Lecture 16

Thursday, February 24, 2011

The semi-classical equation of motion

In real situations, a mono-chromatic wave with a very sharply defined crystal momentum is more a fantasy than a reality. Even when a theoretical description prefers to use a plane wave or a infinitely sharply defined Bloch state, one is advised to always remember that physical situations always involve wave packets due to intrinsic effects such as finite lifetime and extrinsic effects such as experimental conditions imposed (finite sample size, smearing by instrumental resolutions, etc.).

Let us then consider an electron wave packet, which is built up with a distribution of wave vectors, say centered at $\vec{k}$ with a width scale $\Delta\vec{k}$. When the spatial extent of this wave packet $\sim 1/\Delta k$, determined by Heisenberg uncertainty principle, is much smaller than the length scale (the wave length or the decay length) of the applied field, then we have the semi-classical approximation.

In addition, we also generally assume that Δk is not too large. If Δk is too large, then the spatial extent of the wave packet can be as small as the lattice constant, in which case the band structure begins to blur out severely. So, we assume that Δk small compared to the wave vector scale for the energy dispersion itself. If follows from this assumption that the wave packet moves with the group velocity $\vec{v}_g = \frac{1}{\hbar}\frac{d\epsilon_k}{d\vec{k}}$.

In this case, the following semi-classical equation of motion applies.

$$\hbar \frac{d\vec{k}}{dt} = \vec{F}(\vec{r}, \vec{v}_g)$$

where $\vec{r}$ is the mean position, and $\vec{v}_g$ is the group velocity ($\partial\epsilon/\partial\vec{k}$), of the wave packet, and $\vec{F}$ is the classical force at the position $\vec{r}$ and the velocity $\vec{v}_g$. For a particle with charge q, in the presence of the $\vec{E}, \vec{B}$ fields:

$$\hbar \frac{d\vec{k}}{dt} = q\vec{E} + \frac{q}{c}\ \vec{v}_g \times \vec{B}$$

Let us see how this can be derived. Consider $H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi$ where we assume that the length scales associated with $\vec{A}$ and ϕ (wave lengths) are much larger than $1/\Delta k$ of the wave packet. Otherwise, we leave $\vec{A}, \phi$ as unrestricted:

e.g. they can be time dependent.
Consider a $T_{\vec{R}}$ operator, where $T_{\vec{R}} f(\vec{r}) = f(\vec{r} - \vec{R})$, i.e. $T_{\vec{R}}$ is the translation by $\vec{R}$.
Our restriction on $\vec{R}$ is that it is a small lattice vector such that $R \ll$ length scales of the field.
We start from QM:

$$\frac{d\langle T_{\vec{R}}\rangle}{dt} = \frac{i}{\hbar}\langle [H, T_{\vec{R}}]\rangle$$

The left hand side here is trivial. $\langle T_{\vec{R}}\rangle \approx \langle e^{-i\vec{k}\cdot\vec{R}}\rangle = e^{-i\vec{k}\cdot\vec{R}}$.
So, $\frac{d\langle T_{\vec{R}}\rangle}{dt} \approx -i\dot{\vec{k}} \cdot \vec{R} e^{-i\vec{k}\cdot\vec{R}}$.
This is the leading order contribution, a term linear in $\vec{R}$. Our next task is to get the term of the same order on the right hand side.
Let us first consider the 2nd term in the Hamiltonian.

$$\frac{i}{\hbar}\langle [q\phi, T_{\vec{R}}]\rangle = \frac{i}{\hbar} q\langle \phi T_{\vec{R}} - T_{\vec{R}}\phi\rangle = \frac{iq}{\hbar}\langle\{\phi(\vec{r}) - \phi(\vec{r} - \vec{R})\}T_{\vec{R}}\rangle = \frac{iq}{\hbar}\vec{R}\cdot\langle\nabla\phi\, T_{\vec{R}}\rangle$$
$$\approx \frac{iq}{\hbar}\vec{R}\cdot\nabla\phi e^{-i\vec{k}\cdot\vec{R}}$$

