6.730 Physics for Solid State Applications

Lecture 20: Motion of Electronic Wavepackets

Outline

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

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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…

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

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

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...

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

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

$$= f(x - R)$$

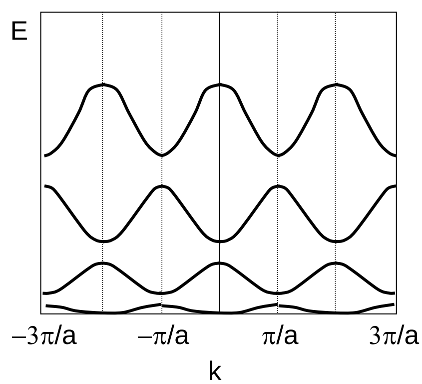
This is just the translation operator...

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

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

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)

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

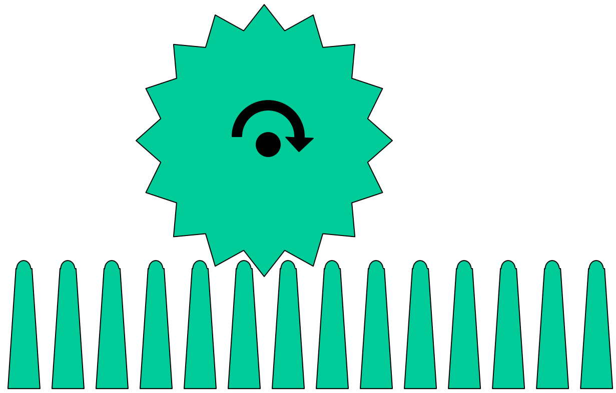
This suggests the operator on the left is just the crystal Hamiltonian !

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

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…

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

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

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

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

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

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

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

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

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

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

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

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

but $< p > \neq \hbar k_0$

Summary

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

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

Bandstructure shows up in here... $\widehat{H}_0 = \sum_{\ell} E_n[R_\ell]\, \widehat{T}_{R_\ell}$

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

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

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