6.730 Physics for Solid State Applications

Lecture 19: Motion of Electronic Wavepackets

Outline

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

Proof of Bloch's Theorem

Step 1: Translation operator commutes with Hamiltonain…
so they share the same eigenstates.

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R})$$

Translation and periodic Hamiltonian commute…

$$T_{\mathbf{R}}H(\mathbf{r})\psi(\mathbf{r}) = \mathbf{H}(\mathbf{r}+\mathbf{R})\psi(\mathbf{r}+\mathbf{R}) = \mathbf{H}(\mathbf{r})\psi(\mathbf{r}+\mathbf{R}) = \mathbf{H}(\mathbf{r})\mathbf{T}_{\mathbf{R}}\psi(\mathbf{r})$$

Therefore,

$$H\psi(\mathbf{r}) = \mathbf{E}\psi(\mathbf{r})$$

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\psi(\mathbf{r})$$

Step 2: Translations along different vectors add…
so the eigenvalues of translation operator are exponentials

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\mathbf{T}_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\mathbf{c}(\mathbf{R}')\psi(\mathbf{r})$$

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{T}_{\mathbf{R}+\mathbf{R}'}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R}+\mathbf{R}')\psi(\mathbf{r})$$

$$c(\mathbf{R}+\mathbf{R}') = \mathbf{c}(\mathbf{R})\mathbf{c}(\mathbf{R}')$$

$$c(\mathbf{R}) = \mathbf{e}^{\mathbf{ik}\cdot\mathbf{R}}$$

$$\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = \mathbf{e}^{\mathbf{ik}\cdot\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{R})$$

Momentum and Crystal Momentum

$$\hat{\mathbf{p}}\,\psi_{n,k} = \hbar k \psi_{n,k} + e^{ik\cdot r}\frac{\hbar}{i}\nabla \tilde{u}_{n,k}(r)$$

$$\hat{\mathbf{p}}\,\psi_{n,k} = e^{ik\cdot r}\hbar\left(k + \frac{1}{i}\nabla\right)\tilde{u}_{n,k}(r)$$

Leads us to, the action of the Hamiltonian on the Bloch amplitude….

$$e^{ik\cdot r}\left(\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k\right)^2 + V(r)\right)\tilde{u}_k(r) = E_k e^{ik\cdot r}\tilde{u}_k(r)$$

$$H_k\tilde{u}_k(r) \equiv \left(\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k\right)^2 + V(r)\right)\tilde{u}_k(r) = E_k\tilde{u}_k(r)$$

k.p Hamiltonian
(in our case q.p)

$$H_k \tilde{u}_k(r) = \left(\frac{\hbar^2}{2m} \left(\frac{1}{i} \nabla + k \right)^2 + V(r) \right) \tilde{u}_k(r)$$

If we know energies as k we can extend this to calculate energies at k+q for small q…

$$H_{k+q} = \frac{\hbar^2}{2m} \left(\frac{1}{i} \nabla + k + q \right)^2 + V(r)$$

$$H_{k+q} = H_k + \frac{\hbar^2}{m} q \cdot \left(\frac{1}{i} \nabla + k \right) + \frac{\hbar^2}{2m} q^2$$

k.p Hamiltonian

$$H_{k+q} = H_k + \frac{\hbar^2}{m} q \cdot \left(\frac{1}{i}\nabla + k\right) + \frac{\hbar^2}{2m} q^2$$

Taylor Series expansion of energies…

$$E_n(k+q) = E_n(k) + \sum_i \frac{\partial E_n}{\partial k_i} q_i + \frac{1}{2} \sum_{ij} \frac{\partial^2 E_n}{\partial k_i \partial k_j} q_i q_j + O(q^3)$$

Matching terms to first order in q…

$$\frac{\partial E_n}{\partial k_i} = \int dr\, \tilde{u}^*_{nk} \frac{\hbar^2}{m} \left(\frac{1}{i}\nabla + k\right)_i \tilde{u}_{nk}$$

$$\frac{\partial E_n}{\partial k_i} = \int dr\, \psi^*_{nk} \frac{\hbar}{m} \widehat{p}_i\, \psi_{nk} = \frac{\hbar}{m} < \widehat{p}_i >$$

