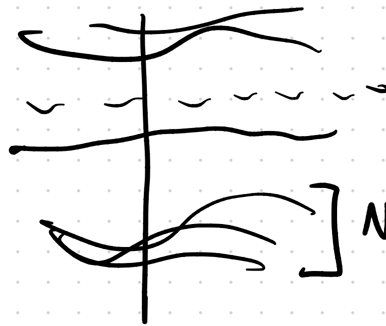
Lecture 16 | Reminder: HW 3 is due next week 10/23

cryst.ehu.es

Last time



N_{occ} filled bands

$$\{|\psi_{nk}\rangle\}_{n=1}^{N_{occ}}$$

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

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

$$P x_i P |f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle [iD_i f]_{nk}$$

$$[D_i f]_{nk} = \frac{\partial f_{nk}}{\partial k_i} - i\sum_{m=1}^{N_{occ}} A_i^{nm}(k) f_{mk}$$

$$A_i^{nm}(k) = \left\langle u_{nk} \middle| \frac{\partial u_{mk}}{\partial k_i} \right\rangle_{cell}$$ vector index

$$i D_i \vec{f}_k = \lambda \vec{f}_k$$

$$\vec{f}_{k+G} = f_k \qquad \vec{G} \in \check{T} \text{ a reciprocal lattice vectors}$$

Simplest case $N_{occ} = 1$

$$A_i(k) = \left\langle u_k \middle| \frac{\partial u_k}{\partial k_i} \right\rangle$$

$$\vec{f}_k \to f_k$$

$$\boxed{\begin{aligned} \lambda f_k &= i \frac{\partial f_k}{\partial k_i} + A_i(k) f_k \\ f_{k+\vec{G}} &= f_k \end{aligned}}$$

$$\vec{k} = \frac{1}{2\pi} k_i \vec{b}_i + \vec{k}_\perp$$

$$f_{\vec{k}} = f(k_j, k_\perp)$$

$$\lambda = \lambda(k_\perp)$$

$$\lambda(k_\perp) f(k_j, k_\perp) = i \frac{\partial f(k_j, k_\perp)}{\partial k_j} + A(k_j, k_\perp) f(k_j, k_\perp)$$

ansatz $\quad f(k_j, \vec{k}_\perp) = g(k_j, \vec{k}_\perp) e^{i \int_{k_0}^{k_j} dk_j' A_i(k_j, k_\perp)}$

$$i \frac{\partial}{\partial k_j} g(k_j, \vec{k}_\perp) = \lambda(\vec{k}_\perp) g(k_j, \vec{k}_\perp)$$

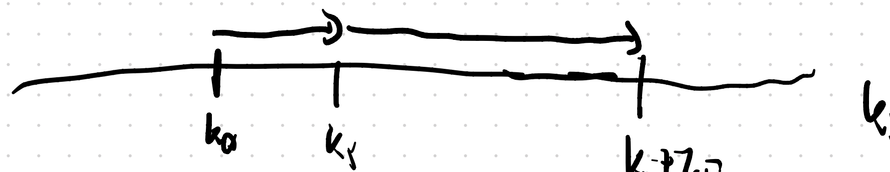
$$g(k_j, k_\perp) = C(\vec{k}_\perp) e^{-i \lambda(k_\perp) k_j}$$

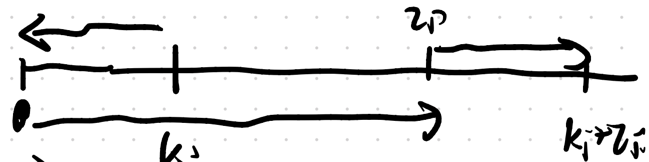
$$\boxed{f(k_j, k_\perp) = C(k_\perp) e^{i \int_{k_0}^{k_j} dk_j' A_i(k_j', \vec{k}_\perp) - i \lambda(k_\perp) k_j}}$$

