6.730 Physics for Solid State Applications

Lecture 21: Effective Mass Theorem and Impurity States

Outline

- Review of Last Time
- Detailed Look at the Translation Operator
- Electronic Wavepackets
- Effective Mass Theorem
  & Semiclassical Equations of Motion

March 29, 2004

Properties of the Translation Operator

Definition of the translation operator…and its Bloch eigenfunctions

$$\widehat{T}_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R}) \qquad \widehat{T}_{\mathbf{R}}\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$$

T_R commutes with the lattice Hamiltonian (V_{ext}=0) and with other T_R

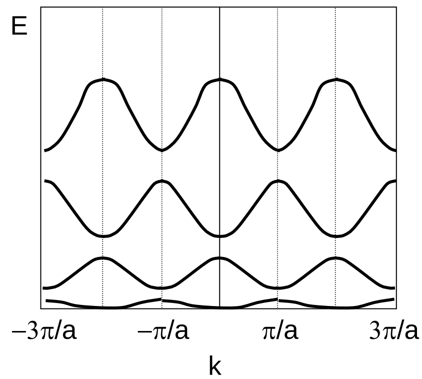
$$[\widehat{T}_{\mathbf{R}}, H(\mathbf{r})] = \mathbf{0} \qquad [\widehat{T}_{\mathbf{R}_1}, \widehat{T}_{\mathbf{R}_2}] = 0$$

Representation of the translation operator…

$$T_{-\mathbf{R}} f(\mathbf{r}) = e^{-\mathbf{R}\cdot\nabla_{\mathbf{r}}} f(\mathbf{r}) = f(\mathbf{r}-\mathbf{R})$$

Another Look at Electronic Bandstructure

$$E_n(k) = E_n(k + K_i)$$



As we will see, it is often convenient to represent the bandstructure by its inverse Fourier series expansion...

$$E_n(k) = \sum_\ell E_n[R_\ell] e^{ik\cdot R_\ell}$$

Translation Operator and Lattice Hamiltonian

From before, the eigenvalue equation for the translation operator is....

$$\hat{T}_{R_\ell}\psi(r) = e^{ik\cdot R_\ell}\psi(\mathbf{r})$$

If we multiply this by the Fourier coefficients of the bandstructure...

$$E_n[R_\ell]\,\hat{T}_{R_\ell}\psi(r) = E_n[R_\ell]\,e^{ik\cdot R_\ell}\psi(\mathbf{r})$$

...and sum over all possible lattice translations...

$$\sum_\ell E_n[R_\ell]\,\hat{T}_{R_\ell}\psi(r) = \underbrace{\sum_\ell E_n[R_\ell]\,e^{ik\cdot R_\ell}}_{E_n(k)}\,\psi(\mathbf{r})$$

...we see that the eigenvalue on the left is just the bandstructure (energy)

$$\sum_\ell E_n[R_\ell]\,\hat{T}_{R_\ell}\psi(r) = E_n(k)\,\psi(\mathbf{r})$$

This suggests the operator on the left is just the crystal Hamiltonian !

$$\hat{H}_0 = \sum_\ell E_n[R_\ell]\,\hat{T}_{R_\ell}$$

No wonder $[\hat{H}_0, \hat{T}_R] = 0$

Alternate Form of the Hamiltonian

$$\widehat{H}_0 = \sum_\ell E_n[R_\ell]\,\widehat{T}_{R_\ell} = \sum_\ell E_n[R_\ell]\,e^{\mathbf{R}\cdot\nabla_\mathrm{r}}$$

and $$E_n(k) = \sum_\ell E_n[R_\ell]e^{ik\cdot R_\ell}$$

Comparing leads us to conclude that the Hamiltonian can be written as

$$\widehat{H}_o = E_n(-i\nabla_r)$$

Meaning that if we can find an expression for $E_n(\mathbf{k})$, then just let

$$\mathbf{k} \longrightarrow -i\nabla$$

Alternate Form of the Bloch Hamiltonian

$$\widehat{H}_o = \frac{\widehat{p}^2}{2m} + V_{\text{periodic}}(\mathbf{r}) = \mathbf{E_n}(-\mathbf{i}\nabla_\mathbf{r})$$

Example 1. $E_n(k) = -A\cos(ka)$

$$\widehat{H}_o = -A\,\cos(-ia\frac{d}{dx}) = -\frac{A}{2}\left(e^{a\frac{d}{dx}} + e^{-a\frac{d}{dx}}\right)$$

Example 2. $E_n(k) = a + bk + ck^2$

$$\widehat{H}_o = a - ia\frac{d}{dx} - c\frac{d^2}{dx^2}$$

Therefore, use the band structure to find the Bloch Hamiltonian near a certain value of crystal momentum k.