[BEGIN]: Optional reading. The above is enough to show $\dot{\vec{k}} = q\vec{E}$.
Now, consider the first term in the Hamiltonian, which is more complicated.

$$\frac{i}{2m\hbar}\left\langle\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 T_{\vec{R}} - T_{\vec{R}}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2\right\rangle$$
$$= \frac{i}{2m\hbar}\left\langle\left\{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 - \left(\vec{p} - \frac{q}{c}\vec{A}(\vec{r} - \vec{R})\right)^2\right\}T_{\vec{R}}\right\rangle$$
$$\approx \frac{i}{2m\hbar}\left\langle\left\{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 - \left(\vec{p} - \frac{q}{c}\vec{A} + \frac{q}{c}(\vec{R}\cdot\nabla)\vec{A}\right)^2\right\}T_{\vec{R}}\right\rangle$$
$$\approx \frac{i}{2m\hbar}\left\langle\left\{-\frac{q}{c}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\cdot(\vec{R}\cdot\nabla)\vec{A} - \frac{q}{c}\left((\vec{R}\cdot\nabla)\vec{A}\right)\cdot\left(\vec{p} - \frac{q}{c}\vec{A}\right)\right\}T_{\vec{R}}\right\rangle$$
$$\approx \frac{i}{2m\hbar}(-2)\frac{q}{c}\, m\vec{v}_g\cdot(\vec{R}\cdot\nabla)\vec{A}\, e^{-i\vec{k}\cdot\vec{R}}$$
$$= -\frac{iq}{\hbar c}\left\{\vec{R}\cdot(\vec{v}_g \times \vec{B}) + \vec{R}\cdot\left(\frac{d\vec{A}}{dt} - \frac{\partial\vec{A}}{\partial t}\right)\right\}e^{-i\vec{k}\cdot\vec{R}}$$

$\vec{p} - \frac{q}{c}\vec{A} \approx m\vec{v}_g$ for the wave packet

$$\vec{v}\cdot(\vec{R}\cdot\nabla)\vec{A} = v_j R_i \partial_i A_j = \delta_{il}\delta_{jk} v_k R_l \partial_i A_j = (\epsilon_{mij}\epsilon_{mlk} + \delta_{ik}\delta_{jl}) v_k R_l \partial_i A_j$$
$$= (\vec{R}\times\vec{v})\cdot(\nabla\times\vec{A}) + \vec{R}\cdot(\vec{v}\cdot\nabla)\vec{A} = (\vec{R}\times\vec{v})\cdot\vec{B} + \vec{R}\cdot\left(\frac{d\vec{A}}{dt} - \frac{\partial\vec{A}}{\partial t}\right) = \vec{R}\cdot(\vec{v}\times\vec{B}) + \vec{R}\cdot\left(\frac{d\vec{A}}{dt} - \frac{\partial\vec{A}}{\partial t}\right)$$

So, collecting all terms:

$$-i\dot{\vec{k}}\cdot\vec{R} = \frac{iq}{\hbar}\vec{R}\cdot\nabla\phi - \frac{iq}{\hbar c}\left\{\vec{R}\cdot(\vec{v}_g\times\vec{B}) + \vec{R}\cdot\left(\frac{d\vec{A}}{dt} - \frac{\partial\vec{A}}{\partial t}\right)\right\}$$

Taking $\vec{R}$ to be $\vec{a}, \vec{b}, \vec{c}$, of the Bravais lattice, we have the vector identity:

$$\hbar\dot{\vec{k}} = -q\nabla\phi + \frac{q}{c}\left(\vec{v}_g \times \vec{B} + \frac{d\vec{A}}{dt} - \frac{\partial\vec{A}}{\partial t}\right)$$

With $\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t}$, we have $\frac{d}{dt}\left(\hbar\vec{k} - \frac{q}{c}\vec{A}\right) = q\vec{E} + \frac{q}{c}\vec{v}_g \times \vec{B}$.

