Lecture 7

Quantum mechanics of block electrons

a) Operator of coordinate in block representation

Block functions represent a convenient basis for considering the electron dynamics in external fields. For instance, the Hamiltonian without fields \( \hat{H}_{\text{ext}} \) is diagonal in this representation:

\[
\hat{H} \psi_{nk} = E_{nk} \psi_{nk} \Rightarrow \hat{H} = \sum_{nk} E_{nk} |\psi_{nk}\rangle \langle \psi_{nk}|.
\]

In other words, the action of the Hamiltonian on an arbitrary wave function is given by

\[
\hat{H} \sum_{nk} c_{nk} |\psi_{nk}\rangle = \sum_{nk} E_{nk} c_{nk} |\psi_{nk}\rangle,
\]

it is just multiplication of the wave function \( |\psi_{nk}\rangle \) in \( \text{Enk} \) representation \( c_{nk} \) by a number \( E_{nk} \).

What is the analogous rule for the coordinate? After all, we need to know it to formulate dynamics on external fields that do depend on the coordinate.

Reminder: In the situation in the free case:

\( \hat{r} \psi(r) = r \psi(r), \) \( \hat{r} \) is diagonal in \( r \)-representation.
But what is $\hat{v}$ in momentum representation?

$$\hat{v}\psi(r) = \hat{r}\cdot \int dp \, \varphi_p(r) = \int dr \, \varphi_r \cdot e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} = \int dr \, \varphi_r \cdot r \, e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}}.$$

$\hat{v}$ in $p$-representation must act on the wave function in $p$-representation $\varphi_p$.

$$r \, e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} = \frac{\partial}{\partial \varphi_p} e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} = -\frac{\partial}{\partial \varphi_p} e^{-\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \Rightarrow$$

$$\Rightarrow \hat{v} \psi = \int dp \left[ \varphi_p \cdot \frac{\partial}{\partial \varphi_p} e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \right] = \int dp \, \frac{\partial}{\partial \varphi_p} \varphi_p \cdot e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}}.$$ 

Therefore, $\left[ \hat{r}, \hat{p} \right] = i\hbar$, well-known relation.

This is in accord with $[\hat{r}, \hat{p}] = i\hbar$, of course.

So what is $\hat{v}$ in block representation?

Let's play the same game:

$$\hat{v}\psi = \hat{r}\cdot \sum_{\nu p} \varphi_{\nu p}(r) = \sum_{\nu p} \varphi_{\nu p} \cdot r \, e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \psi_{\nu p}.$$

Now $r \, e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \psi_{\nu p}(r) = \frac{\partial}{\partial \varphi_{\nu p}} (e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \psi_{\nu p}) +$

$$+ \frac{i\hbar}{2\hbar} \varphi_{\nu p} \cdot e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \varphi_{\nu p}$$
Thus
\[ 
\psi = \sum_{\mathbf{p}} C_{\mathbf{p}} \left[ -i \hbar \partial_{\mathbf{p}} \psi_{\mathbf{p}} + i \hbar e^{i \mathbf{p} \cdot \mathbf{r} / \hbar} \partial_{\mathbf{r}} \psi_{\mathbf{p}} \right] = 
\]
\[ 
= \n \sum_{\mathbf{p}} \frac{d^{3} \mathbf{p}}{(2\pi)^{3} \hbar} \left( i \hbar \partial_{\mathbf{p}} C_{\mathbf{p}} \right) \psi_{\mathbf{p}} + 
\]
\[ 
+ \n \sum_{\mathbf{p}} \frac{d^{3} \mathbf{p}}{(2\pi)^{3} \hbar} C_{\mathbf{p}} i \hbar e^{i \mathbf{p} \cdot \mathbf{r} / \hbar} \partial_{\mathbf{r}} \psi_{\mathbf{p}}. 
\]

To massage the second term, we note that \( \partial_{\mathbf{r}} \psi_{\mathbf{p}}(\mathbf{r}) \) is a periodic function of \( \mathbf{r} \) on the principal cell, like \( \psi_{\mathbf{p}}(\mathbf{r}) \) itself. It can be expanded in the basis of \( \psi_{\mathbf{p}} \):

\[ 
i \hbar \partial_{\mathbf{p}} \psi_{\mathbf{p}} = \sum_{\mathbf{n}} \psi_{\mathbf{p}} \Delta_{\mathbf{n}} \psi_{\mathbf{n}} = \sum_{\mathbf{n}} \psi_{\mathbf{n}} \Delta_{\mathbf{n}} \psi_{\mathbf{p}} = \sum_{\mathbf{n}} \Delta_{n,n'} \psi_{n'} \psi_{\mathbf{n}}. \]