Wavefunction of Electronic Wavepacket

The eigenfunction for $k \sim k_0$ are approximately...

$$\psi_{n,k}(r) = e^{ik\cdot r} u_{n,k}(r)$$

$$\approx e^{ik\cdot r} u_{n,k_0}(r)$$

$$\approx e^{i(k-k_0)\cdot r} \psi_{n,k_0}(r)$$

A wavepacket can therefore be constructed from Bloch states as follows...

$$\psi_n'(r,t) = \sum_{k \text{ near } k_o} c_n(k,t)\psi_{n,k}(r)$$

$$\approx \underbrace{\sum_{k \text{ near} k_o} c_n(k,t) e^{i(k-k_0)\cdot r}}_{F_n(r,t)} \psi_{n,k_0}(r)$$

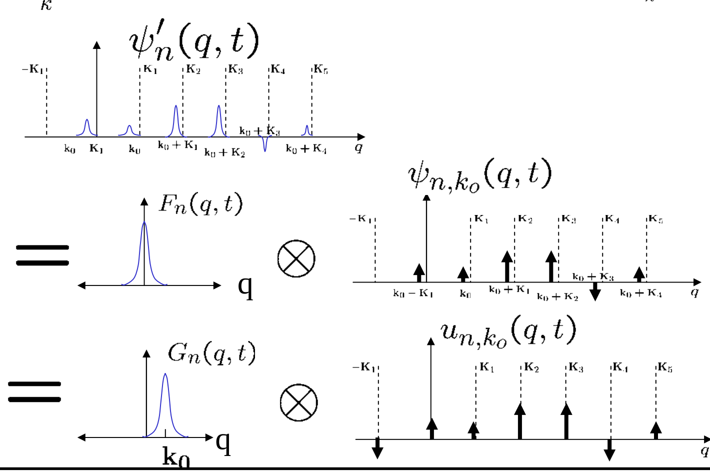
F is a slowly varying function...

Wavefunction of Electronic Wavepacket

$$\psi_n'(r,t) \approx F_n(r,t)\psi_{n,k_0}(r) = G_n(r,t) u_{n,k_0}(r)$$

F & G are slowly varying functions...

$$F_n(r,t) = \sum_k c_n(k,t) e^{i(k-k_o)\cdot r} \qquad G_n(r,t) = e^{-ik_o\cdot r} F_n(k,t) = \sum_k c_n(k,t) e^{ik\cdot r}$$



Wavefunction of Electronic Wavepacket

$$\psi'_n(r,t) = \underbrace{F_n(r,t)}_{\text{envelope function}} \quad \underbrace{\psi_{n,k_0}(r)}_{\text{Bloch function}}$$

$$\psi'_n(r,t) = \underbrace{G_n(r,t)}_{\text{envelope function}} \quad \underbrace{u_{n,k_0}(r)}_{\text{Bloch amplitude}}$$

And $$G_n(r,t) = e^{-ik_o \cdot r} F_n(k,t)$$

Since we construct wavepacket from a small set of k's...

$$\Delta k \ll \frac{2\pi}{a} \quad \text{and} \quad \Delta r \gg a$$

...the envelope function must vary slowly...wavepacket must be large...

$$\Delta r \gg a$$

Action of Crystal Hamiltonian on Wavepacket

$$\widehat{H}_0 \, \psi'_{n,k} = \widehat{H}_0 \left(G_n(r,t) u_{n,k_0}(r) \right)$$

$$= \sum_\ell E_n(R_\ell) \, \widehat{T}_{R_\ell} \left(G_n(r,t) u_{n,k_0}(r) \right)$$

$$= \sum_\ell E_n(R_\ell) \, G_n(r + R_\ell, t) u_{n,k_0}(r + R_\ell)$$

$$= u_{n,k_0}(r) \sum_\ell E_n[R_\ell] G_n(r + R_\ell, t)$$

$$= u_{n,k_0}(r) \underbrace{\sum_\ell E_n[R_\ell] \, \widehat{T}_{R_\ell}}_{H_0} \, G_n(r,t)$$

$$= u_{n,k_0}(r) \, \widehat{H}_0 \, G_n(r,t)$$

It appears that the Hamiltonian only acts on the slowly varying amplitude...