While this form is consistent with the classical limit ($\hbar\vec{k}$ is an average of the canonical momentum for each plane wave component of the wave packet, up to a constant reciprocal vector, and so $\frac{d}{dt}\left(\hbar\vec{k} - \frac{q}{c}\vec{A}\right) \approx \frac{d}{dt}\left(m\vec{v}_g\right)$), it is <u>not</u> $\frac{d}{dt}\left(\hbar\vec{k}\right) = \vec{F}\left(\vec{r},\vec{v}_g\right) = q\vec{E} + \frac{q}{c}\vec{v}_g \times \vec{B}$. Also, our derivation resulted in a gauge dependent form, which is clearly not desirable. The resolution of this problem is complicated, and is sketched in the following paragraph.

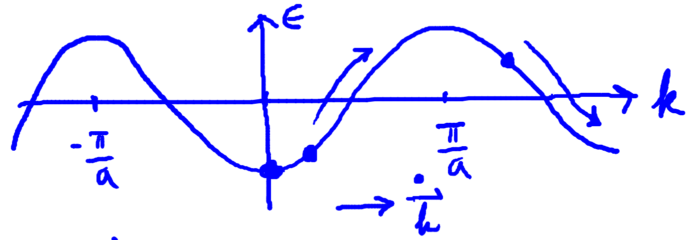
According to Zak, Phys. Rev. 168, 686 ('68), the semi-classical equation of motion should read as $\hbar\frac{d}{dt}\left[\vec{k}\right] = q\vec{E} + \frac{q}{c}\left[\frac{\partial\epsilon_n(\vec{k})}{\partial\vec{k}}\right] \times \vec{B}$ where [] means replacing $\vec{k} \to \vec{k} - i\frac{q}{2\hbar c}\vec{B} \times \frac{\partial}{\partial\vec{k}}$ (his derivation is for a constant $\vec{B}$ field and single band). $\vec{A} = \frac{1}{2}\vec{B} \times \vec{r}$ for a constant $\vec{B}$ field, and so $\vec{k} - i\frac{q}{2\hbar c}\vec{B} \times \frac{\partial}{\partial\vec{k}}$ can be thought of as related to $\vec{k} - \frac{q}{\hbar c}\vec{A}$ since one might expect $\vec{r}$ to be something like $i\frac{\partial}{\partial\vec{k}}$. As a matter of fact, Zak works in the representation that diagonalize both $T\left(\vec{R}\right) = e^{-i\vec{p}\cdot\vec{R}/\hbar}$ (translation operator in real space) and $T^*\left(\vec{G}\right) = e^{-i\vec{x}\cdot\vec{G}}$ (translation operator in momentum space). Since these two operators commute, it is possible to find the $\vec{k}, \vec{q}$ representation, where $\vec{k}$ labels the eigenvalue of $T\left(\vec{R}\right)$, $e^{-i\vec{k}\cdot\vec{R}}$, and $\vec{q}$ labels the eigenvalue of $T^*\left(\vec{G}\right)$, $e^{-i\vec{q}\cdot\vec{G}}$. In this representation, he obtains $\vec{p} = -i\hbar\frac{\partial}{\partial\vec{q}}$ and $\vec{r} = i\frac{\partial}{\partial\vec{k}} + \vec{q}$. He further finds that, in the presence of the magnetic field, the semi-classical equation $\hbar\frac{d}{dt}\vec{k} = q\vec{E} + \frac{q}{c}\,v_g\left(\vec{k}\right) \times \vec{B}$ has to be interpreted as $\vec{k}$ meaning $\left[\langle\vec{k}\rangle\right]$, where [] means the replacement of $\vec{k} \to \vec{k} - i\frac{q}{2\hbar c}\vec{B} \times \frac{\partial}{\partial\vec{k}}$. So, it is not really $\vec{k}$ when there is a magnetic field. However, this can be understood as a simple "re-mapping" or "re-labeling" of $\vec{k}$. Besides, the magnitude of the 2nd term is generally very small: $\frac{q}{2\hbar c}Ba \sim \frac{e\hbar}{2mc}B\frac{mc^2}{(\hbar c)^2}a \sim \mu_B B\ \frac{1}{4\ \text{eV}\ \text{Å}} \sim O(10^{-3})\ \text{Å}^{-1}$ (a is the lattice constant $\sim O\left(\frac{\partial}{\partial\vec{k}}\right)$, and μ_B is the Bohr magneton $= 6 \times 10^{-9}$ eV/gauss. The strongest B field that one can generate in a laboratory $\sim 10^6$ gauss; On the other hand, the term $\frac{q}{\hbar c}A \sim \frac{q}{\hbar c}Br$ is *not* necessarily small, since $r \gg a$.)

