Lecture 15

Announcement: HW 3 extended until 10/23

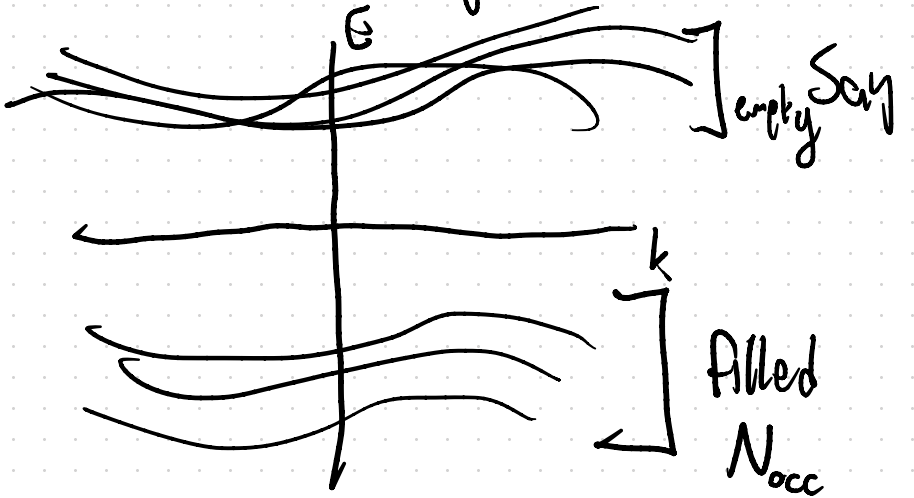
Two stories

1. A Hamiltonian, invariant under a space group $G \rightarrow$ Bloch's theorem $\rightarrow$ a set of delocalized $\psi_{nk}(\vec{r}) = e^{ikr} u_{nk}(r)$

2. "Chemistry" approach: start w/ atoms, bond to form a crystal "donate" e⁻s to form bands $\rightarrow$ band structure built up from localized states

(2) → (1) straightforward · Write down Schrödyer eqn for all atoms and electrons → turn the crank → energies and eigenstates

How about going from (1) → (2)



Say we have an insulator

$E_{nk}, |\psi_{nk}\rangle$

Can we find localized orbitals from linear combinations of $\{|\psi_{nk}\rangle\}_{n=1}^{N_{occ}}$

We can start by looking at $\hat{x}$

P - projection operator onto N_{occ} filled states

$$P|\psi_{nk}\rangle = \begin{cases} |\psi_{nk}\rangle & \text{if } n = 1, \dots, N_{occ} \\ 0 & \text{otherwise} \end{cases}$$

$P\hat{x}P$ - projected position operator

$\langle \psi_{nk} | P\hat{x}P | \psi_{mk'} \rangle$ only nonzero if $n, m \in \{1, \dots, N_{occ}\}$

$$= \int d^3r \left(\psi_{nk}(\vec{r})\right)^* \vec{r}\, \psi_{mk'}(\vec{r})$$

Problem - $\psi_{nk}(r)$ not normalizable

and $\vec{r} \to \infty$

Continuum normalization: $\langle \psi_{nk} | \psi_{mk'} \rangle = \delta_{nm} \delta(k-k') \frac{(2\pi)^3}{v}$

v - volume of the primitive unit cell

$$|\vec{e}_1 \cdot (\vec{e}_2 \times \vec{e}_3)|$$

$$\int_{BZ} d^3k = \frac{(2\pi)^3}{v}$$

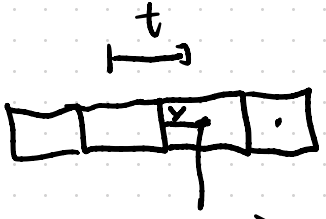
choose $|\psi_{n k+\vec{G}}\rangle = |\psi_{n\vec{k}}\rangle$ for all $\vec{G} \in \mathcal{T}$

let k and k' both be in the first BZ

$$\sum_{t \in T} e^{i(k-k')\cdot \vec{t}} = \frac{(2\pi)^3}{v} \sum_{G \in \mathcal{T}} \delta(k-k'-\vec{G})$$