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

Energy Surface for 2-D Crystal

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

In 2-D, circular energy contours result in $< \mathbf{v_n(k)} >$ parallel to $\mathbf{k}$

Energy Surface for 2-D Crystal

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

In general, for higher lying energies $< \mathbf{v_n(k)} >$ is not parallel to $\mathbf{k}$

Semiclassical Equation of Motion

$$\frac{d < \hat{T}_R >}{dt} = \frac{i}{\hbar}\langle[\hat{V}_{ext}, \hat{T}_R]\rangle = eE\frac{i}{\hbar}\langle[\hat{r}, \hat{T}_R]\rangle$$

Plugging in this commutation relation into the equation of motion…

$$\frac{d < \hat{T}_R >}{dt} = eE\frac{i}{\hbar}\langle[\hat{r}, \hat{T}_R]\rangle$$

$$= eER\,\frac{i}{\hbar}\langle\hat{T}_R\rangle$$

Solving the simple differential equation…

$$\langle\hat{T}_R\rangle = e^{ieE\,R\,t/\hbar}$$

From Bloch's Thm. We know the eigenvalues of T_R…

$$T_R\psi(r) = e^{ikR}\psi(r) \qquad \langle\hat{T}_R\rangle = e^{ik\,R}$$

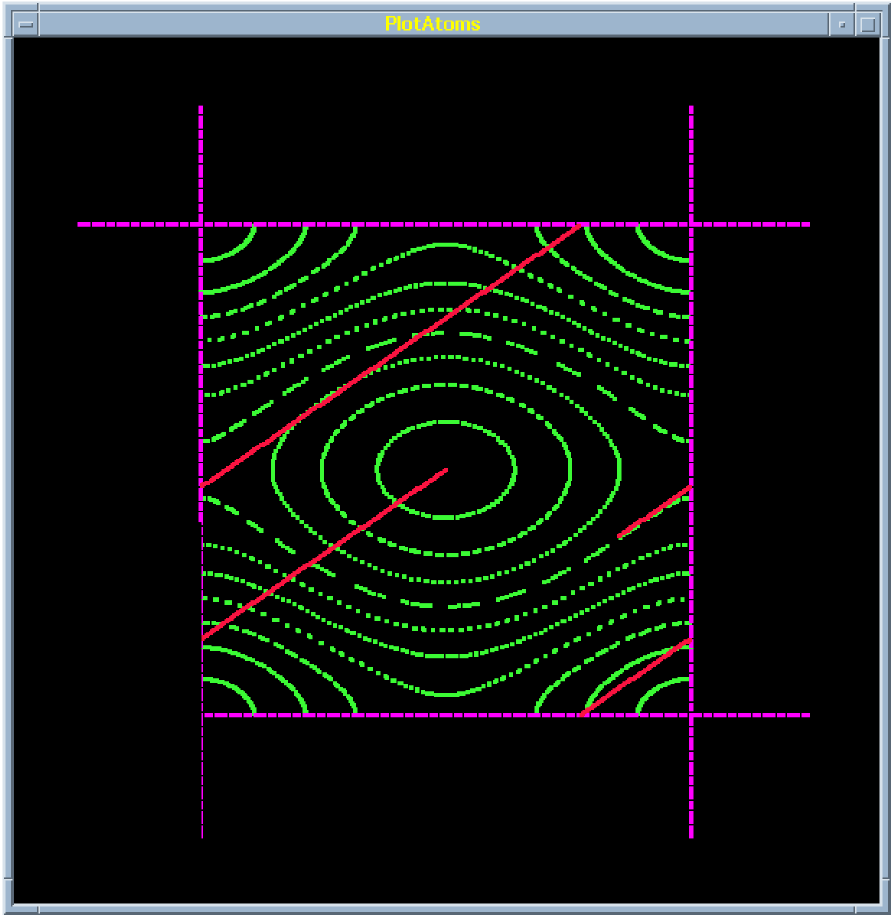
$$k = \frac{eE}{\hbar}t + k_0$$

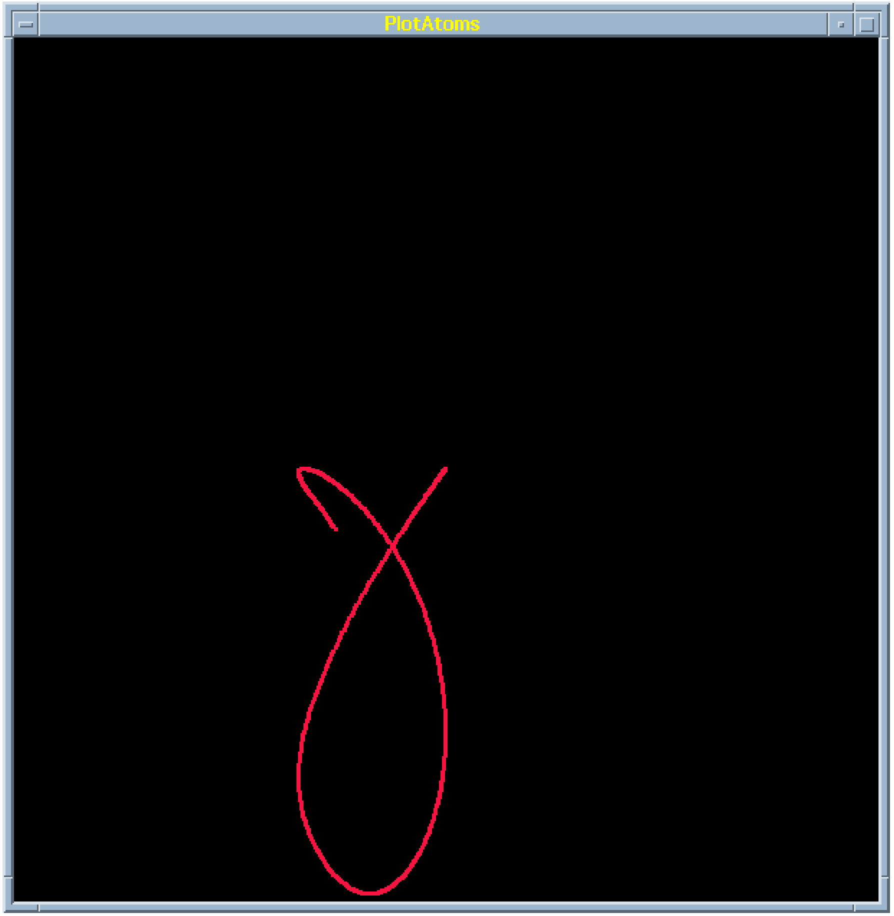
$$eE = \hbar\frac{dk}{dt}$$