$$f(k_j+2\pi, \vec{k}_\perp) = f(k_j, \vec{k}_\perp)$$

$$e^{i\int_{k_0}^{k_j+2\pi} dk_j' A_j(k_j', k_\perp) - i\lambda(k_\perp)(\cancel{k_j}+2\pi)} = e^{i\int_{k_0}^{k_j} dk_j A_j(k_j, \vec{k}_\perp) \cancel{- i\lambda(k_\perp)k_j}}$$

$$e^{i\lambda(k_\perp)2\pi} = e^{i\left[\int_{k_j}^{k_j+2\pi} dk_j A_j(k_j,k_\perp) - \cancel{\int_{k_0}^{k_j} dk_j A_j(k_j,k_\perp)}\right]}$$





$$e^{i\lambda(k_\perp)2\pi} = e^{i\int_0^{2\pi} dk_j A_j(k_j,k_\perp)} = e^{i\varphi(k_\perp)}$$

$\varphi(k_\perp)$ Berry phase

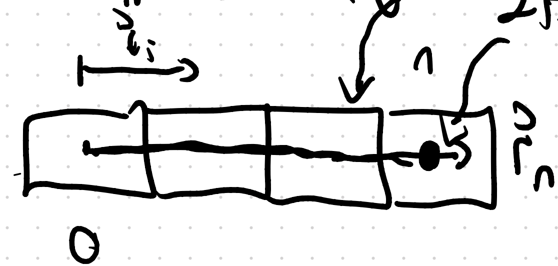
$$\lambda(k_\perp) = \frac{\varphi(k_\perp)}{2\pi} + n$$

$$x_i = \frac{\vec{x} \cdot b_i}{2\pi}$$

$$\vec{x} = x_i \vec{t}_i + \vec{x}_\perp$$

Px_iP has eigenvalues $n + \frac{\varphi(k_\perp)}{2\pi}$

$P\vec{t}_i x_i P$ has eigenvalues $\vec{r}_n(k_\perp) = \vec{t}_i \left(n + \frac{\varphi(k_\perp)}{2\pi}\right)$



Berry phase gives the displacement of $\vec{r}_n$ relative to the center of the unit cell

Eigenfunctions $|W_{n\vec{k}_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_i \, |\psi_k\rangle e^{i\left[\int_{k_0}^{k_j} dk_i' A_i(k_i, k_\perp) - \frac{k_j \varphi(k_\perp)}{2\pi} - nk_j\right]}$

$$P x_j P |W_{nk_\perp}\rangle = \left(n + \frac{\varphi(k_\perp)}{2\pi}\right) |W_{n\vec{k}_\perp}\rangle$$

Hybrid Wannier functions localised in the x_j direction

$b_i \cdot \vec{t}_\perp = 0$

$$U_{\vec{t}_\perp} |W_{n\vec{k}_\perp}\rangle = e^{-i\vec{k}_\perp \cdot \vec{t}_\perp} |W_{nk_\perp}\rangle$$

Localization: $\Omega[f] = \langle f | P x_i^2 P | f\rangle - |\langle f | P x_i P | f\rangle|^2$ $\quad P|f\rangle = |f\rangle$

$$x_i^2 = x_i x_i = x_i P x_i + x_i (1-P) x_i$$

$$\Omega[f] = \langle f|Px_iPx_iP|f\rangle - |\langle f|Px_iP|f\rangle|^2$$

Vanishes when $|f\rangle = |W_{nk_\perp}\rangle$

$$+ \langle f|Px_i(1-P)x_iP|f\rangle$$

Hybrid Wannier functions minimize $\Omega[f]$

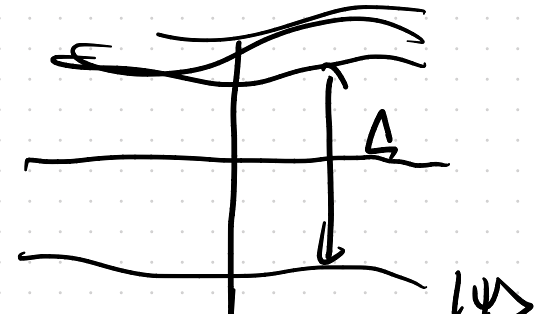
$$|\tilde{\psi}_{\vec{k}}\rangle = |\psi_k\rangle e^{i\int_{k_0}^{k_j} dk_j' A(k_j', k_\perp) - \frac{k_j \varphi(k_\perp)}{2\pi}}$$

