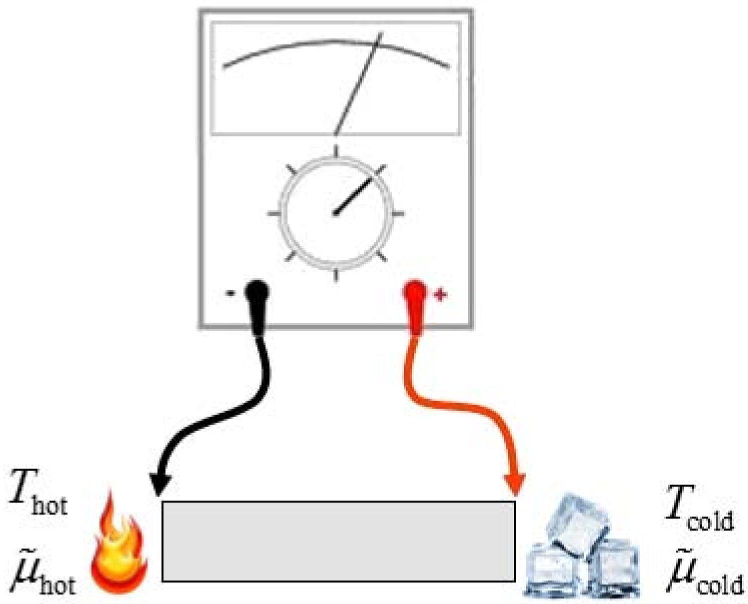
Transport

Seebeck effect

$$\nabla_{\vec{r}}\tilde{\mu} = -S\nabla_{\vec{r}}T$$



$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k$$

$$\vec{j}_{\text{elec}} = 0 \qquad \vec{B} = 0$$

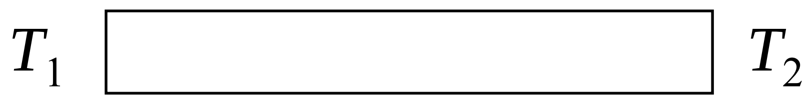
Seebeck effect

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu}+\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T\right)\right)d^3k.$$

$$\begin{bmatrix}\frac{\partial\tilde{\mu}}{\partial x}\\ \frac{\partial\tilde{\mu}}{\partial y}\\ \frac{\partial\tilde{\mu}}{\partial z}\end{bmatrix} = -\begin{bmatrix}S_{xx} & S_{xy} & S_{xz}\\ S_{yx} & S_{yy} & S_{yz}\\ S_{zx} & S_{zy} & S_{zz}\end{bmatrix}\begin{bmatrix}\frac{\partial T}{\partial x}\\ \frac{\partial T}{\partial y}\\ \frac{\partial T}{\partial z}\end{bmatrix}$$

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_i\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\begin{pmatrix}-S_{xj}\\ -S_{yj}\\ -S_{zj}\end{pmatrix}+\frac{E(\vec{k})-\mu}{T}\hat{e}_j\right)\right)d^3k$$

Thermal conductivity again



Open boundary conditions

A heat current will also flow in this case. The expression for the heat current is,

$$\vec{j}_Q = -\frac{1}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\left(E(\vec{k})-\mu\right)\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu}+\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T\right)\right)d^3k.$$

In this experiment, the electrochemical potential and the temperature gradient are related by $\nabla_{\vec{r}}\tilde{\mu} = -S\nabla_{\vec{r}}T$ so this is inserted into the expression for the heat current.

$$\vec{j}_Q = -\frac{1}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\left(E(\vec{k})-\mu\right)\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(-S\nabla_{\vec{r}}T+\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T\right)\right)d^3k.$$

The thermal conductivity in this case is,

$$K_{ij} = -\frac{1}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\left(E(\vec{k})-\mu\right)\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_i\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(-S\hat{e}_j+\frac{E(\vec{k})-\mu}{T}\hat{e}_j\right)\right)d^3k.$$

new term

Thermoelectric effects

Seebeck effect:
A thermal gradient causes a thermal current to flow. This results in a voltage which sends the low entropy charge carriers back to the hot end.