$$\mathbf{F}_{\mathbf{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

Electron Motion in a Uniform Electric Field

2-D Crystal





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

Properties of the Translation Operator

Definition of the translation operator…

$$\hat{T}_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R})$$

Bloch functions are eigenfunctions of the lattice translation operator…

$$\hat{T}_{\mathbf{R}}\psi(\mathbf{r}) = \mathbf{c}(\mathbf{R})\psi(\mathbf{r})$$

$$c(\mathbf{R}) = \mathbf{e}^{\mathbf{ik}\cdot\mathbf{R}}$$

Lattice translation operator commutes with the lattice Hamiltonian (V_{ext}=0)

$$[\hat{T}_{\mathbf{R}}, H(\mathbf{r})] = \mathbf{0}$$

The translation operator commutes with other translation operators…

$$[\hat{T}_{\mathbf{R}_1}, \hat{T}_{\mathbf{R}_2}] = 0$$

Properties of the Translation Operator

Lets see what the action of the following operator is…

$$\left[e^{-R\frac{\partial}{\partial x}}\right] f(x) = \left(1 - R\frac{\partial}{\partial x} + \frac{1}{2!}R^2\frac{\partial^2}{\partial x^2} - \frac{1}{3!}R^3\frac{\partial^3}{\partial x^3} + \cdots\right) f(x)$$