[END]: Optional reading.

Bloch Oscillation

Surprisingly, the semi-classical equation above predicts that if a partially filled band is subjected to a constant DC electric field, then an AC response may be obtained.

This is easy to see if there was one wave packet moving on a single band in one dimension.



$$\dot{\vec{k}} = \frac{q}{\hbar}\vec{E} = \text{const.}$$

According to the semi-classical EOM, **the wave vector simply changes at a constant rate**, under a constant $\vec{E}$ field, but without the $\vec{B}$ field. So, given a band sketched above, the wave packet will simply trace the dispersion relation, going up and coming down and repeating indefinitely, while the wave vector changes steadily. Why does this mean an AC current? The current density is $nq\vec{v}_g$ ($q = -e$ for the electron wave packet), where $n =$ number density, and $\vec{v}_g$ is the group velocity. Notice how the group velocity increases to a positive number, decreases to zero at $k = \pi/a$, and then reverses its direction, and then decreases further before increasing to 0 again ($k = 2\pi/a$). Thus the current is definitely an AC current. Given the band structure (which may not be a single cosine function in general), we expect that the AC current will contain harmonics of the $2\pi/T$, where T is the period: the time it takes for $\Delta k = 2\pi/a$. Since the rate at which k changes is constant ($|qE|/\hbar$), $T = \frac{2\pi\hbar}{a|qE|}$. This is the so-called **Bloch oscillation**.

Each wave packet causes such an AC current, and the frequency of the current will not change when the same type of AC current is caused by a very many number of electron wave packets.

When would a Bloch oscillation be observed? $T \ll \tau$, where τ is the relaxation time. For a small T, one would like to have a large a (a nanoscale superstructure -- an artificial crystal -- rather than a natural crystal) and a large $|E|$ (semi-conductor instead of a metal). In semiconductors, τ is on the order of pico-seconds, and a superstructure with $a \sim 50$ Å and $E \sim 5 \times 10^4$ V/cm, giving $T \sim 0.2$ pico-seconds, will be enough.

Motion of charged particle in a $\vec{B}$ field

$\tau \sim 0.2$ pico-seconds, will be enough.

