Lecture 15 | Recap: looking @ eigenstates of $P x_i P$

Single band: $P = \frac{V}{(2\pi)^3}\int d^3k\, |\psi_k\rangle\langle\psi_k|$

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

$$\varphi(k_\perp) = \int_0^{2\pi} dk_i\, A_i(k_i, \vec{k}_\perp) \quad \text{- Berry phase}$$

$$P x_i P |W_n \vec{k}_\perp\rangle = \left(n + \frac{1}{2\pi}\varphi(\vec{k}_\perp)\right)|W_n k_\perp\rangle$$

indexes unit cells in the

displacement relative to the origin of the unit

$\vec{t}_i$ direction cel

How localized are the $|W_{n\vec{k}_\perp}\rangle$?

We can compute $\Omega_{ii} = \langle W_{n\vec{k}_\perp} | x_i^2 | W_{nk_\perp}\rangle$

$$- |\langle W_{n\vec{k}_\perp} | x_i | W_{nk_\perp}\rangle|^2$$

$$x_i^2 = x_i [P + (I d - P)] x_i \qquad I d - P \equiv Q$$

projects onto all unoccupied states

$$\Omega_{ii} = \langle W_{n\vec{k}_\perp} | P x_i Q x_i P | W_{nk_\perp}\rangle$$

if P is a projection operator, $P^2 = P$

$$\cancel{+\left[\langle W_{nk_\perp}|Px_iPx_iP|W_{nk_\perp}\rangle - \left|\langle W_{nk_\perp}|Px_iP|W_{nk_\perp}\rangle\right|^2\right]} \to 0$$

$$Px_iPx_iP = (Px_iP)(Px_iP)$$

if $Px_iP|W_{nk_\perp}\rangle = \lambda|W_{nk_\perp}\rangle$

$\to$ Ω_{ii} is minimized for Hybrid Wannier functions

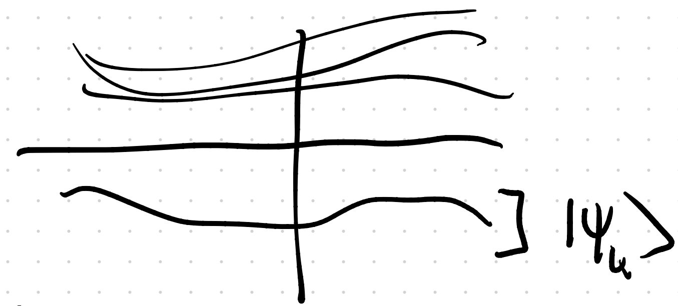
$$|W_{n\vec{k}_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_i \left(\underbrace{|\psi_k\rangle \, e^{i\left[\int_{k_0}^{k_i} dk_i' \, A_i(k_i,\vec{k}_\perp) - \frac{k_i}{2\pi}\varphi(k_\perp)\right]}}_{\equiv\, |\tilde{\psi}_k\rangle} \right) e^{-ik_i n}$$

$$|\tilde{\psi}_{k+G}\rangle = |\tilde{\psi}_k\rangle$$

for $G \in \check{T}$

$$|W_{nk_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_i \, |\Psi_k\rangle e^{-ik_i n}$$

if $|\Psi_k\rangle$ is separated from all all eigenstates of the Hamiltonian by an energy gap

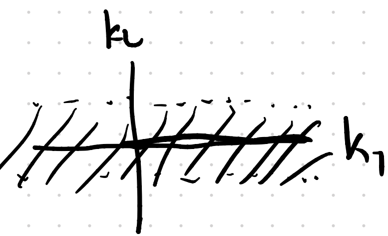


Then it can be shown (Kohn, Phys Rev 1959
des Cloizeaux 1963, 1964)

that we can view $|\tilde{\Psi}_{\vec{k}}\rangle$ as a fn of $\vec{k}_\perp$, and