$$= \frac{(2\pi)^3}{v}\delta(k-k')$$

Normalisation: $\delta_{nm}\delta(k-k')\frac{(2\pi)^3}{v} = \int d^3r\ \psi^*_{nk}(r)\psi_{mk'}(r)$



$$= \int d^3r \left(e^{ik\cdot r}u_{nk}(r)\right)^* \left(e^{ik'\cdot r}u_{mk'}(r)\right)$$

$$= \int d^3r\, e^{i(k'-k)\cdot r}\, u^*_{nk}(r)\,u_{mk'}(r)$$

$$= \sum_t \int_{cell} d^3y\, e^{i(k'-k)\cdot t}\, e^{i(k'-k)\cdot y}\, u^*_{nk}(y)\,u_{mk'}(y)$$

$$= \frac{(2\pi)^3}{v}\delta(k-k')\int_{cell} d^3y\, u^*_{nk}(y)\,u_{mk}(y)$$

$$\langle u_{nk} | u_{mk} \rangle_{cell} = \int_{cell} d^3r \, u^*_{nk}(r) u_{mk}(r) = \delta_{nm}$$

$\mu = x, y, z$

$$\langle \psi_{nk} | p_x^\mu p | \psi_{mk'} \rangle = \int d^3r \, \psi^*_{nk}(\vec{r}) \, p^\mu \, \psi_{mk'}(\vec{r})$$

$$= \int d^3r \, r^\mu e^{i(k'-k)\cdot r} \, u^*_{nk}(r) u_{mk'}(r)$$

$$= \int d^3r \; i \frac{\partial}{\partial k^\mu} \left(e^{i(k'-k)\cdot r} \right) u^*_{nk}(r) u_{mk'}(r)$$

$$= i \frac{\partial}{\partial k^\mu} \left[\int d^3r \, \psi^*_{nk}(r) \psi_{mk'}(r) \right] - i \int d^3r \, e^{i(k'-k)\cdot r} \frac{\partial u^*_{nk}(r)}{\partial k^\mu} u_{mk'}(r)$$

$$= i\frac{(2\pi)^3}{\tau}\delta_{nm}\frac{\partial}{\partial k^\mu}\delta(k-k') - i\sum_{\text{cell}\in T}\int_{\text{cell}} dy\, e^{i(k'-k)\cdot(y+t)}\frac{\partial u^*_{nk}(y)}{\partial k^\mu}u_{mk'}(y)$$

$$= i\frac{(2\pi)^3}{\tau}\left[\delta_{nm}\frac{\partial}{\partial k^\mu}\delta(k-k') + \delta(k-k')\int_{\text{cell}} dy\; u^*_{nk}(r)\frac{\partial u_{mk}(y)}{\partial k^\mu}\right]$$

$$= \frac{(2\pi)^3}{\tau}\left[i\delta_{nm}\frac{\partial}{\partial k^\mu}\delta(k-k') + \delta(k-k')A^{nm}_\mu(k)\right] = \langle\psi_{nk}|p_\mu|\psi_{mk'}\rangle$$

$$\rightsquigarrow A^{nm}_\mu(k) = i\int_{\text{cell}} d^3y\; u^*_{nk}(y)\frac{\partial u_{mk}(y)}{\partial k^\mu}$$

Berry connection

$$= i\left\langle u_{nk}\middle|\frac{\partial u_{mk}}{\partial k^\mu}\right\rangle_{\text{cell}}$$

$$P = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}|$$

Lets define a wavepacket $$|f\rangle = \frac{v}{(2\pi)^3}\int d^3k' \sum_{m=1}^{N_{occ}} |\psi_{mk'}\rangle f_{mk'}$$

$$P x^\mu P |f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}| x^\mu |f\rangle$$

$$= \sum_{m=1}^{N_{occ}} \int d^3k' \left(\frac{v}{(2\pi)^3}\right)^2 \int dk \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}| x^\mu |\psi_{mk'}\rangle f_{mk'}$$

$$= \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle \left(i\frac{\partial f_{nk}}{\partial k^\mu} + \sum_m A^{nm}_\mu(k) f_{mk} \right)$$

$$\simeq \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle [iD_\mu f]_{nk} \qquad D_\mu = \frac{\partial}{\partial k^\mu} - iA_\mu$$