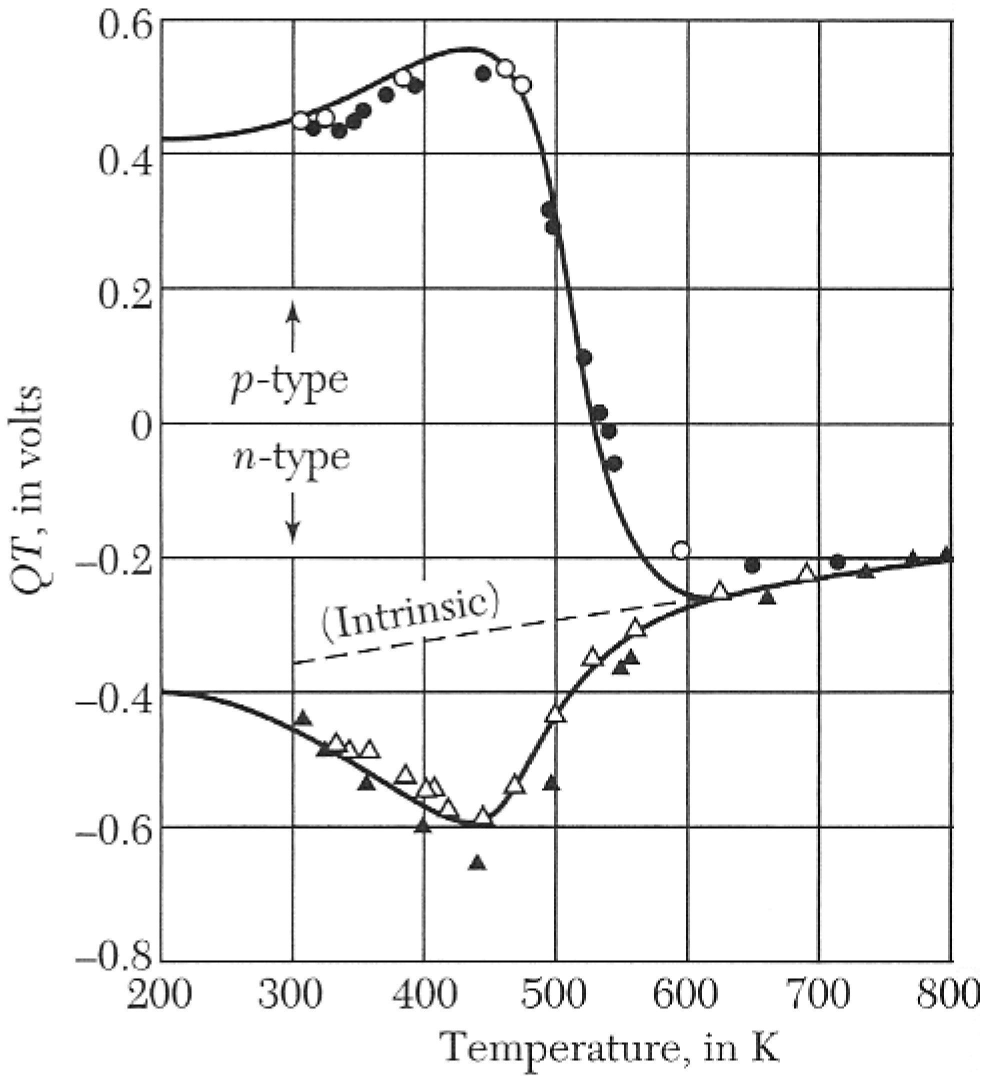
$$\nabla \tilde{\mu} = -S \nabla T$$

S is the absolute thermal power (often also called Q). The sign of the voltage (electrochemical potential, electromotive force) is the same as the sign of the charge carriers.

The Seebeck effect can be used to make a thermometer. The gradient of the temperature is the same along both wires but the gradient in electrochemical potential differs.

