartmann
http://ww1.iucr.org/comm/cteach/pamphlets/18/index.html

International Tables for Crystallography
http://it.iucr.org/

Kittel chapter 3: elastic strain

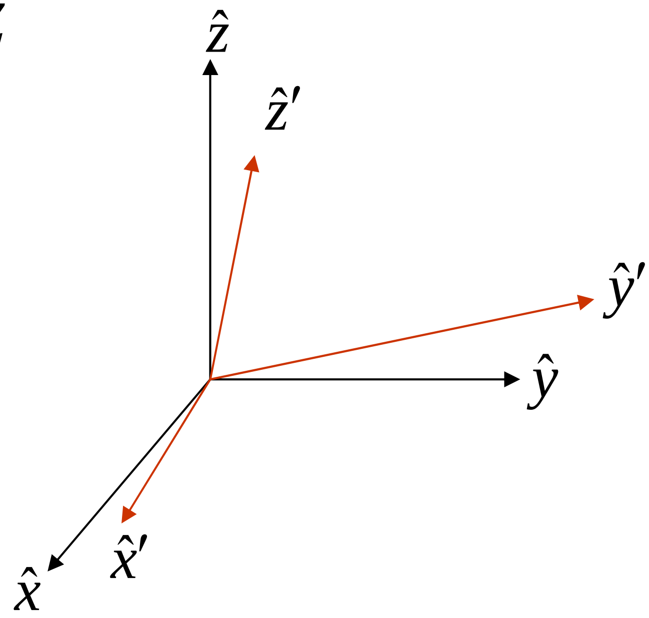
Strain

A distortion of a material is described by the strain matrix

$$x' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$

$$y' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$

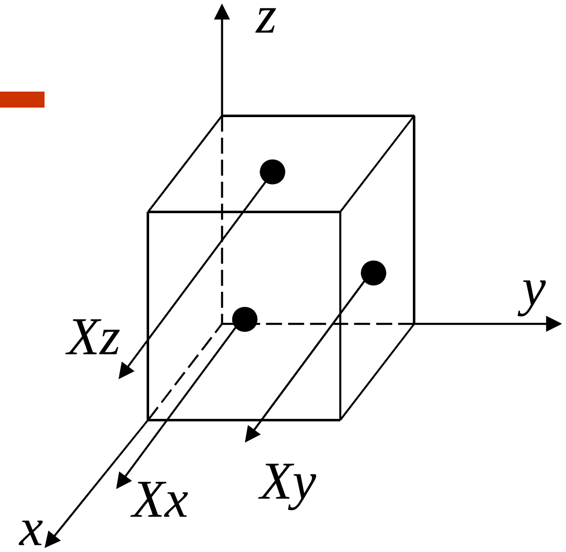
$$z' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$



Stress

9 forces describe the stress

Xx, Xy, Xz, Yx, Yy, Yz, Zx, Zy, Zz



Xx is a force applied in the *x*-direction to the plane normal to *x*

Xy is a sheer force applied in the *x*-direction to the plane normal to *y*

stress tensor:

$$\sigma = \begin{bmatrix} \frac{X_x}{A_x} & \frac{X_y}{A_y} & \frac{X_z}{A_z} \\ \frac{Y_x}{A_x} & \frac{Y_y}{A_y} & \frac{Y_z}{A_z} \\ \frac{Z_x}{A_x} & \frac{Z_y}{A_y} & \frac{Z_z}{A_z} \end{bmatrix}$$

Stress is force/m^2

Stress and Strain

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$$

The stress - strain relationship is described by a rank 4 stiffness tensor. The inverse of the stiffness tensor is the compliance tensor.

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

Einstein convention: sum over repeated indices.

$$\varepsilon_{xx} = s_{xxxx}\sigma_{xx} + s_{xxxy}\sigma_{xy} + s_{xxxz}\sigma_{xz} + s_{xxyx}\sigma_{yx} + s_{xxyy}\sigma_{yy}$$
$$+ s_{xxyz}\sigma_{yz} + s_{xxzx}\sigma_{zx} + s_{xxzy}\sigma_{zy} + s_{xxzz}\sigma_{zz}$$

Statistical Physics

Microcannonical Ensemble: Internal energy is expressed in terms of extrinsic quantities $U(S, M, P, \varepsilon, N)$.

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial U}{\partial P_k} dP_K + \frac{\partial U}{\partial M_l} dM_l$$

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

The normal modes must be solved for in the presence of electric and magnetic fields.