$$|W_{nk_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_j\, |\tilde{\psi}_{\vec{k}}\rangle e^{-ink_j}$$

$$\langle \tilde{u}_k | \frac{\partial \tilde{u}}{\partial k_j}\rangle = \left(\cancel{\langle u_k | \frac{\partial u_k}{\partial k}\rangle} + i\cancel{A_i(\vec{k})} - \frac{1}{2\pi}\varphi(k_\perp)\right)$$

$$= \frac{1}{2\pi}\varphi(k_\perp)$$

Diagonalizing $P x_i P$ tells us how to pick the best/smoothest phase for $|\tilde{\Psi}_k\rangle$



Kohn, Phys Rev 1959

des Cloizeaux, 1963, 1964

if we have a gap $|\tilde{\Psi}_{k_i, k_2}\rangle$ as a function of $k_i = k_1 + i k_2$

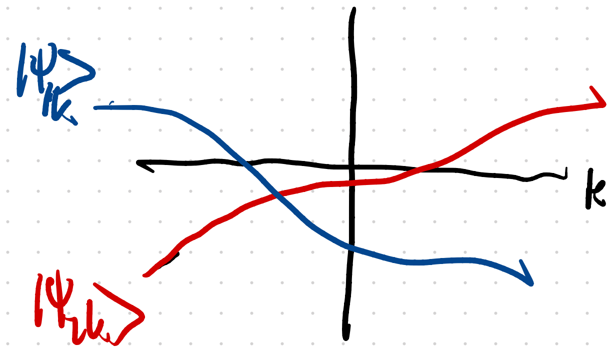
$k_2 \in [-\varkappa, \varkappa]$

$\varkappa \sim \sqrt{\Delta}$

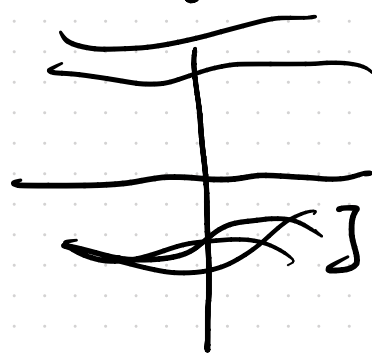
inverting F.T.

$$|\Psi_k\rangle = \sum_n |W_{nk_2}\rangle e^{i(k_1+ik_2)n} \Rightarrow |W_{nk_2}\rangle \text{ is exponentially decaying } |W_{nk_2}\rangle \propto e^{-n|k_2|}$$

$|W_{nk_\perp}\rangle$ is exponentially localized in the x_j direction



Now - general case



$\Big]N_{occ}$ $\{|\psi_{ak}\rangle,\ a=1,\dots,N_{occ}\}$

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

We want

vector index

$$|W_{an k_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_i \sum_{b=1}^{N_{occ}} |\psi_{b k_i, k_\perp}\rangle f^{b}_{an}(k_i, k_\perp)$$

band index unit cell index

label the eigenvalue

$$P x_i P |W_{ank_\perp}\rangle = \lambda_{an}(k_\perp)|W_{ank_\perp}\rangle$$

$$\boxed{\begin{aligned} i D_i \vec{f}_{an}(k_i,k_\perp) &= \lambda_{an}(k_\perp) f_{an}(k_i,k_\perp) \\ \vec{f}_{an}(k_i+2\pi,k_\perp) &= \vec{f}_{an}(k_i,k_\perp) \end{aligned}}$$

$$\lambda_{an}(k_\perp) f^b_{an}(k_i, k_\perp) = i \frac{\partial f^b}{\partial k_i} + \sum_{c=1}^{N_{occ}} A_i^{bc} f^c_{an}(k_i, k_\perp)$$