Thermocouple

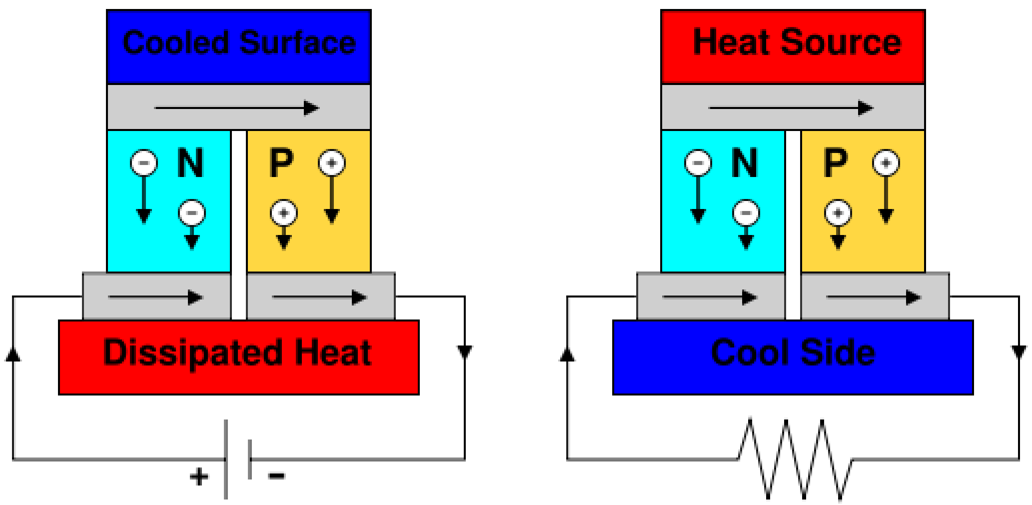
Thermoelectric effects



Intrinsic Q is negative because electrons have a higher mobility.

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.

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

Hall effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

$$\nabla_{\vec{r}}T = 0$$

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k$$

$$R_{lmn} = \frac{\nabla_{\vec{r}}\tilde{\mu}_l}{e j_m B_n}.$$

$$R_{lmn} = \left[\frac{e^2}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_m\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\hat{e}_l + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\hat{e}_n\right)\right)d^3k\right]^{-1}$$

Nerst effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

$$\vec{j}_{\text{elec}} = 0$$

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

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

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_i\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\begin{pmatrix} eN_{xyz} \\ eN_{yyz} \\ eN_{zzz}\end{pmatrix} + \frac{E(\vec{k})-\mu}{T}\hat{y} + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\hat{z}\right)\right)d^3k.$$

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.

Ettingshausen effect

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

The sample is electrically grounded so $\nabla_{\vec{r}}\tilde{\mu} = 0$.

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

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

Probability current in 1-D

The normalized probability current density:

$$S = \frac{-i\hbar}{2m} \frac{\psi^* \dfrac{d\psi}{dx} - \psi \dfrac{d\psi^*}{dx}}{\int_0^L \psi^* \psi \, dx}$$

$$j = -eS = -nev$$

$$n = \frac{1}{Na}$$

$$v = NaS$$

$$v_k = -v_{-k} = \frac{-i\hbar a}{2m} \frac{\psi^* \dfrac{d\psi}{dx} - \psi \dfrac{d\psi^*}{dx}}{\int_0^a \psi^* \psi \, dx}$$