More explicitly,
\[ 
\Delta_{n,n'} = \int d\mathbf{r} \psi^{*}_{n'}(\mathbf{r}) \frac{\hbar^{2}}{2m} \psi_{n}(\mathbf{r}), \quad \text{and} \]
\[ 
i \hbar \partial_{\mathbf{p}} \psi_{n}(\mathbf{r}) = \sum_{n'} \Delta_{n,n'} \psi_{n'}(\mathbf{r}). \]
this may we get
\[ \sum_n \int \sqrt{\frac{\hbar}{2m}} \ C_{np} \ ei^{i \frac{p \cdot \vec{r}}{\hbar}} \cdot i \hbar \ \partial_p \ \Psi_{np} = \]
\[ = \sum_n \int \sqrt{\frac{\hbar}{2m}} \ C_{np} \ e^{i \frac{p \cdot \vec{r}}{\hbar}} \cdot \frac{1}{\sqrt{N}} \ \sum \Omega_{nn'} \cdot \Psi_{np}(\vec{r}) = \]
\[ = \sum_n \int \sqrt{\frac{\hbar}{2m}} \ \left[ \Omega_{nn'} \ C_{np} \right] e^{i \frac{p \cdot \vec{r}}{\hbar}} \cdot \Psi_{np} \]
\[ \text{C_{new}} \quad \text{Y_{np}} \]

We see that the total effect of \( \hat{p} \) is
\[ \hat{r} = i \hbar \ \frac{\partial}{\partial p} \cdot S_{np} + \Omega_{nn'}(\vec{p}), \text{ where} \]
\[ \Omega_{nn'}(\vec{p}) = \int d \vec{s} \ U_{np}^* \ (\vec{s}) \left( i \hbar \ \frac{\partial}{\partial \vec{p}} \ U_{np} (\vec{s}) \right) \leftrightarrow \]
\[ \leftrightarrow \quad i \hbar \ \left< \Psi_{np} \left| \frac{\partial}{\partial \vec{p}} \right| \Psi_{np} \right> \]

when the motion of a particle is restricted to a single

When the motion of a particle is restricted to a single
field, \( \Omega_{nn'}(\vec{p}) \) acts like vector potential in momentum space.
Indeed, we get

\[ \hat{p}_n = \frac{i}{\hbar} \frac{\partial}{\partial R_n} + \hat{\mathbf{a}}(\mathbf{R}) \]

\[ \mathbf{p} = \mathbf{P} - \mathbf{e} \mathbf{A}(\mathbf{R}) \]

\( \hat{\mathbf{a}}(\mathbf{R}) \) is called Berry connection.

\( \hat{\mathbf{A}}(\mathbf{R}) \) is gauge dependent: \( U \rightarrow e^{i\mathbf{F} \cdot \mathbf{A}} U \), changes \( \hat{\mathbf{A}} \).

Example: motion in electric field

\[ \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) - e\mathbf{E} \cdot \mathbf{R} \]

In Bloch representation this looks like

\[ \hat{H} = \sum_{\mathbf{k}, \mathbf{p}} \varepsilon_{\mathbf{n}\mathbf{p}} \langle \mathbf{n}\mathbf{p} | - e \mathbf{E} \cdot \sum_{\mathbf{m}\mathbf{p}} \left[ \frac{i}{\hbar} \frac{\partial}{\partial \mathbf{m}\mathbf{p}} + \mathbf{A}_{\mathbf{n}\mathbf{m}\mathbf{p}}(\mathbf{R}) \right] \otimes \langle \mathbf{n}\mathbf{p} | \rangle \]

Let us assume that band \( \mathbf{n} \) is well-separated in energy from the rest of the bands. Then it is plausible that if the electric field is not too large, the electron will stay in band \( \mathbf{n} \) (adiabatic approximation).
When projected onto with hand, it gives

\[ H_\nu = E_\nu \rho - eE \vec{R}_{\text{canonical}} = -eE \vec{Q}_n(\vec{p}) \]

the canonical EOM contain how the leading in \( t \) correction due to \( \theta_n(\vec{p}) (\vec{a} \times \vec{t}) \) - long term in the velocity.

\[ \dot{R}_\nu = \frac{\partial H}{\partial \vec{p}_\nu} = \frac{\partial E_\nu}{\partial \vec{p}_\nu} - eE \beta \frac{\partial \vec{Q}_n}{\partial \vec{p}_\nu} \]

\[ \dot{p}_\nu = -\frac{\partial H}{\partial R_\nu} = eE \quad \text{the usual equation.} \]

Basically, we see that we recover the usual eq. of if we neglect \( \theta_n(\vec{p}) \), that is \( R = R \), and \( \dot{R}_\nu = \dot{p}_\nu = \frac{\partial E_\nu}{\partial \vec{p}_\nu} \).