$$= f(x) - Rf'(x) + \frac{1}{2!}R^2 f''(x) - \frac{1}{3!}R^3 f'''(x) + \cdots$$

$$= f(x - R)$$

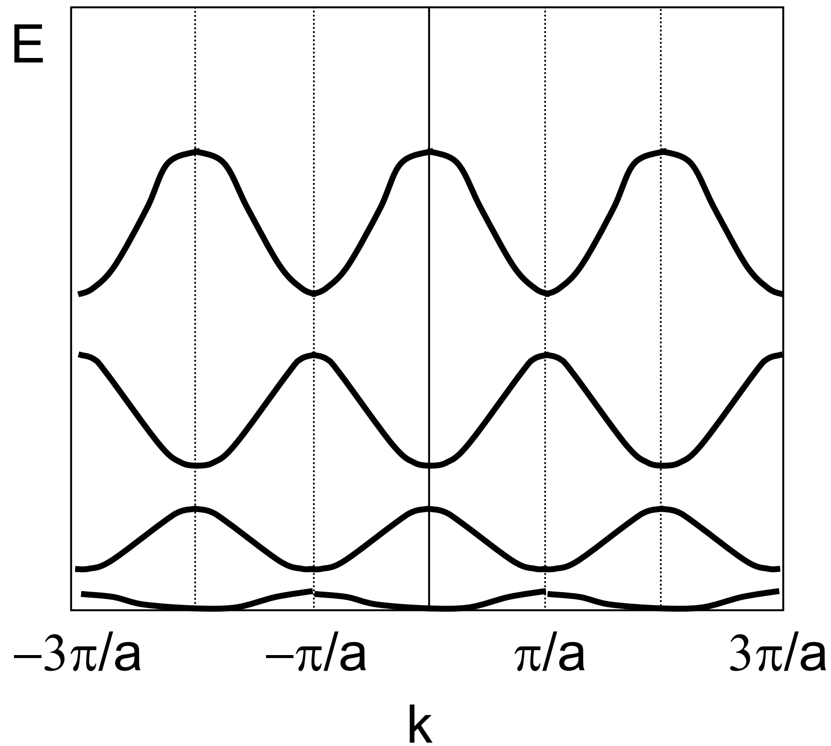
This is just the translation operator…

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

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

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)

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

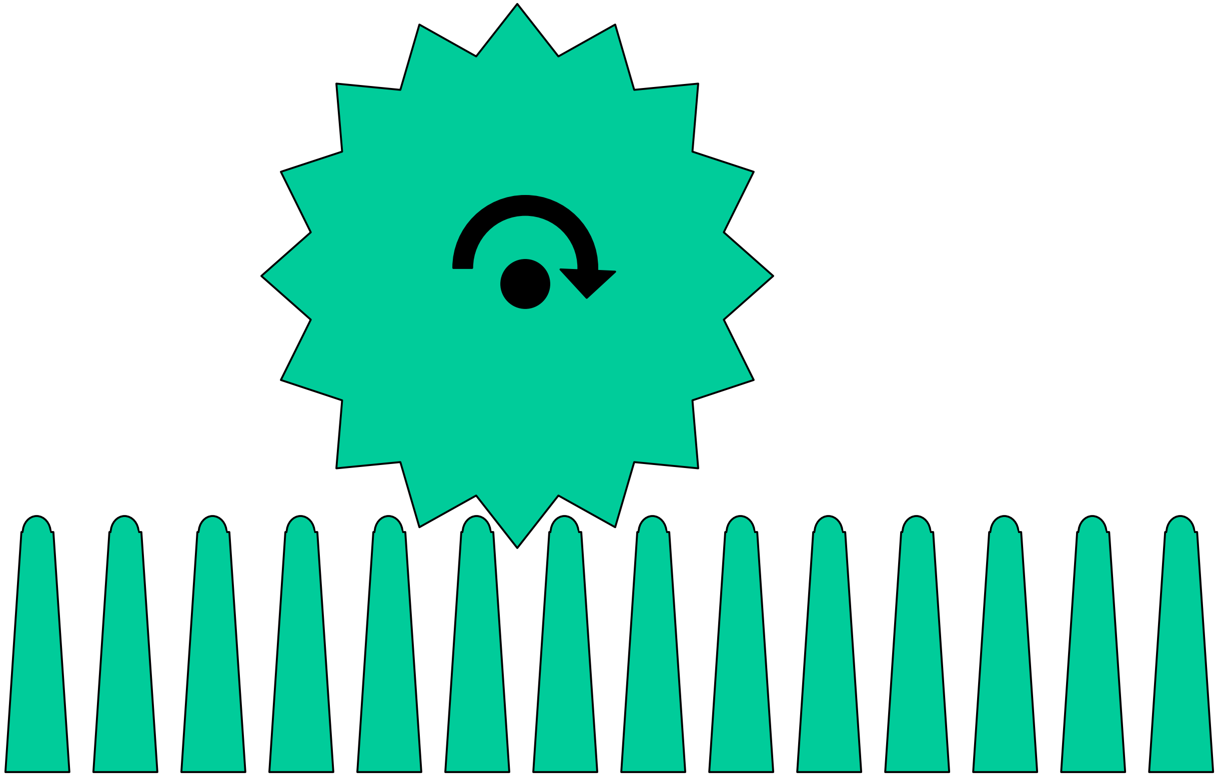
This suggests the operator on the left is just the crystal Hamiltonian !