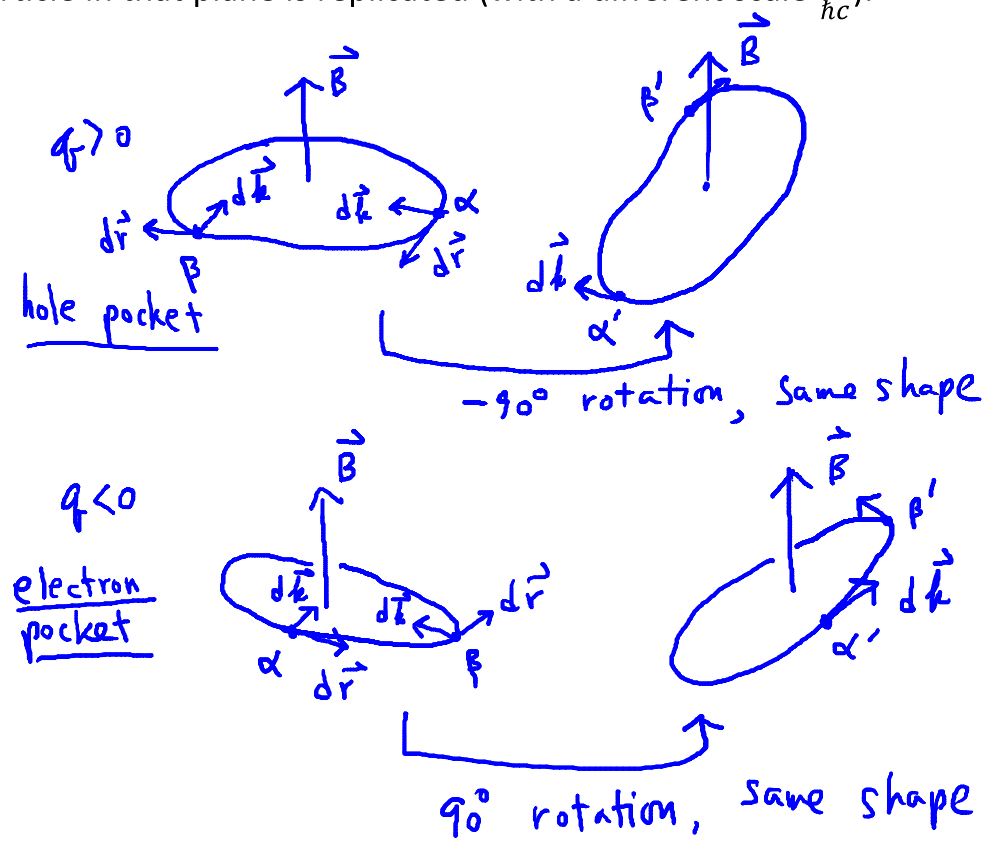
Motion of charged particle in a $\vec{B}$ field

Let us consider a complementary situation when $\vec{E} = 0$ but $\vec{B} =$ constant. Classically, we know that this means a circular motion with the cyclotron frequency $\omega_c = \frac{qB}{mc}$. We shall now see what happens in the quantum case.

First, let us look at the equation of motion: $\hbar\dot{\vec{k}} = \frac{q}{c}\vec{v} \times \vec{B}$. Rewriting this $\hbar\frac{d\vec{k}}{dt} = \frac{q}{c}\frac{d\vec{r}}{dt} \times \vec{B}$, we get

$$d\vec{k} = \frac{q}{\hbar c} d\vec{r} \times \vec{B}$$

What does this mean? Suppose $q > 0$. Let us say that there is a real space path that is followed by this wave packet $(d\vec{r})$. We consider a planar motion only, where the plane is perpendicular to the field. [The particle can have a finite constant velocity parallel to the field.] This equation means that the path of the particle in that plane is replicated (with a different scale $\frac{qB}{\hbar c}$).



It is important to realize that the shape of the orbit above is determined by the crossection of the constant energy surface. Why? (1) $\hbar\dot{\vec{k}} = \frac{q}{c}\vec{v} \times \vec{B}$ means that $\dot{\vec{k}} \cdot \vec{B} = 0$, meaning that the $\vec{k}$ component along the direction of $\vec{B}$ is constant (so the motion in $\vec{k}$ space is strictly two dimensional, while the motion in $\vec{r}$ space can be three dimensional with a constant velocity along the direction of $\vec{B}$). (2) $\frac{d\epsilon_{\vec{k}}}{dt} = \frac{\partial\epsilon_{\vec{k}}}{\partial\vec{k}} \cdot \dot{\vec{k}} = \vec{v} \cdot \dot{\vec{k}} = \frac{q}{c}\vec{v} \cdot \left(\vec{v} \times \vec{B}\right) = 0$. That is, the magnetic field doesn't do any work, as well-known. So a given band structure completely determines the motion of a wave packet.