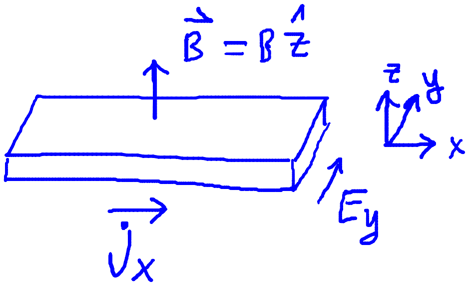
Lecture 12

Thursday, February 11, 2010

Now, we consider Hall effect for free electrons and electrons in a crystalline environment.

Hall Effect



In this experiment, a B field is applied perpendicular to the sample (a "Hall bar"), say the z axis, while a current is induced by an electric field along the x axis. As the charge carrier experiences the Lorentz force, it will acquire some momentary current along the y direction. In the steady state, the Hall bar will develop a charge accumulation at the edges and the corresponding electric field E_y. The Hall coefficient R_H is defined as

$$R_H = \frac{E_y}{j_x B}$$

Within the free electron model, it is straightforward to calculate R_H. As before, we use the semi-classical equation of motion (which we will prove couple of lectures later): $\vec{F} = \hbar\dot{\vec{k}}$ with $\vec{F} = -e\left(\vec{E} + \frac{1}{c}\vec{v}_{\vec{k}} \times \vec{B}\right)$. Here, $\vec{v}_{\vec{k}}$ is the group velocity at $\vec{k}$, i.e. $\hbar\vec{k}/m$ for the current theory. Defining the drift velocity $\vec{v}$ as before (i.e. as the average of $\vec{v}_{\vec{k}}$ over all electrons) we get

$$m\frac{d\vec{v}}{dt} = -e\left(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}\right)$$

where $\vec{v}$ is the drift velocity. Note the transition from $\vec{v}_{\vec{k}}$ ($\sim$ Fermi velocity) to $\vec{v}$ (a very tiny fraction of Fermi velocity). As before, we apply the relaxation time approximation, which can be implemented by making the substitution $\frac{d}{dt} \to \frac{d}{dt} + \frac{1}{\tau}$. This substitution can be best understood as considering $\vec{v}$ as being related to the probability that the electron distribution will survive without collision $P(t)$: $P(t)\left(1 - \frac{dt}{\tau}\right) = P(t + dt)$ and so $\frac{dP}{dt} = -\frac{P}{\tau}$. Thus, in the absence of an external force, $\frac{d\vec{v}}{dt} + \frac{\vec{v}}{\tau} = 0$. In the presence of an external force

$$\frac{d\vec{v}}{dt} + \frac{\vec{v}}{\tau} = \frac{\vec{F}}{m}$$

In the current problem, we have

$$\frac{d\vec{v}}{dt} + \frac{\vec{v}}{\tau} = -\frac{e}{m}\left(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}\right)$$

We look for a steady state solution ($\frac{d\vec{v}}{dt} = 0$) with $v_y = v_z = 0$, $\vec{B} = B\hat{z}$, and $E_z = 0$.

$$v_x = -\frac{\tau e}{m} E_x$$
$$v_y = 0 = -\frac{\tau e}{m}\ (E_y - \frac{1}{c} v_x B)$$

The first equation is what we already know. $j_x = -nev_x = \sigma E_x$, with $\sigma = \frac{ne^2\tau}{m}$. The second equation means: $\frac{E_y}{v_x B} = \frac{1}{c}$. Thus, $R_H = \frac{E_y}{j_x B} = -\frac{1}{nec}$.

$$R_H = -\frac{1}{nec}$$

This is the famous Hall coefficient (in the SI unit, $R_H = -\frac{1}{ne}$). The simplicity of this equation is the result of the simple model, the free electron model. While this theory is marvelously successful in many ways, it also comes short in important ways. According to this model, note that R_H is always negative. This is not true in general can be seen in Table 4. For instance, the Hall coefficient is positive for Be, Al, In, and As. It is also very large for Sb and Bi. All these anomalies need to be explained by the "band theory" which we will now explore. A more fundamental failure of the free electron theory is the inability to explain why certain substances such as Si, diamond or GaAs become insulators/semiconductors.

Bloch Theorem (Waves in crystal IV)

This is the fundamental theorem for waves in crystal, namely particles in crystal. The good news is that we already covered it, in "Waves in Crystal I" (Lecture 06). In the context of electrons, the following statement is more suitable.