$$\hat{H}_0 = \sum_\ell E_n(R_\ell)\,\hat{T}_{R_\ell}$$

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

Electron Wavepacket in Periodic Potential

Wavepacket in a dispersive media… $\mathbf{v_g} = \nabla_{\mathbf{k}}\omega(\mathbf{k})$



So long as the wavefunction has the same short range periodicity as the underlying potential, the electron can experience smooth uniform motion at a constant velocity.

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…

$$\psi'_n(r,t) = \sum_k c_n(k,t) \psi_{n,k}(r)$$

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

$$\psi'_n(r,t) \approx e^{-ik_0\cdot r} G_n(r,t) \psi_{n,k_0}(r) = G_n(r,t) u_{n,k_0}(r)$$

G is a slowly varying function…

$$G_n(r,t) = \sum_k c_n(k,t) e^{ik\cdot r}$$

Wavefunction of Electronic Wavepacket

$$\psi'_n(r,t) = e^{ik_0\cdot r} \underbrace{G_n(r,t)}_{\text{envelope function}} \underbrace{\psi_{n,k_0}(r)}_{\text{Bloch function}}$$

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

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

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

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

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

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

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

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

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…

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

Normalization of the Envelope Function

$$1 = \int \psi_n'^*(r,t)\psi_n'(r,t)d^3r$$

$$= \int G_n^*(r,t)G_n(r,t)\, u_{n,k_0}^*(r)u_{n,k_0}(r)d^3r$$

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

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

$$1 = \frac{1}{V_{\text{box}}}\sum_m G_n^*(R_m,t)G_n(R_m,t)\Delta$$

$$1 \approx \frac{1}{\text{V}_{\text{box}}}\int_{\text{box}} G_n^*(r,t)G_n(r,t)d^3r$$

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

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

$$< G_n(r,t)|\frac{\hbar}{i}\nabla_r|G_n(r,t) >$$

$$= \int_{box} \sum_{k'} c_n^*(k',t)\, e^{-ik'\cdot r} \frac{\hbar}{i}\nabla_r \left(\sum_{k''} c_n(k'',t) e^{ik''\cdot r} \right) d^3r$$

$$= \sum_{k'} \sum_{k''} c_n^*(k',t) c_n(k'',t) \hbar k'' \int_{box} e^{i(k''-k')\cdot r} d^3r$$

$$= \sum_{k'} \sum_{k''} c_n^*(k',t) c_n(k'',t) \hbar k'' \delta_{k',k''} V_{box}$$

$$= V_{box} \sum_{k'} |c_n^*(k',t)|^2 \hbar k' \approx V_{box} |c_n^*(k_0,t)|^2 \hbar k_0$$

$$< G_n(r,t)|G_n(r,t) > \quad = V_{box} \sum_{k'} |c_n^*(k',t)|^2 \approx V_{box} |c_n^*(k_0,t)|^2$$

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

but $< p > \neq \hbar k_0$

Summary

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

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

Bandstructure shows up in here… $\hat{H}_0 = \sum_{\ell} E_n(R_\ell)\, \hat{T}_{R_\ell}$

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

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

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