Effective Mass Theorem

If we can consider an external potential (eg. electric field) on the crystal...

$$\hat{H} = \hat{H}_0 + \hat{V}_{ext}$$

$$\left(\hat{H}_0 + \hat{V}_{ext}(r)\right)\ \psi'_{n,k}(r,t) = i\hbar \frac{\partial \psi'_{n,k}(r,t)}{\partial t}$$

The influence of the external field on the wavepacket...

$$\psi'_n(r,t) \approx G_n(r,t) u_{n,k_0}(r)$$

$$u_{n,k_0}(r)\ \left(\hat{H}_0 + \hat{V}_{ext}(r)\right)\ G_n(r,t) = i\hbar\, u_{n,k_0}(r)\, \frac{\partial G_n(r,t)}{\partial t}$$

We can solve Schrodinger's equation just for the envelope functions...

$$\left(\hat{H}_0 + \hat{V}_{ext}(r)\right)\ G_n(r,t) = i\hbar\, \frac{\partial G_n(r,t)}{\partial t}$$

Effective Mass Theorem

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Recall that $\hat{H}_o = E_n(-i\nabla_r)$

So that we find what is known as the ***Effective Mass Theorem***:

$$\left(E_n(-i\nabla_r) + \hat{V}_{ext}(r)\right)\ G_n(r,t) = i\hbar\, \frac{\partial G_n(r,t)}{\partial t}$$

Likewise, we find an alternate form of the ***Effective Mass Theorem***:

$$\left(E_n(k_o - i\nabla_r) + \hat{V}_{ext}(r)\right)\ F_n(r,t) = i\hbar\, \frac{\partial F_n(r,t)}{\partial t}$$

Normalization of the Envelope Function $G_n(r,t)$

$$1 = \int \psi_n'^*(r,t)\psi_n'(r,t)d^3r$$
$$= \int G_n^*(r,t)G_n(r,t)\, u_{n,k_0}^*(r)u_{n,k_0}(r)d^3r$$

Since the envelope is slowly varying...it is nearly constant over the volume of one primitive cell...

$$1 \approx \sum_m G_n^*(R_m,t)G_n(R_m,t)\int_\Delta u_{n,k_0}^*(r)u_{n,k_0}(r)d^3r$$
$$1 = \frac{1}{V_{\text{box}}}\sum_m G_n^*(R_m,t)G_n(R_m,t)\Delta$$
$$1 \approx \frac{1}{V_{\text{box}}}\int_{\text{box}} G_n^*(r,t)G_n(r,t)d^3r$$

$$< G_n(r,t)|G_n(r,t) >= V_{\text{box}}$$

What is the Position of Wavepacket ?

Proof that...$\langle\hat{\mathbf{r}}(t)\rangle_G \approx \langle\hat{\mathbf{r}}(t)\rangle$

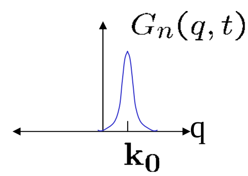
$$< r(t) >= \frac{< \psi_n'(r,t)|\hat{r}|\psi_n'(r,t) >}{< \psi_n'(r,t)|\psi_n'(r,t) >}$$
$$= \int_{V_{\text{Box}}} G_n^*(r,t)G_n(r,t)u_{n,k_0}^*(r)\; r\; u_{n,k_0}(r)d^3r$$
$$\approx \sum_m G_n^*(R_m,t)G_n(R_m,t)\int_\Delta u_{n,k_0}^*(r)\,[r+R_m]\,u_{n,k_0}(r)d^3r$$
$$\approx \sum_m G_n^*(R_m,t)G_n(R_m,t)\,R_m\int_\Delta u_{n,k_0}^*(r)u_{n,k_0}(r)d^3r$$
$$= \sum_m G_n^*(R_m,t)\frac{1}{N}R_m\,G_n^*(R_m,t) \approx \frac{1}{N\Delta}\sum_m G_n^*(R_n,t)\,R_n\,G_n(R_n,t)\Delta$$
$$= \frac{< G_n(r,t)|r|G_n(r,t) >}{< G_n(r,t)|G_n(r,t) >} = \langle\hat{r}(t)\rangle_G$$