To get the \( E_\nu \). For physical coordinate, we note that

\[ \dot{R}_\nu = \dot{R}_\nu + \frac{\partial E_\nu}{\partial \vec{p}_\nu} \vec{p}_\nu \]

and obtain

\[ \dot{R}_\nu = \frac{\partial E_\nu}{\partial \vec{p}_\nu} + eE_b (\frac{\partial \vec{a}_\nu}{\partial \vec{p}_\nu} - \frac{\partial \vec{a}_\nu}{\partial \vec{p}_\nu}) = \frac{\partial E_\nu}{\partial \vec{p}_\nu} - F_{\vec{p}_\nu} E_\nu \]

\[ \frac{\partial \vec{a}_\nu}{\partial \vec{p}_\nu} - \frac{\partial \vec{a}_\nu}{\partial \vec{p}_\nu} = F_{\vec{p}_\nu} - \text{anti-sym. tensor} \]

As in the case of real vector potential,

\[ F_{\vec{p}_\nu} = E_{\vec{p}_\nu} \vec{Q}_\nu, \quad \vec{Q}_\nu = E_{\vec{p}_\nu} \vec{a}_\nu - \frac{\partial E_{\vec{p}_\nu}}{\partial \vec{p}_\nu} \vec{a}_\nu \]

\[ \vec{S}_\nu = \text{curl } E_{\vec{p}_\nu} \vec{a}_\nu \]
The gauge-independent vector \( \mathbf{\Omega} \) is called "Berry curvature" - this is the analog of the magnetic field in the momentum space.

Finally,

\[
\mathbf{\Gamma} = \frac{\partial \mathbf{E}}{\partial \mathbf{p}} - \mathbf{e} E \times \mathbf{\Omega}_n
\]

\[
\mathbf{\Omega}_n = \mathbf{e} E
\]

I added the "-" sign on 09/23/2013.

\( \delta \mathbf{V} = -\mathbf{e} E \times \mathbf{\Omega}_n \) is called the anomalous velocity. It may cause deflection of \( \mathbf{E} \), and will eventually cause the Hall effect. This will be the subject of our studies pretty soon.

For now, let us discuss how the velocity operator changes in the absence of \( \mathbf{E} \), but with allowance for inelastic transitions.

By definition,

\[
\hat{\mathbf{V}} = \hat{\mathbf{r}} = i\hbar \left[ \hat{\mathbf{r}}, \hat{F} \right]
\]

we have

\[
\hat{F} = \sum_{nP} \left( \frac{i}{\hbar} \frac{\partial}{\partial \mathbf{p}} \right) \mathbf{S}_{n'n'} + \mathbf{\Omega}_{n'n'}(\mathbf{p}) \right|_{\mathbf{p}} \times \mathbf{\Omega}_{n'}.
\]
Let us calculate the commutator of the first term:

\[
\frac{i}{\hbar} \left[ \hat{\mathbf{H}}, \hat{\mathbf{r}} \right] = \frac{i}{\hbar} \sum_{n,p} \left( \left[ \hat{E}_n, \frac{\partial}{\partial \mathbf{p}} \right] \delta_{nm} \right) \langle n|p \rangle \langle n|p \rangle = \\
= \sum_{n,p} \frac{2\mathbf{E}_n \cdot \mathbf{p}}{\partial \mathbf{p}} \langle n|p \rangle \langle n|p \rangle.
\]

This is the diagonal contribution we obtained many times.

The second term in \( \hat{\mathbf{r}} \):

\[
\frac{i}{\hbar} \left[ \hat{\mathbf{H}}, \hat{\mathbf{\Omega}} \right] = \frac{i}{\hbar} \left[ \sum_{n,p} \mathbf{E}_n \langle n|p \rangle \langle n|p \rangle \mathbf{\Omega}_{n''} \right] \langle n'|p' \rangle \langle n'|p' \rangle = \\
= \frac{i}{\hbar} \sum_{n''} \left( \mathbf{E}_n \cdot \mathbf{\Omega}_{n''} \right) \langle n'|p' \rangle \langle n'|p' \rangle.
\]

Finally, for \( n = n' \):

\[
\langle n|p \rangle \langle n|p \rangle = \frac{\partial \mathbf{E}_n}{\partial \mathbf{p}};
\]

for \( n \neq n' \):

\[
\langle n|p \rangle \langle n|p \rangle = \frac{i}{\hbar} \left( \mathbf{E}_n - \mathbf{E}_n \right) \mathbf{\Omega}_{n''}.
\]