

# 22. Transport

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# Transport phenomena

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Bloch waves

Crystal momentum

Group velocity

Boltzmann equation

Electrical conductivity

Thermal conductivity

Hall effect

Peltier effect

Seebeck effect

Ettingshausen effect

Nerst effect

- **Transport**

- Thermoelectric effects
- Crystal momentum
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- Relaxation time approximation
- Current densities
- Electrochemical potential
- Electrical conductivity
- Thermoelectric currents
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- Hall effect
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# Bloch waves

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Any wave function:  $\psi(\vec{r}) = \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$

$$\psi(\vec{r}) = \sum_{\vec{k} \in 1\text{BZ}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

Bloch wave:  $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

$$\psi(\vec{r}) = \sum_{\vec{k} \in 1\text{BZ}} \psi_{\vec{k}}(\vec{r})$$

$$\mathbf{T}\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot(\vec{r}+\vec{a})} u_{\vec{k}}(\vec{r} + \vec{a}) = e^{i\vec{k}\cdot\vec{a}} e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{a}} \psi_{\vec{k}}(\vec{r})$$

Bloch waves are eigenfunctions of the Hamiltonian

## Bloch waves in 1-D

It is instructive to consider a one-dimensional crystal at this point since the dispersion relation  $E(\vec{k})$  can be readily calculated numerically in one-dimension. 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,

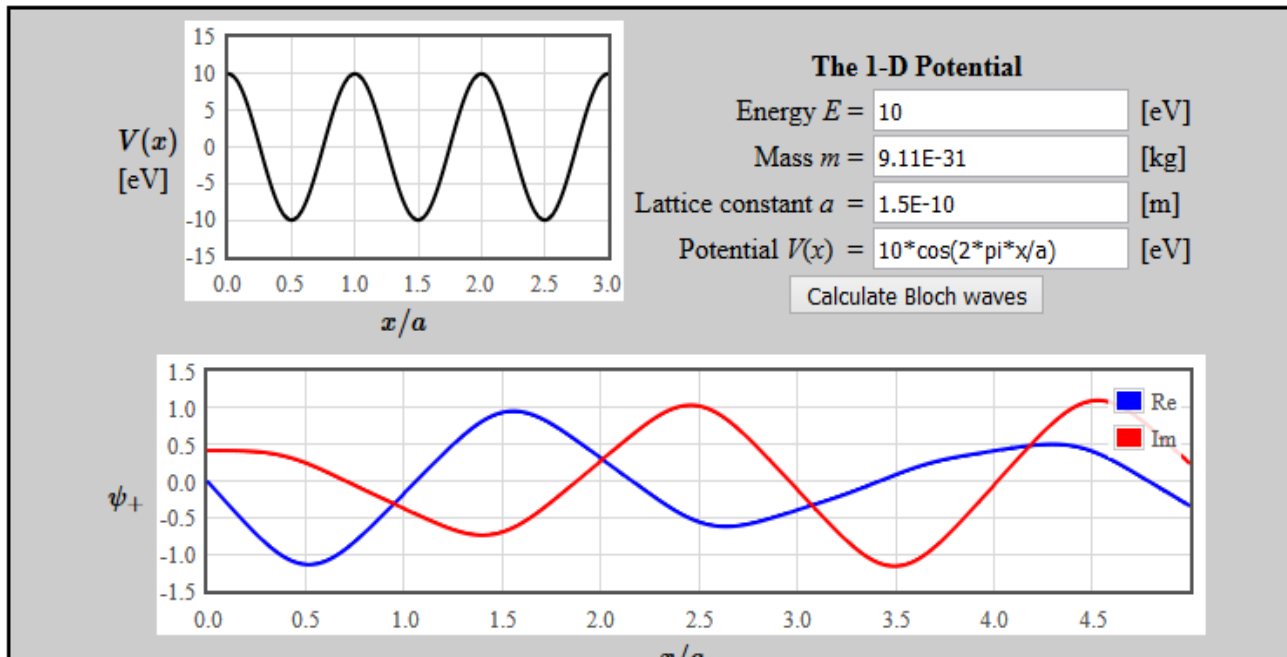
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

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,

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

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.



# Crystal momentum $\hbar\vec{k}$

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Ehrenfest theorem: 
$$i\hbar\frac{d}{dt}\langle\mathbf{A}\rangle = \langle[\mathbf{A}, \mathbf{H}]\rangle$$

translation operator 
$$T\psi(\vec{r}) = \psi(\vec{r} + \vec{a})T$$

$\langle T \rangle$  is a constant of motion  
for a perfect crystal 
$$i\hbar\frac{d}{dt}\langle\mathbf{T}\rangle = \langle[\mathbf{T}, \mathbf{H}_0]\rangle = 0.$$

Consider an external force 
$$\vec{F} = -\nabla U \quad U = -F_x x - F_y y - F_z z$$

$$i\hbar\frac{d}{dt}\langle\mathbf{T}\rangle = \langle[\mathbf{T}, \mathbf{H}_0 - F_x x - F_y y - F_z z]\rangle.$$