What is the Momentum of Wavepacket

$$< p >_G = \frac{< G_n(r,t)|\widehat{p}|G_(r,t) >}{< G_n(r,t)|G_n(r,t) >}$$

$$= \frac{< G_n(q,t)|\hbar q|G_(q,t) >}{< G_n(q,t)|G_n(q,t) >}$$

$$\approx \hbar k_0$$



$$< p >_G = \hbar \mathbf{k_o}$$

but $$< p > \neq \hbar k_0$$

Summary Wavepacket properties

Without explicitly knowing the Bloch functions, we can solve for the envelope functions...

$$\left(E_n(-i\nabla_r) + \widehat{V}_{ext}(r)\right) G_n(r,t) = i\hbar \frac{\partial G_n(r,t)}{\partial t}$$

or $$\left(E_n(k_o - i\nabla_r) + \widehat{V}_{ext}(r)\right) F_n(r,t) = i\hbar \frac{\partial F_n(r,t)}{\partial t}$$

The envelope functions are sufficient to determine the expectation of position and crystal momentum for the system...

$$< r(t) >_G = \frac{< G_n(r,t)|r|G_n(r,t) >}{< G_n(r,t)|G_n(r,t) >} = < r(t) >$$

$$< p >_G = \frac{< G_n(r,t)|\widehat{p}|G_(r,t) >}{< G_n(r,t)|G_n(r,t) >} \approx \hbar k_0$$

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From Lecture 19 recall that the Semiclassical Equations of Motion are

$$\frac{d}{dt} < \mathbf{r}(t) > = < \mathbf{v_n}(\mathbf{k}) > = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n}(\mathbf{k}) \qquad \mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

We could have also proved the last statement as a Erhenfest with G(r,t) !

$$\frac{d}{dt} < p >_G = \frac{d}{dt}\hbar k_0 = < -\frac{\partial}{\partial x}V_{ext} >_G = < F_{ext} >_G$$

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Semiclassical Equations of Motion:

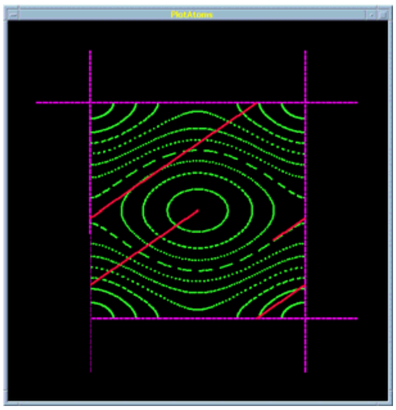
$$\frac{d}{dt} < \mathbf{r}(t) > = < \mathbf{v_n}(\mathbf{k}) > = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n}(\mathbf{k})$$

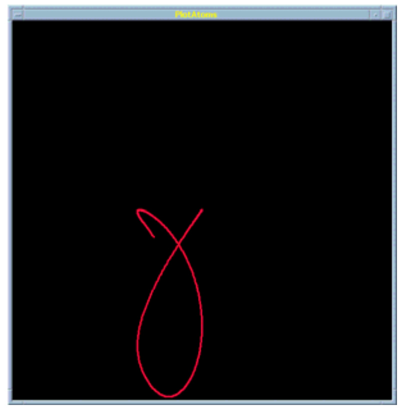
$$\mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