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Bloch Theorem, Form 1: The Hamiltonian eigen-state for a particle in a crystal can be written as

$$\psi_{n\vec{k}}(\vec{r}) = \exp\left(i\vec{k}\cdot\vec{r}\right) u_{n\vec{k}}(\vec{r})$$

where $u_{n\vec{k}}(\vec{r})$ is a lattice periodic function i.e. $u_{n\vec{k}}\left(\vec{r}+\vec{R}\right) = u_{n\vec{k}}(\vec{r})$.

Bloch Theorem, Form 2: The Hamiltonian eigen-state for a particle in a crystal can be chosen so that

$$\psi_{n\vec{k}}\left(\vec{r}+\vec{R}\right) = \exp\left(i\vec{k}\cdot\vec{R}\right)\psi_{n\vec{k}}(\vec{r})$$

Bloch Theorem, Form 3: (NFE)

The Hamiltonian eigen-state for a particle in a crystal can be chosen so that

$$\psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_n\left(\vec{k}+\vec{G}\right)\exp\left(i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}\right)$$

Bloch Theorem, Form 4: (TB)

$$\psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{R}} \exp\left(i\vec{k}\cdot\vec{R}\right)\phi_n\left(\vec{r}-\vec{R}\right)$$

$$\phi_n\left(\vec{r}-\vec{R}\right) = \frac{1}{V_{BZ}}\int_{BZ} d\vec{k}e^{-i\vec{k}\cdot\vec{R}}\psi_{n\vec{k}}(\vec{r}) \quad \text{(Wannier orbital)}$$

Here, n = branch index or band index (polarization, optical or acoustical for phonons; band/symmetry index for electrons). In the case of phonons, for a given $\vec{k}$, there are a finite number of branches. In the case of electrons, there are infinite number of branches.

Note on Form 4: This is the Fourier expansion of $\psi_{n\vec{k}}$ as a periodic function <u>of $\vec{k}$</u>. The Wannier orbital is just the coefficient of the Fourier series. Use $\int_{V_c} d\vec{r}e^{i\vec{G}\cdot\vec{r}} = V_c\delta_{\vec{G},0}$ (Lecture 06), with $\vec{G}\to\vec{R}$ and $\vec{r}\to\vec{k}$! Since $\frac{1}{V_{BZ}}\int_{BZ} d\vec{k}e^{-i\vec{k}\cdot\vec{R}}\psi_{n\vec{k}}(\vec{r})$ is invariant under $\vec{r}\to\vec{r}+\vec{R}'$ and $\vec{R}\to\vec{R}+\vec{R}'$, ϕ_n is a function of $\vec{r}-\vec{R}$.

All of these forms are equivalent. It is quite easy to go from Form 1 to Form 2, or from Form 4 to Form 1. It is also very easy to go from Form 3 to Form 4. Going

All of these forms are equivalent. It is quite easy to go from Form 1 to Form 2, or from Form 4 to Form 1. It is also very easy to go from Form ~~2~~ 3 to Form ~~3~~ 4. Going from Form 2 to Form 3 is not that difficult either. Here, we will do that here, thus proving Bloch's theorem and the equivalence of all four forms.

What does Form 2 mean? When you have a function $f(\vec{r})$, the function $f(\vec{r}-\vec{R})$ is a result of translating that function by $\vec{R}$. Let us call this operation $T_{\vec{R}}$. Form 2 means that $T_{\vec{R}}\psi_{n\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{R}}\psi_{n\vec{k}}(\vec{r})$, that is $\psi_{nk}(\vec{r})$ is an eigenstate of the translation operator $T_{\vec{R}}$. As we learn in QM, if two operators commute and if both operators can be diagonalized, then the two operators can be simultaneously diagonalized. Bloch states are those simultaneous eigenstates for the Hamiltonian and $T_{\vec{R}}$. This is the statement of Form 2.

What is the most general form of $T_{\vec{R}}$ eigenstates? Start with $e^{i\vec{k}\cdot\vec{r}}$. Since, however, we are considering a lattice translation, any $\vec{k}+\vec{G}$ will be equivalent. Thus, $\sum_{\vec{G}} C_{n\vec{k}}(\vec{G})\exp\left(i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}\right)$ is the most general form. This is how we go from Form 2 to Form 3, at the same time identifying the eigenvalue of $T_{\vec{R}}$.

Crystal momentum

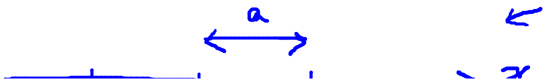
In QM, the translational operator is $e^{-\frac{ip\Delta x}{\hbar}}$, the rotational operator (translation in angle) is $e^{-\frac{iL_z\Delta\phi}{\hbar}}$, and the time evolution operator (translation in time) is $e^{-\frac{iH\Delta t}{\hbar}}$. So, the fact that the eigenvalue of $T_{\vec{R}}$ is given by $e^{-i\vec{k}\cdot\vec{R}}$ is not surprising at all. In this case, $\hbar\vec{k}$ not the momentum, but the crystal momentum, a conserved quantity for a *discrete* translational symmetry.