↑ covariant derivative

on wavepackets, $[x^\mu, \cdot]$ acts like a covariant derivative

covariant w.r.t change of basis

$$|\psi'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |\psi_{mk}\rangle U_{mn}(k) \qquad U(k) \in N_{occ} \times N_{occ} \text{ unitary matrix}$$

$$U_{mn}(k+G) = U_{mn}(k)$$

$$P' = \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi'_{nk}\rangle\langle\psi'_{nk}|$$

$$= \frac{v}{(2\pi)^3} \int d^3k \sum_{m,n=1}^{N_{occ}} |\psi_{mk}\rangle U_{mn}(k) U^{\dagger}_{ln} \langle \psi_{ek}| \quad \delta_{ml}$$

$$= P$$

P is invariant under $U(N_{occ})$ gauge transformation

$$|f\rangle = \frac{v}{(2\pi)^3} \int d^3k \sum_{n=1}^{N_{ec}} f_{nk} |\psi_{nk}\rangle = \frac{v}{(2\pi)^3} \int d^3k \sum_{m=1}^{N_{ec}} f'_{mk} |\psi'_{mk}\rangle$$

$$\vec{f}'_k = U^{\dagger}(k) \vec{f}_k$$

$$|\psi'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |\psi_{mk}\rangle U_{mn}(k) \quad \text{def}$$

$$|u'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |u_{mk}\rangle U_{mn}(k)$$

Berry connection

$$A'^{mn}_{m}(k) = i \langle u'_{nk} | \frac{\partial}{\partial k^m} u'_{mk} \rangle_{cell}$$

$$= i \sum_{l,p=1}^{N_{occ}} U^{\dagger}_{nl}(k) \langle u_{lk} | \left(\frac{\partial}{\partial k^m} \left(|u_{pk}\rangle U_{pn}(k) \right) \right)$$

$$= [U^{\dagger} A_m(k) U]^{nn} + i \left[U^{\dagger} \frac{\partial U}{\partial k^m} \right]^{nn}$$ ← transforms like a gauge field / vector potential

$$[D_m \vec{f}]'_{nk} = U^{\dagger}(k) [D_m f]$$

$$= U^{\dagger}(k) D_\mu [U f']$$

$$= U^{\dagger}(k) \left[\frac{\partial}{\partial k^\mu} (U f') - i A_\mu U f' \right]$$

$$= \frac{\partial f'}{\partial k^\mu} - i U^{\dagger} A_\mu U f' + U^{\dagger} \frac{\partial U}{\partial k^\mu} f'$$

$$= \frac{\partial f'}{\partial k^\mu} - i A'_\mu f' \equiv D'_\mu f'$$

D_μ is covariant under basis transformations

Given e^-s in our occupied states, what values can we find if we measure the position of an electron

$$P_{x^m} P$$

How localized (in position) can we make an electron just using $\{|\psi_{nk}\rangle\}_{n=1}^{N_{occ}}$

→ Eigenstates & Eigenvalues of $P_{x^m} P$

$$P_{x^m} P |f\rangle = \lambda |f\rangle$$

$$\|$$

$$\frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{bc}} |\psi_{nk}\rangle [iD_n f]_{nk} = \frac{v}{(2\pi)^3}\int d^3k\, |\psi_{nk}\rangle \lambda f_{nk}$$

$$iD_n f_{nk} = \lambda f_{nk}$$

$$f_{nk+G} = f_{nk}$$

lattice coordinates: $x_i = \frac{1}{2\pi}\vec{b}_i \cdot \vec{x}$

$\vec{b}_i$ ↑ primitive reciprocal lattice vector

$$\vec{x} = x_1\vec{e}_1 + x_2\vec{e}_2 + x_3\vec{e}_3$$

e_i - primitive lattice vectors

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 \qquad k_i = \vec{e}_i \cdot \vec{k}$$

$k_j \in [-\pi, \pi)$

$$P_{x_i} P |f\rangle = \lambda f$$

$$D_i f = \frac{\partial}{\partial k_i} \vec{f} - i A_i(k) \vec{f} = \lambda \vec{f}$$

$$f_{nk+G} = f_{nk}$$

Simplest case: $N_{occ} = 1$