Semiclassical Equations of Motion

$$< \mathbf{v_n(k)} > = \frac{< \mathbf{p} >}{\mathbf{m}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathbf{E_n(k)}$$

$$\mathbf{F_{ext}} = \hbar \frac{\mathbf{dk}}{\mathbf{dt}}$$





http://www.physics.cornell.edu/sss/ziman/ziman.html

Semiclassical Equations of Motion

$$< \mathbf{v_n(k)} > = \frac{< \mathbf{p} >}{\mathbf{m}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathbf{E_n(k)}$$

$$\mathbf{F_{ext}} = \hbar \frac{\mathbf{dk}}{\mathbf{dt}}$$

Lets try to put these equations together....

$$a(t) = \frac{dv}{dt} = \frac{1}{\hbar} \frac{\partial}{\partial t} \frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar} \frac{\partial^2 E_N(k)}{\partial k^2} \frac{dk}{dt}$$

$$= \left[\frac{1}{\hbar^2} \frac{\partial^2 E_N(k)}{\partial k^2} \right] F_{\text{ext}}$$

Looks like Newton's Law if we define the mass as follows...

$$m^*(k) = \hbar^2 \left(\frac{\partial^2 E_N(k)}{\partial k^2} \right)^{-1}$$

dynamical effective mass

→ mass changes with k...so it changes with time according to k

Dynamical Effective Mass (3D)

Extension to 3-D requires some care,

F and a don't necessarily point in the same direction

$$\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1}\mathbf{F}_{\text{ext}} \quad \text{where} \quad \overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

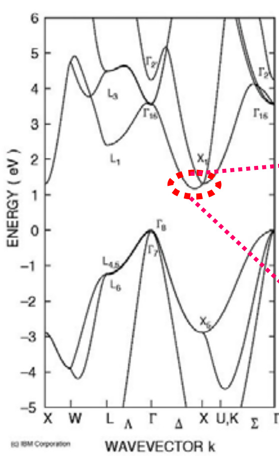
$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{pmatrix}\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$$

Dynamical Effective Mass (3D)

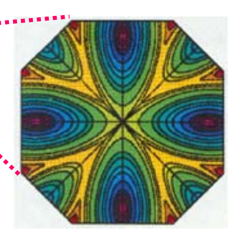
Ellipsoidal Energy Surfaces

Fortunately, energy surfaces can often be approximate as...

$$E_N(k) = E_c + \frac{\hbar^2}{2}\left(\frac{(k_x - k_x^0)^2}{m_t} + \frac{(k_y - k_y^0)^2}{m_t} + \frac{(k_z - k_z^0)^2}{m_l}\right)$$



Silicon



$$\overline{\overline{\mathbf{M}}}^{-1} = \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} \end{pmatrix}$$

$$\overline{\overline{\mathbf{M}}} = \begin{pmatrix} m_t & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_l \end{pmatrix}$$

http://csmr.ca.sandia.gov/workshops/nacdm2002/viewgraphs/Conor_Rafferty_NACDM2002.pdf

Summary Wavepacket properties

A. Without explicitly knowing the Bloch functions, solve for the envelope function.

$$\left(E_n(-i\nabla_r) + \widehat{V}_{ext}(r)\right) G_n(r,t) = i\hbar \frac{\partial G_n(r,t)}{\partial t}$$

or $$\left(E_n(k_o - i\nabla_r) + \widehat{V}_{ext}(r)\right) F_n(r,t) = i\hbar \frac{\partial F_n(r,t)}{\partial t}$$

$$< r(t) >_G = \frac{< G_n(r,t)|r|G_n(r,t) >}{< G_n(r,t)|G_n(r,t) >} = < r(t) > \qquad < p >_G = \frac{< G_n(r,t)|\widehat{p}|G_(r,t) >}{< G_n(r,t)|G_n(r,t) >} \approx \hbar k_0$$

B. Alternatively, use the **Semiclassical Equations of Motion** for a slowly varying external force are

$$\frac{d}{dt} < \mathbf{r}(t) > = < \mathbf{v_n}(\mathbf{k}) > = \frac{\mathbf{1}}{\hbar} \nabla_{\mathbf{k}} \mathbf{E_n}(\mathbf{k})$$

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F_{ext}}$$

Combing these equations give $\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1} \mathbf{F}_{\text{ext}}$ where $\overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2} \frac{\partial^2 E_N}{\partial k_i \partial k_j}$