

# Probability current in 1-D

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The normalized probability current density:

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

$$j = -eS = -nev$$

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

$$v = NaS$$

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

## 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,

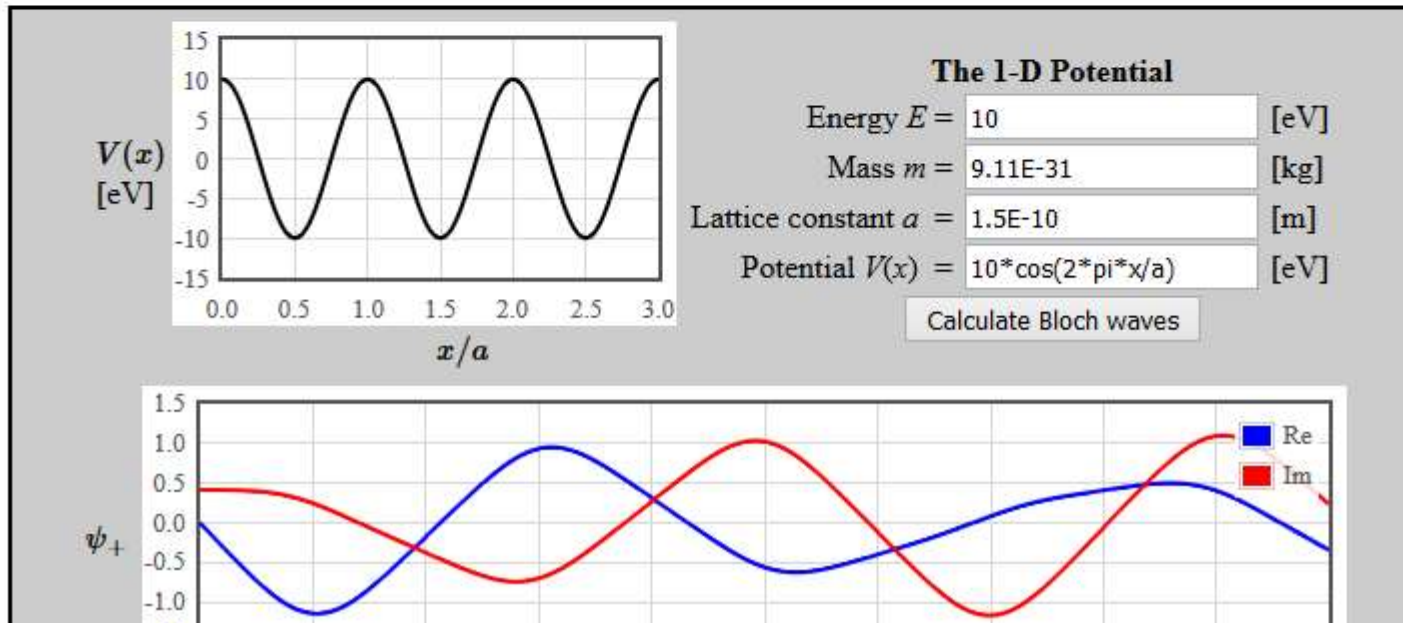
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \quad (1)$$