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,

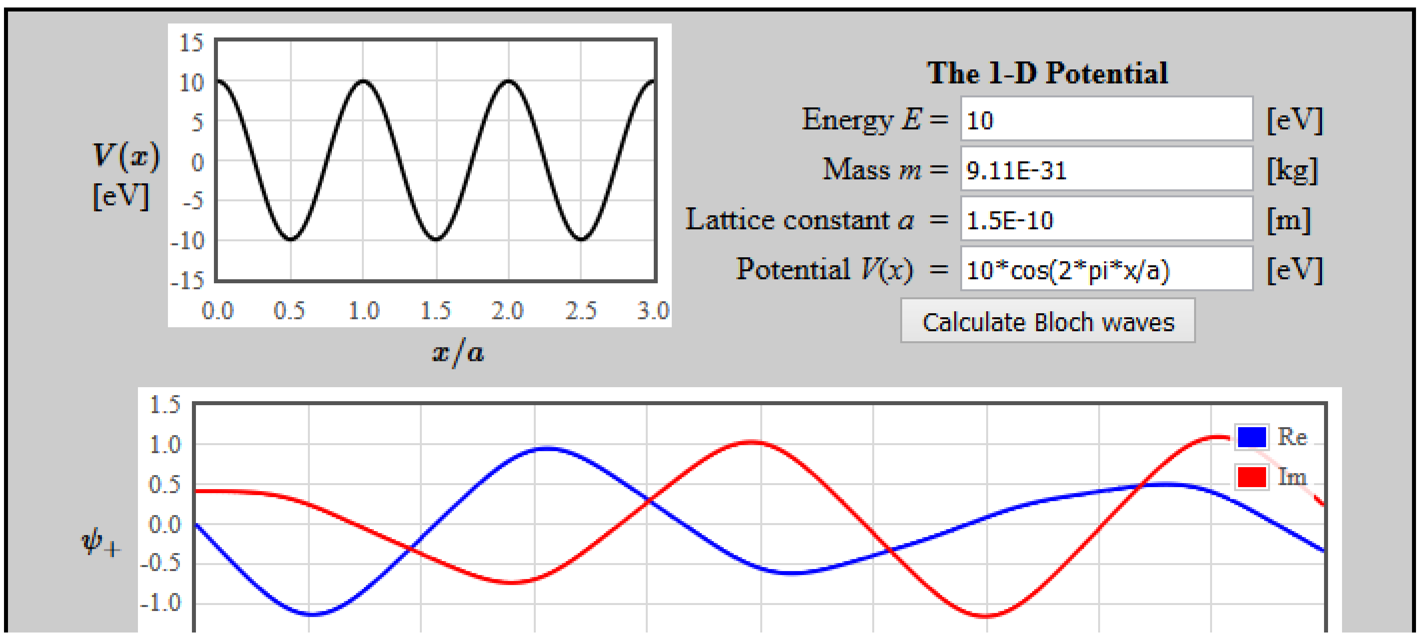
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \tag{1}$$

