Mohor dB electrons within lattices

In general, an electron in the Bloch state with energy $E_n(k)$ has expectation value of velocity:

$$\langle \vec{v} \rangle = \frac{1}{\hbar} \nabla_k E_n(k)$$

where

$$\nabla_k E = \frac{\partial E}{\partial k_x} \hat{x} + \frac{\partial E}{\partial k_y} \hat{y} + \frac{\partial E}{\partial k_z} \hat{z}$$

and this can be used to determine current density

$$\vec{J} = \frac{1}{V} \sum (-e) \langle \vec{v} \rangle$$

all electron states.

This has the consequence that completely filled bands do not contribute to electrical conduction. Thus insulators have bands which are entirely full or else completely empty. Recall that the number of $E$ values in the Brillouin zone is exactly equal to the number of primitive lattice sites, $N$. Thus the number of electron states in one band is $2N$. In monatomic crystals, the primitive cells contain one atom. If this atom has an odd number of electrons, then at least one band is partially filled. Thus atoms in the first column of the periodic table do not form insulators.
Motion of electrons in electric + magnetic fields

Consider an electron in a periodic lattice subject to external fields.

\[ \text{ion} \quad \text{ion} \]
\[ \text{electron} \]

In general the electron interacts with the lattice via electric + magnetic fields provided by the lattice, \( \hat{E}_{\text{lattice}} \) and \( \hat{B}_{\text{lattice}} \). Suppose that additional magnetic fields are provided by external objects. Denote these \( \hat{E}_{\text{ext}} \) and \( \hat{B}_{\text{ext}} \).

The total electric + magnetic fields are:

\[ \hat{E}_{\text{total}} = \hat{E}_{\text{lattice}} + \hat{E}_{\text{ext}} \]

etc.,... However, the framework of Bloch states accounts for the lattice fields, and we now ask about the effects of the external fields on the electron in these Bloch states.

An argument due to Ashcroft + Mermin suggests the general rule:

\[ \hbar \frac{d\hat{p}}{dt} = -e \left[ \hat{E}_{\text{ext}} + \langle \hat{\nabla} \rangle \times \hat{B}_{\text{ext}} \right] \]

and a simple version when \( \hat{B} = 0 \) appears in Omori. Note that this is identical to the classical rule:

\[ \frac{dp}{dt} = -e \left[ \hat{E}_{\text{ext}} + \hat{\nabla} \times \hat{B}_{\text{ext}} \right] \]

provided that

\[ \hat{p} = \hbar \hat{\mathbf{r}}. \]
We may be inclined to say that $\vec{p}$ is the electron momentum but (2) only includes the external fields and not the lattice fields. Thus it is not the total momentum of the electron. However, it is known as the crystal momentum.

Electron in an external electric field. (one dimension)

Suppose that $\vec{B}_{\text{ext}} = 0$. Thus:

$$\frac{i}{\hbar} \frac{d\vec{p}}{dt} = -e \vec{E}_{\text{ext}}.$$

Now

$$\langle \frac{dE}{dk} \rangle = \frac{1}{T} \frac{dE}{dk}.$$

$$\Rightarrow \langle \alpha \rangle = \frac{d\langle v \rangle}{dt} = \frac{1}{T} \frac{dt}{d\alpha} \frac{dE}{dk}$$

$$= \frac{1}{\hbar} \langle \frac{-e}{k} \rangle \vec{E}_{\text{ext}} \frac{dE}{dk^2}.$$

which implies that

$$\langle \alpha \rangle \frac{\hbar}{\alpha} \frac{d^2E}{dk^2} = -e \vec{E}_{\text{ext}}.$$

corresponding to a particle with effective mass

$$M^* = \frac{\hbar^2}{d^2E}$$
Example: NFE bottom of band.

Consider the case where an electron occupies a state at the bottom of a band. Then

\[ E = \text{const} + \frac{\hbar^2}{2m'} \alpha k^2 \]

where \( \alpha = 1 + \frac{4E_{p}}{E_{g}} \) energy at bottom / \( E_{g} \) gap.

Thus the effective mass is:

\[ M* = \frac{\hbar^2}{2m'} \alpha = \frac{M}{\alpha}. \]

At the top of a band we get:

\[ E = \text{const} - \frac{\hbar^2}{2m'} \alpha k^2 \]

\[ \Rightarrow m^* = \frac{M}{\alpha}. \]

These are masses which including the effects of the periodic lattice potential. They are not the mass of an isolated electron, but in a crystal we cannot isolate the electron; we can only probe it with external fields. The internal interactions between the crystal and lattice will always affect the apparent mass.

\begin{align*}
\text{Free:} & \quad \text{measure mass via } E \frac{\partial}{\partial \theta} \\
\text{field dynamics} & \quad \Rightarrow M_0 \\
\text{Crystal:} & \quad \text{measure via } E \frac{\partial}{\partial \theta} \\
\text{field dynamics} & \quad m^* \end{align*}