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,

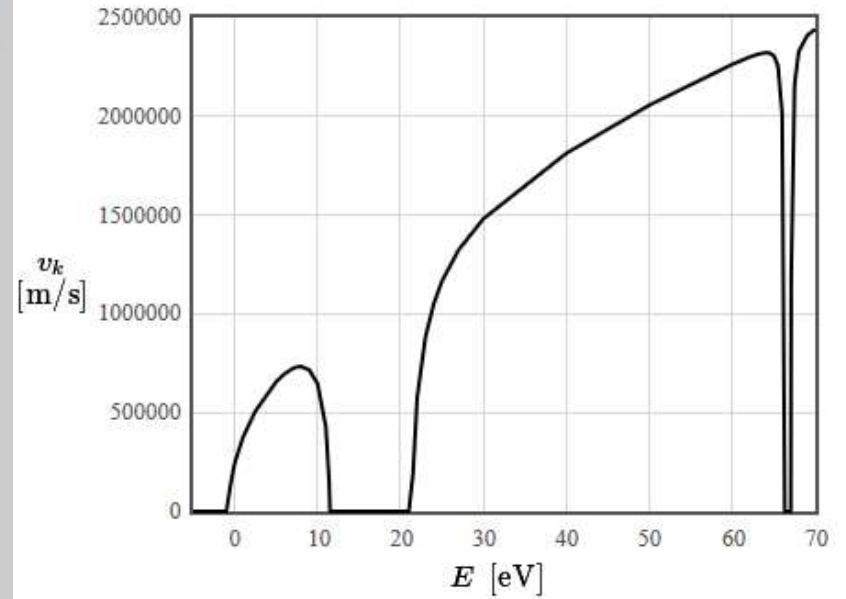
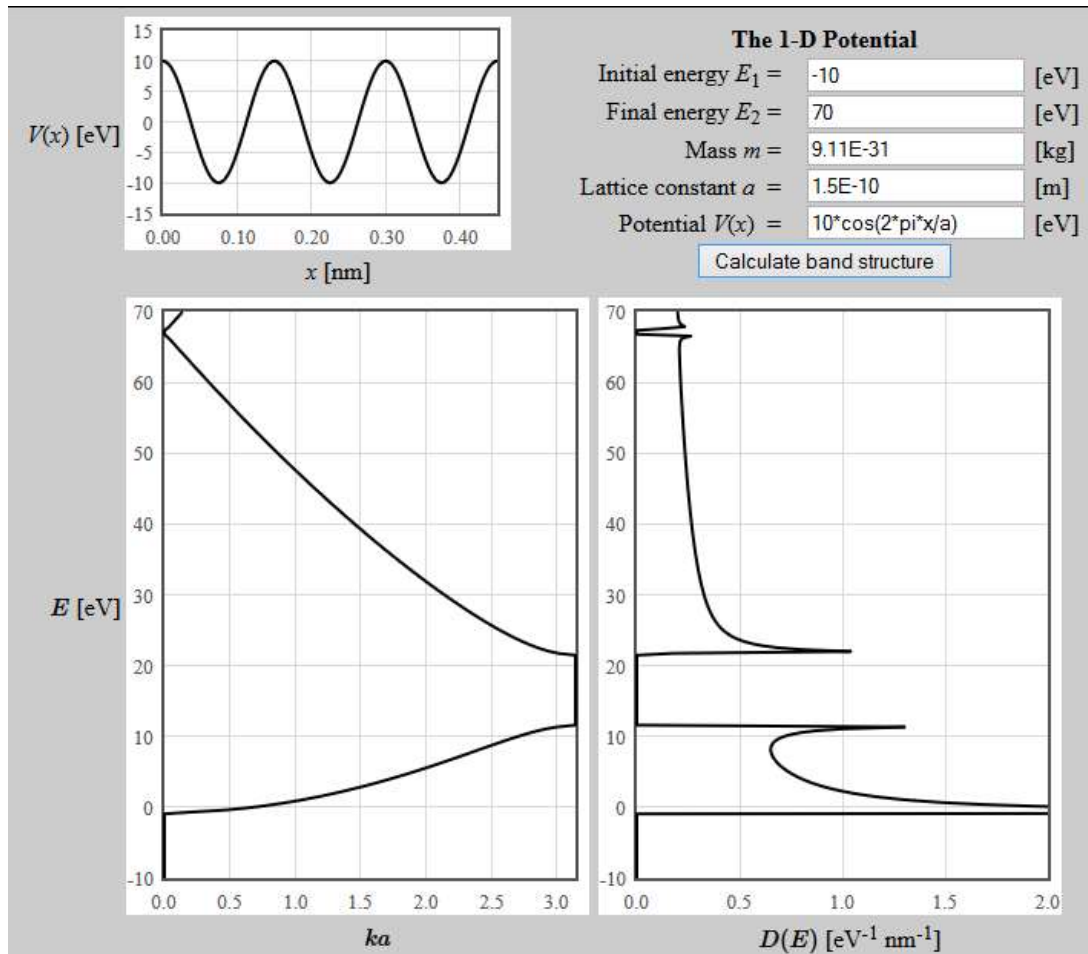
$$\psi = e^{ikx} u_k(x). \quad (2)$$

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



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

# Electrical current

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In the Drude model, the current density is,

$$\vec{j}_{elec} = -en\vec{v}_d$$

$n$  is the electron density, and  $\vec{v}_d$  is the drift velocity (the average velocity of the electrons)

To calculate the current density from the microscopic states:

$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

velocity of electron state  $k$       density of states      probability that the state  $k$  is occupied

$D(|\vec{k}|) \neq D(\vec{k}) = \frac{2}{(2\pi)^3}$       spin

# Boltzmann equation (see Kittel appendix F)

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There is a function  $f(\vec{k}, \vec{r}, t)$  that gives the probability that state  $k$  is occupied at position  $r$  and time  $t$ .

In equilibrium, for a uniform system,  $f$  is the Fermi function.