The dynamical origin of the Bloch theorem

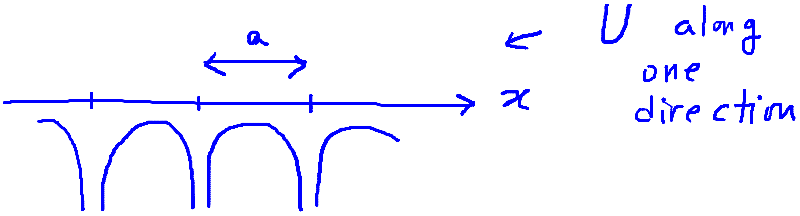
The total Hamiltonian of the system is

$$H = T + U = \frac{p^2}{2m} + U$$

$$U\left(\vec{r}+\vec{R}\right) = U(\vec{r})$$



← U along one



For plane wave basis $|\vec{k}\rangle$, the matrix element $\langle\vec{k}'|U|\vec{k}\rangle = 0$ unless $\vec{k}' = \vec{k} + \vec{G}$. This is easy to see

$$|\vec{k}\rangle \rightarrow \underbrace{\frac{1}{\sqrt{V}}}_{\text{normalization factor}} e^{i\vec{k}\cdot\vec{r}}$$

$$\langle\vec{k}'|U|\vec{k}\rangle = \frac{1}{V}\int d\vec{r}\, e^{-i\vec{k}'\cdot\vec{r}}\, U(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

$$\vec{r} = \vec{r}' + \vec{R} \quad = \frac{1}{V} e^{-i(\vec{k}'-\vec{k})\cdot\vec{R}} \int d\vec{r}'\, e^{-i\vec{k}'\cdot\vec{r}'}\, U(\vec{r}')\, e^{i\vec{k}\cdot\vec{r}'}$$

$$= e^{-i(\vec{k}'-\vec{k})\cdot\vec{R}} \langle\vec{k}'|U|\vec{k}\rangle$$

$$\therefore \langle\vec{k}'|U|\vec{k}\rangle = 0 \quad \text{unless} \quad \underbrace{e^{-i(\vec{k}'-\vec{k})\cdot\vec{R}} = 1}_{\vec{k}'-\vec{k}=\vec{G}}$$

What is this condition? $\vec{k}' - \vec{k} = \vec{G}$ is the Bragg diffraction condition or the crystal momentum conservation condition for a scattering! In general, we can call this condition a **Bragg scattering/reflection** condition as diffraction means elastic, while in general scattering includes inelastic processes.

So, what does this mean? First, note that $|\vec{k}\rangle$ diagonalizes the kinetic energy operator T. Second, U is block-diagonal in the plane wave basis where each block is given by the basis states $\{\vec{k}+\vec{G}\}$. What one knows for sure is then that the eigenstate of the Hamiltonian can be written as $\sum_{\vec{G}} C_{n\vec{k}}(\vec{G}) \exp\left(i(\vec{k}+\vec{G})\cdot\vec{r}\right)$ (Form 3). By the way, in this picture, it is easy to understand that there will be an infinite number of states given by different n's, as the number of basis states in the block, $\{\vec{k}+\vec{G}\}$, is as many as the number of plane waves $\exp\left(i(\vec{k}+\vec{G})\cdot\vec{r}\right)$.

In general, one can see that this problem is unsolvable, since each block is an infinite dimensional matrix. Amazingly, the Kronig-Penney Model is an exactly solvable model, which is thus interesting. However, it is not very important for a conceptual understanding. And so, it is left for your reading.

Bragg scattering and Bragg diffraction

So, the electrons (or any particles) go through a Bragg scattering $\vec{k}' - \vec{k} = \vec{G}$ due to the crystal potential. What is the condition for the Bragg diffraction? It is that $|\vec{k}'| = |\vec{k}|$. This means $|\vec{k} + \vec{G}| = |\vec{k}|$. For what $\vec{k}$ values does this condition satisfied? For $\vec{k}$ on Brillouin zone boundaries! (Not just the 1st BZ, but the 2nd BZ, and the 3rd, and on and on.) So, elastic scatterings can happen at the BZ boundaries, while inelastic scatterings happen at other places in the $\vec{k}$ space.