Momentum and effective mass

What is the physical significance of $k$?

Free space has continuous translational invariance. It can be shown this leads to conservation of momentum.

For free electrons: $\psi_k(\hat{r}) = e^{i\hat{k} \cdot \hat{r}}$

$\hbar \hat{k}$ is momentum.

But in a crystal, momentum is not strictly conserved. Coherent Bragg scattering with the crystal lattice occurs --> any $\hat{G}$ can be added or subtracted to $k$.

Recall the Bloch functions: $\psi_k(\hat{r})$

Consider some scattering process involving a photon or phonon with wavevector $\hat{k}$

The space part of the matrix element has the form:

$$\int \psi_{k'}^*(\hat{r}) e^{i\hat{k'} \cdot \hat{r}} \psi_k(\hat{r}) d^3r$$

$$= \int U_{k'}^*(\hat{r}) U_k(\hat{r}) e^{i(\hat{k'} + \hat{k} - \hat{k}) \cdot \hat{r}} d^3r$$

Now the $U_k$ functions are periodic:

$$U_k(\hat{r}) = \sum_G C(k - G) e^{i\hat{G} \cdot \hat{r}}$$

so the integral vanishes unless:

$$\text{for some } \hat{G}$$

This is the modified conservation law for crystal momentum, $\hbar \hat{k}$.
i.e., $\hbar \mathbf{k}$, the crystal momentum, is conserved modulo any reciprocal lattice vector, $\mathbf{G}$. How about the good old momentum operator: $\hat{p} = -i\hbar \hat{\nabla}$?

**proof**

Take S-eqn:

$$\langle \Psi_k | \nabla_k (H - E) | \Psi_k \rangle = 0$$

Note that:

Using the chain rule:

$$\nabla_k (H - E) | \Psi_k \rangle = -(\nabla_k E | \Psi_k \rangle + (H - E) \nabla_k | \Psi_k \rangle$$

so,

$$-\nabla_k E | \Psi_k \rangle + \langle \Psi_k | (H - E) \nabla_k | \Psi_k \rangle = 0 \quad (1)$$

Also, we can write:

$$\nabla_k | \Psi_k \rangle = \nabla_k U_k \mathbf{e}^{i \mathbf{k} \cdot \mathbf{\hat{r}}} = i \mathbf{\hat{r}} U_k \mathbf{e}^{i \mathbf{k} \cdot \mathbf{\hat{r}}} + \mathbf{e}^{i \mathbf{k} \cdot \mathbf{\hat{r}}} \nabla U_k \quad (2)$$

Then:

$$\langle H - E | i \mathbf{k} \cdot \mathbf{\hat{r}} | \Psi_k \rangle = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V - E \right] i \mathbf{k} \cdot \mathbf{\hat{r}} | \Psi_k \rangle$$

$$= \left[ -\frac{\hbar^2}{2m} \nabla \cdot \nabla | \Psi_k \rangle \right] + \left[ \frac{\hbar^2}{2m} | \nabla | \Psi_k \rangle + i | \Psi_k \rangle \right]$$

$$= \left[ \frac{\hbar^2}{2m} \left[ i \mathbf{\hat{r}} \nabla | \Psi_k \rangle + i \nabla | \Psi_k \rangle + i \nabla | \Psi_k \rangle \right] \right]$$
Combining:

\[(H - E)i\hbar \Psi_k = \imath \hbar (H - E)\Psi_k - \frac{\hbar^2}{m} \nabla \Psi_k\]

\[\implies (H - E)i\hbar \Psi_k = -\frac{\hbar^2}{m} \nabla \Psi_k\]  \hspace{1cm} (3)

From (1):

\[\nabla_k E = \langle \Psi_k | (H - E) \nabla_k | \Psi_k \rangle\]

insert (2), (3)

\[\nabla_k E = \langle \Psi_k | (H - E) \nabla_k | \Psi_k \rangle - \frac{\hbar^2}{m} \nabla \Psi_k = \langle \Psi_k | (H - E) \nabla_k | \Psi_k \rangle e^{ik \cdot \mathbf{r}_k} \equiv 0\]

by hermiticity of \(H\)

Finally, since \(\langle \Psi_k | \partial | \Psi_k \rangle = -i\hbar \langle \Psi_k | \nabla | \Psi_k \rangle\):

This important relation connects the electron velocity to the bandstructure.

Now look at momentum in yet another way.

Apply a force \(\mathbf{F}\). The amount of work done is:

\[dE = \nabla_k E \cdot d\mathbf{k} = \hbar \mathbf{v} \cdot d\mathbf{k}\]

Newton’s law for crystal momentum:
What about \( \frac{d\mathbf{v}}{dt} \)?

\[
\frac{dv_j}{dt} = \frac{d(1 \partial E)}{dt} = \frac{1}{\hbar^2} \sum_{i} \frac{\partial}{\partial k_i} \left( \frac{\partial E}{\partial k_j} \right) \frac{dk_i}{dt}
\]

\[
= \frac{1}{\hbar^2} \sum_{i} \frac{\partial^2 E}{\partial k_i \partial k_j} F_i
\]

Define an “effective mass” tensor:

\[
\frac{1}{m^*_{ij}} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}
\]

For an isotropic band:
Holes

Filled valence band

negative $m^*$, missing electron $\xi_{me}$

\[
q_h = -q_e = e
\]

\[
m_h^* = -m_{me}^*
\]

\[
\tilde{\nu}_h = \tilde{\nu}_e
\]