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,

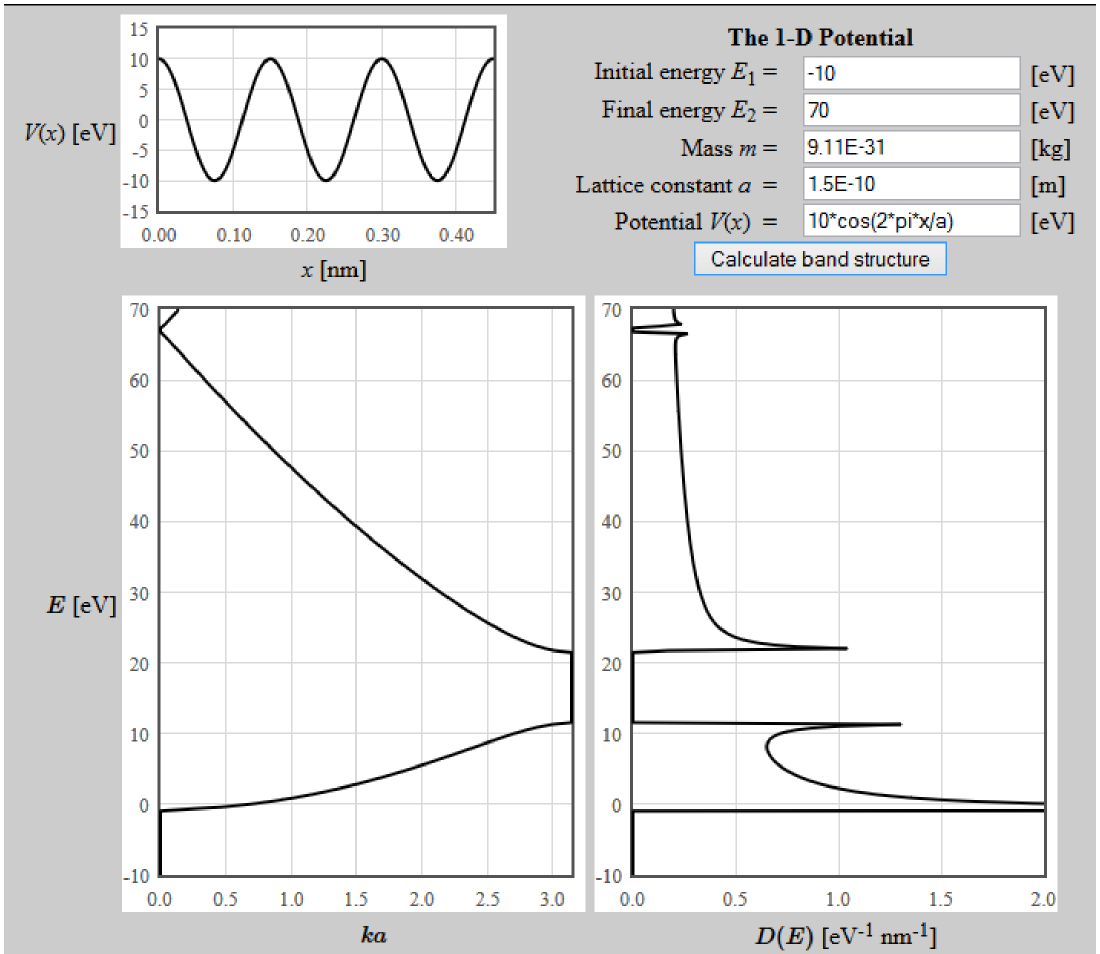
$$\psi = e^{ikx}u_k(x). \tag{2}$$

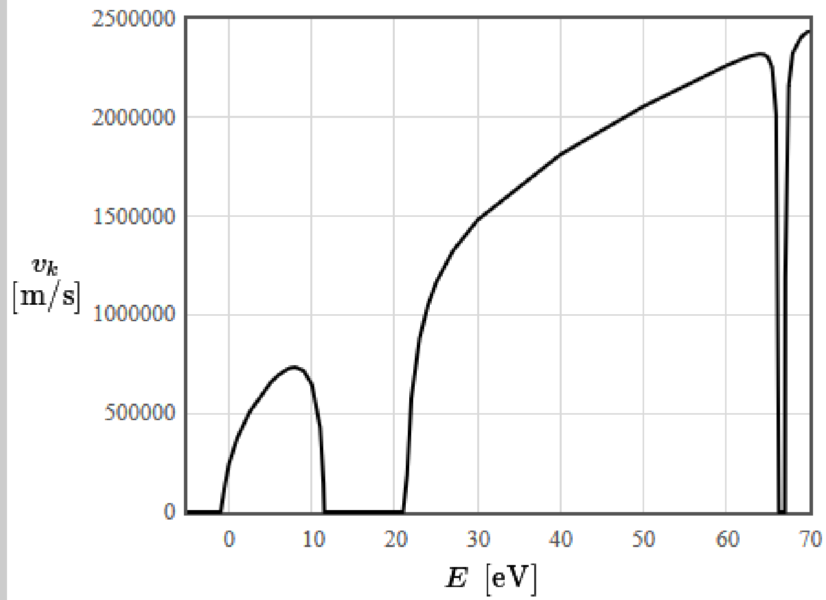
where k is the wavenumber and $u_k(x)$ is a periodic function with periodicity a.

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.



Velocity of *k*-states





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

Student Projects

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

Numerically calculate a transport property for a one dimensional material.