Since  $[\mathbf{T}, \mathbf{H}_0] = [\mathbf{H}_0, \mathbf{T}] = 0$ , this is,

$$i\hbar\frac{d}{dt}\langle\mathbf{T}\rangle = \langle-\mathbf{T}(F_x x + F_y y + F_z z) + (F_x x + F_y y + F_z z)\mathbf{T}\rangle$$

# Crystal momentum

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$$i\hbar \frac{d}{dt} \langle \mathbf{T} \rangle = \langle -\mathbf{T}(F_x x + F_y y + F_z z) + (F_x x + F_y y + F_z z)\mathbf{T} \rangle.$$

Allow  $\mathbf{T}$  to act on  $(F_x x + F_y y + F_z z)$ ,

$$\begin{aligned} i\hbar \frac{d}{dt} \langle \mathbf{T} \rangle &= \langle -(F_x(x + a_x) + F_y(y + a_y) + F_z(z + a_z))\mathbf{T} + (F_x x + F_y y + F_z z)\mathbf{T} \rangle \\ &= \langle -(F_x a_x + F_y a_y + F_z a_z)\mathbf{T} \rangle \end{aligned}$$

Here  $a_x, a_y, a_z$  are integer steps in the periodic lattice. As  $(F_x a_x + F_y a_y + F_z a_z)$  is a constant,

$$i\hbar \frac{d}{dt} \langle \mathbf{T} \rangle = -(F_x a_x + F_y a_y + F_z a_z) \langle \mathbf{T} \rangle.$$

# Crystal momentum

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$$i\hbar \frac{d}{dt} \langle \mathbf{T} \rangle = -(F_x a_x + F_y a_y + F_z a_z) \langle \mathbf{T} \rangle.$$

For a Bloch wave  $\langle \mathbf{T} \rangle = \langle e^{-i\vec{k}\cdot\vec{r}} u_{\vec{k}}^* | \mathbf{T} | e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}} \rangle = e^{i\vec{k}\cdot\vec{a}} \langle e^{-i\vec{k}\cdot\vec{r}} u_{\vec{k}}^* | e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}} \rangle = e^{i\vec{k}\cdot\vec{a}},$

$$i\hbar \frac{d}{dt} e^{i\vec{k}\cdot\vec{a}} = -(F_x a_x + F_y a_y + F_z a_z) e^{i\vec{k}\cdot\vec{a}}.$$

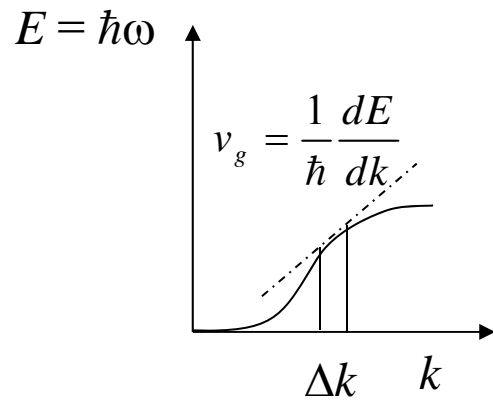
The external force will cause the momentum of the electron to change so  $\vec{k}$  will be time dependent. Performing the differentiation with respect to time,

$$-\hbar \left( \frac{dk_x}{dt} a_x + \frac{dk_y}{dt} a_y + \frac{dk_z}{dt} a_z \right) e^{i\vec{k}\cdot\vec{a}} = -(F_x a_x + F_y a_y + F_z a_z) e^{i\vec{k}\cdot\vec{a}}.$$