lets introduce a matrix $W^{(k_\perp)}_{k_i \leftarrow k_0}$

$$\boxed{\begin{gathered} i \frac{\partial W_{k_i \leftarrow k_0}}{\partial k_i} = -A_i(k_i, k_\perp) W^{(k_\perp)}_{k_i \leftarrow k_0} \\ W_{k_0 \leftarrow k_0}(k_\perp) = \mathrm{Id} \end{gathered}}$$

given W $\quad f^b_{an}(k_i, k_\perp) = \sum_{c=1}^{N_{occ}} W^{bc}_{k_i \leftarrow k_0}(k_\perp)\, g^c_{an}(k_i, k_\perp)$

Solved by a <u>path-ordered exponential</u>

$$W_{k_j \leftarrow k_0}(k_\perp) = P e^{i\int_{k_0}^{k_j} dk_i A_i(k_i, k_\perp)}$$

Path ordering: $$W_{k_2 \leftarrow k_0}(k_\perp) = W_{k_2 \leftarrow k_1}(k_\perp)\, W_{k_1 \leftarrow k_0}(k_\perp)$$

$$W^\dagger_{k_1 \leftarrow k_0}(k_\perp) = W_{k_0 \leftarrow k_1}(k_\perp)$$

using the ansatz

$$i \frac{\partial g^{b}_{an}}{\partial k_i} = \lambda_{an}(k_\perp)\, g^{b}_{an}(k)$$

$$\vec{g}_{an} = \vec{C}(k_\perp, k_0)\, e^{-i\lambda_{an}(k_\perp) k_i}$$

$$f^{b}_{an}(k_j, k_\perp) = \sum_{c=1}^{N_{occ}} W^{bc}_{k_j \leftarrow k_0} C^{c}_{an}(k_\perp, k_0) e^{-j\lambda_{an}(k_\perp) k_j}$$

$$f^{b}_{an}(k_j + 2\pi, k_\perp) = f^{b}_{an}(k_j, k_\perp)$$

$$e^{-2\pi j \lambda_{an}(k_\perp)} W_{k_j+2\pi \leftarrow k_0}(k_\perp) \cdot \vec{C}_{an}(k_\perp) = W_{k_j \leftarrow k_0}(k_\perp) \cdot \vec{C}_{an}(k_\perp)$$

$$\shortparallel$$

$$W_{k_j+2\pi \leftarrow k_0+2\pi}(k_\perp) \, W_{k_0+2\pi \leftarrow k_0}(k_\perp)$$

$$W_{k_0+2\pi \leftarrow k_0}(k_\perp) \cdot \vec{C}_{an}(k_\perp) = e^{2\pi j \lambda_{an}(k_\perp)} \vec{C}_{an}(k_\perp)$$

$\Rightarrow \vec{C}_{an}(k_\perp, k_0)$ is an eigenvector of $W_{k_0+2\pi \leftarrow k_0}(k_\perp)$

with eigenvalue $e^{2\pi i \lambda_{an}(k_\perp)}$

eigenvalues of $W_{k_0+2\pi \leftarrow k_0}(k_\perp)$ are $e^{i\varphi_a(k_\perp)}$ ← non-abelian Berry phase

$P_{x_j}P$ eigenvalues $\lambda_{an}(k_\perp) = n + \frac{\varphi_a(k_\perp)}{2\pi}$

$$|W_{ank_\perp}\rangle = \frac{1}{2\pi} \sum_{b,c=1}^{N_{occ}} \int_{k_0}^{k_0+2\pi} dk_j \, |\psi_{bk_j}\rangle e^{-\left[\frac{\varphi_a(k_\perp)}{2\pi}+n\right]k_j} W^{bc}_{k_j \leftarrow k_0}(k_\perp) \, \vec{C}_a(k_\perp, k_0)$$

where $\vec{C}_a(k_1, k_0)$ is an eigenvector of
$W_{k_0+2\pi \leftarrow k_0}(k_1)$ w/ eigenvalue $e^{i\varphi_a(k_1)}$