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EE230 - Solid State Electronics *Prof. J. Bokor*

Momentum and effective mass

<u>What is the physical significance of *k*?</u>

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

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

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

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

Recall the Bloch functions:

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

The space part of the matrix element has the form:

$$\int \Psi^*_{k_f}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \Psi_{k_i}(\vec{r}) d^3r$$

$$= \int U^*_{k_f}(\vec{r}) U_{k_i}(\vec{r}) e^{i(\vec{k}_i + \vec{k} - k_f) \cdot \vec{r}} d^3r$$

Now the U_k functions are periodic:

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

so the integral vanishes unless:

for some $\vec{G}$

This is the modified conservation law for crystal momentum, $\hbar\vec{k}$.

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

<u>proof</u>

Take S-eqn:

Then:

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

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,

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

Also, we can write:

$$\nabla_k|\Psi_k\rangle = \nabla_k U_k e^{i\vec{k}\cdot\vec{r}} = i\vec{r}U_k e^{i\vec{k}\cdot\vec{r}} + e^{i\vec{k}\cdot\vec{r}}\nabla_k U_k \qquad (2)$$

Then:

$$(H-E)i\vec{r}|\Psi_k\rangle = \left[\underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{\downarrow} + V - E\right]i\vec{r}|\Psi_k\rangle$$

$$\frac{-\hbar^2}{2m}\vec{\nabla}\cdot\vec{\nabla}(i\vec{r})|\Psi_k\rangle$$

$$\frac{-\hbar^2}{2m}\vec{\nabla}\cdot[i\vec{r}\vec{\nabla}|\Psi_k\rangle + i|\Psi_k\rangle]$$

$$\frac{-\hbar^2}{2m}[i\vec{r}\nabla^2|\Psi_k\rangle + i\vec{\nabla}|\Psi_k\rangle + i\vec{\nabla}|\Psi_k\rangle]$$

Combining:

$$(H-E)i\vec{r}|\Psi_k\rangle = \cancelto{0}{i\vec{r}(H-E)|\Psi_k\rangle} - i\frac{\hbar^2}{m}\vec{\nabla}|\Psi_k\rangle$$

$$(H-E)i\vec{r}|\Psi_k\rangle = -i\frac{\hbar^2}{m}\vec{\nabla}|\Psi_k\rangle \qquad (3)$$

From (1):

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

insert (2), (3)

$$\nabla_k E = -i\frac{\hbar^2}{m}\langle\Psi_k|\vec{\nabla}|\Psi_k\rangle + \cancelto{0}{\langle\Psi_k|(H-E)e^{i\vec{k}\cdot\vec{r}}\vec{\nabla}|U_k\rangle}$$

by hermiticity of H

Finally, since $\langle\Psi_k|\vec{p}|\Psi_k\rangle = -i\hbar\langle\Psi_k|\vec{\nabla}|\Psi_k\rangle$:

This important relation connects the electron velocity to the bandstructure.

Now look at momentum in yet another way.

Apply a force $\vec{F}$. The amount of work done is:

also

$$dE = \vec{\nabla}_k E \cdot d\vec{k} = \hbar\vec{v}\cdot d\vec{k}$$

Newton’s law for <u>crystal</u> momentum:

What about $\frac{d\vec{v}}{dt}$?

$$\frac{dv_j}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial E}{\partial k_j}\right) = \frac{1}{\hbar}\sum_i \frac{\partial}{\partial k_i}\left(\frac{\partial E}{\partial k_j}\right)\frac{dk_i}{dt}$$

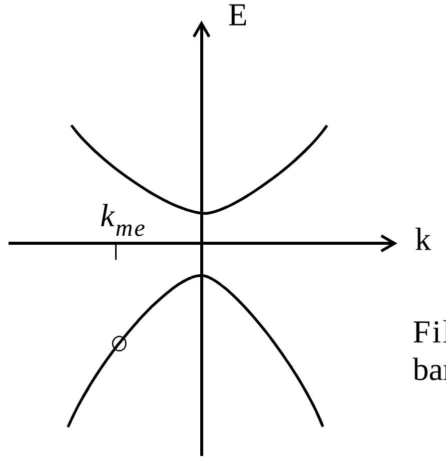
$$= \frac{1}{\hbar^2}\sum_i \frac{\partial^2 E}{\partial k_i \partial k_j} F_i$$

Define an “effective mass” tensor:

$$\frac{1}{m_{ij}^*} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

For an isotropic band:

<u>Holes</u>



Filled valence band

negative m*, missing electron $\vec{k}_{me}$

$$q_h = -q_e = e$$

$$m_h^* = -m_{me}^*$$

$$\vec{v}_h = \vec{v}_e$$