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$

Take the total derivative of  $f$ ,

$$\frac{df(\vec{k}, \vec{r}, t)}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial k_x} \frac{dk_x}{dt} + \frac{\partial f}{\partial k_y} \frac{dk_y}{dt} + \frac{\partial f}{\partial k_z} \frac{dk_z}{dt} + \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt}$$

# Boltzmann equation


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$$\frac{df(\vec{k}, \vec{r}, t)}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial k_x} \frac{dk_x}{dt} + \frac{\partial f}{\partial k_y} \frac{dk_y}{dt} + \frac{\partial f}{\partial k_z} \frac{dk_z}{dt} + \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt}$$

Liouville theorem:  $\frac{df(\vec{k}, \vec{r}, t)}{dt} = 0$

$$\hbar \frac{d\vec{k}}{dt} = \vec{F}_{ext}$$

Boltzmann equation

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \left. \frac{\partial f}{\partial t} \right|_{collisions}$$


Collision term describes the transitions between  $k$  states.

# Relaxation time approximation

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$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \left. \frac{\partial f}{\partial t} \right|_{collisions}$$

In the relaxation time approximation,

$$\left. \frac{\partial f}{\partial t} \right|_{collisions} = \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

If the driving field is turned off, the collision term will drive the system back to equilibrium in time  $\tau$ .

When  $\nabla_k f = \nabla f = 0$  and the initial condition is  $f = f_1$ , the solution to the Boltzmann equation is,

$$f(t) = f_0 + f_1 e^{-t/\tau}$$

# Boltzmann equation: relaxation time approx.

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In the relaxation time approximation.

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

in a stationary state  $\frac{\partial f}{\partial t} = 0$

If the system is not far from equilibrium,  $f \approx f_0$ , and we can substitute  $f_0$  for  $f$  on the right

$$f(\vec{k}) = f_0(\vec{k}) + \frac{\tau(\vec{k}) \vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k}) \vec{v} \cdot \nabla f_0$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$



# Boltzmann equation: relaxation time approx.

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$$f(\vec{k}) \approx f_0(\vec{k}) + \frac{\tau(\vec{k})\vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k})\vec{v} \cdot \nabla f_0$$

$$\nabla f_0 = \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu$$

$$\vec{F}_{ext} = -e(\vec{E} + \vec{v} \times \vec{B})$$

Temperature and chemical potential  
can depend on position

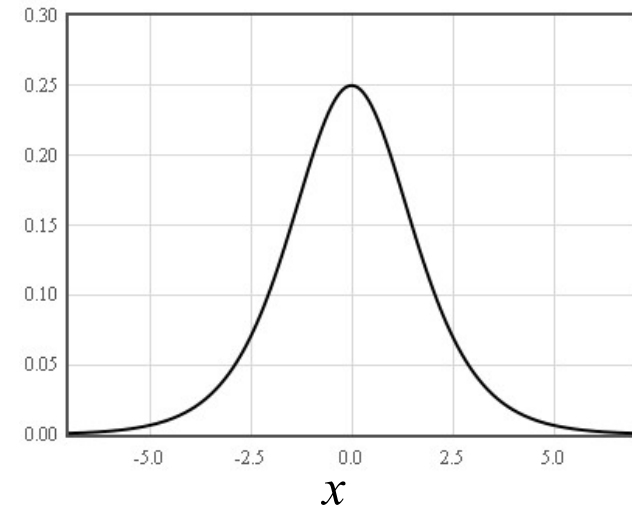
$$f(\vec{k}) \approx f_0(\vec{k}) + \frac{\tau(\vec{k})(-e)(\vec{v} \times \vec{B} + \vec{E}) \cdot \nabla_k f_0}{\hbar} + \tau(\vec{k})\vec{v} \cdot \left( \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu \right)$$

Temperature gradient

Concentration gradient

# Boltzmann equation: relaxation time approx.

$$\frac{\partial f_0}{\partial \mu} = \frac{\frac{1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \quad \frac{\exp(x)}{(\exp(x) + 1)^2}$$



$$\begin{aligned} \nabla_k f_0 &= \frac{\frac{-1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \nabla_k E(\vec{k}) \\ &= -\frac{\partial f_0}{\partial \mu} \nabla_k E(\vec{k}) \end{aligned}$$

$$\begin{aligned} \frac{\partial f_0}{\partial T} &= \frac{\frac{E(\vec{k}) - \mu}{k_B T^2} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \\ &= \frac{\partial f_0}{\partial \mu} \frac{E(\vec{k}) - \mu}{T} \end{aligned}$$

Only the states near the Fermi surface contribute.

# Boltzmann equation: relaxation time approx.

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$$f(\vec{k}) \approx f_0(\vec{k}) + \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} (\vec{v}(\vec{k}) \times \vec{B} + \vec{E}) \cdot \nabla_k E(\vec{k}) + \vec{v}(\vec{k}) \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right)$$

$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

The contribution of  $f_0(k)$  is zero

density of states

$$D(\vec{k}) = \frac{2}{(2\pi)^3} \longleftarrow \text{spin}$$

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