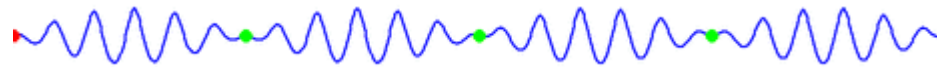
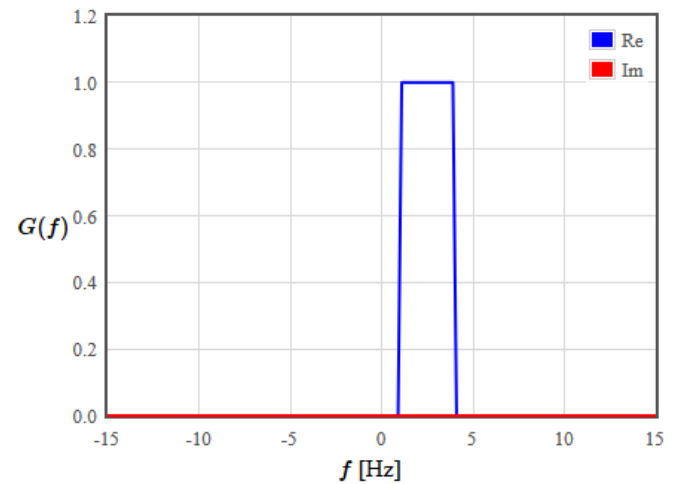
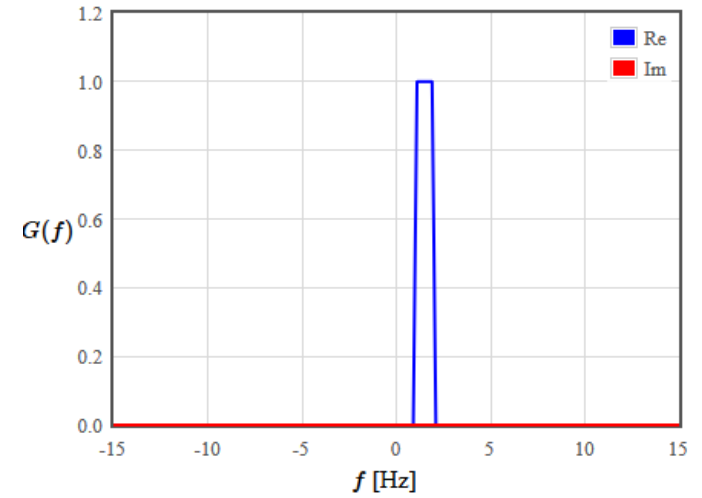
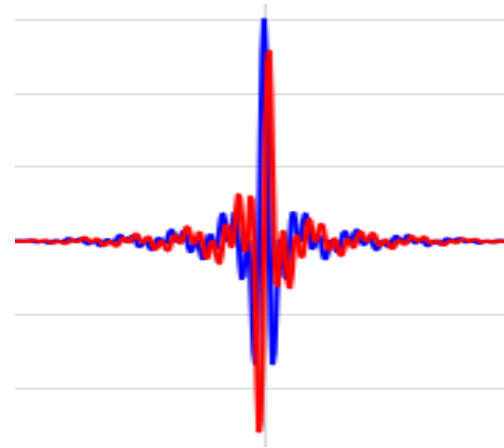
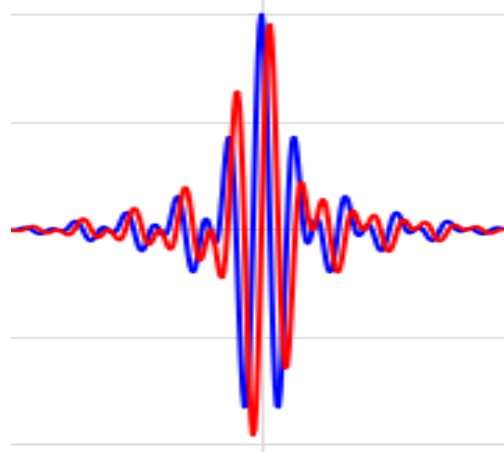
$$\hbar \frac{d\vec{k}}{dt} = \vec{F}_{\text{ext}}.$$



# Group velocity

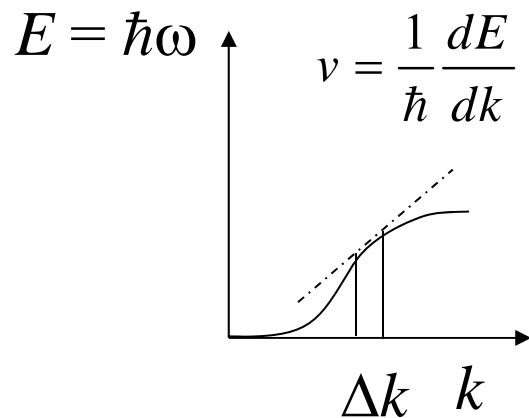


$v_g$  is the velocity of a wave packet  
 $\Delta x \Delta k \sim 1$



[https://en.wikipedia.org/wiki/Phase\\_velocity](https://en.wikipedia.org/wiki/Phase_velocity)

# Group velocity



$$\vec{v}_g = \frac{1}{\hbar} \nabla_{\vec{k}} E$$

$$\frac{d\vec{v}_g}{dt} = \frac{1}{\hbar} \left( \frac{d^2 E}{dk_x dt} \hat{k}_x + \frac{d^2 E}{dk_y dt} \hat{k}_y + \frac{d^2 E}{dk_z dt} \hat{k}_z \right) = \frac{1}{\hbar} \nabla_{\vec{k}}^2 E \frac{d\vec{k}}{dt}$$

$$\frac{d\vec{v}_g}{dt} = \frac{1}{\hbar^2} \nabla_{\vec{k}}^2 E \vec{F}_{ext}$$

$v_g$  is the velocity of a wave packet

$$\Delta x \Delta k \sim 1$$

$$\vec{F}_{ext} = \frac{\hbar^2}{\nabla_{\vec{k}}^2 E(\vec{k})} \frac{d\vec{v}_g}{dt} = m^*(\vec{k}) \vec{a}_g$$

Particles in a semiconductor can be thought of as free particles with an effective mass.

# Wave/particle nature of electrons

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Usually when we think about a current flowing, we imagine the electrons as particles moving along. Really we should be thinking about how the occupation of the wave like eigenstates are changing.

When wave packets are built from the eigenstates, they move like particles with an effective mass.