$$k_i = k_1 + i k_2$$

and $|\tilde{\Psi}_{k_1+ik_2,\vec{k}_\perp}\rangle$ is an analytic function



of $k_1 + i k_2$ for $k_1 \in [0, 2\pi]$

$k_2 \in (-\kappa, \kappa)$ $\kappa \sim \sqrt{\text{energy gap}}$

$$|\tilde{\Psi}_{k_1+ik_2,k_\perp}\rangle = \sum_{n=-\infty}^{\infty} |W_{n k_\perp}\rangle e^{i(k_1+ik_2)n}$$

sum is only convergent if $|W_{n k_\perp}\rangle \sim e^{-\kappa|n|}$

→ Hybrid Wannier fns are exponentially localized,

localization length $\frac{1}{\sqrt{\Delta}}$

$|f\rangle =$ 

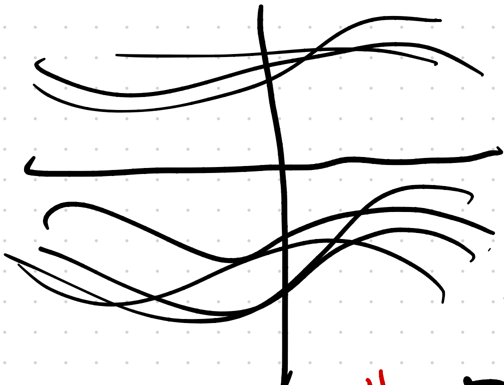
$$\langle f | \hat{\Psi}_{k_1+ik_2, k_2}\rangle = \sum_{n=-\infty}^{\infty} \langle f | W_{nk_1}\rangle e^{i(k_1+ik_2)n}$$

$$= \sum_{n=-\infty}^{\infty} \langle f | W_{nk_1}\rangle e^{ik_1 n} e^{-k_2 n}$$

$$\langle f | W_{nk_1}\rangle \sim e^{-\varkappa |n|}$$

Next: General case

$x_i = \vec{b}_i \cdot \vec{x}$



Filled $|\psi_{ak}\rangle$, $a = 1, \dots, N$

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

unit cell index

band index $1, \dots, N$

We want
$$|W_{an\vec{k}_\perp}\rangle = \frac{1}{2\pi} \int_{k_0}^{k_0+2\pi} dk_i \sum_{b=1}^{N} |\psi_{bk}\rangle f_b^{an}(k_i, k_\perp)$$

s.t.
$$P x_i P |W_{ank_\perp}\rangle = \lambda_{an}(\vec{k}_\perp) |W_{ank_\perp}\rangle$$

$$i\left[D_i f^{an}\right]_{b\vec{k}} = i\left(\frac{\partial f_b^{an}}{\partial k_i} - i\sum_{c=1}^{N} A_i^{bc} f_c^{an}\right) = \lambda_{an}(k_\perp) f_b^{an}$$

To solve this, introduce a matrix $W_{k_i\leftarrow k_0}$ that solves

$$i\frac{\partial W_{k_i\leftarrow k_0}}{\partial k_i} = -A_i(k_i, k_\perp) W_{k_i\leftarrow k_0}$$

c.f. $W \leftrightarrow U(t, t_0)$

$A \leftrightarrow H$

then this is like the Schrödinger equation

$$W_{k_0\leftarrow k_0} = \mathrm{Id}$$

$$\Rightarrow W_{k_i\leftarrow k_0}(k_\perp) = P e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i', \vec{k}_\perp)}$$

"Path ordered exponential"

$$W_{k_2 \leftarrow k_0} = W_{k_2 \leftarrow k_1} W_{k_1 \leftarrow k_0}$$

Now define $$F^{an}_b(k_i, k_\perp) = \sum_{c=1}^{N} W^{bc}_{k_i \leftarrow k_0}(k_\perp)\, g^{an}_c(\vec{k}, k_0)$$

$$\Rightarrow \quad i\frac{\partial}{\partial k_i} g^{an}_c(\vec{k}, k_0) = \lambda_{an}(k_\perp)\, g^{an}_c(\vec{k})$$

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

Now enforce periodicity

$$f_b^{na}(k_i+2\pi, \vec{k}_\perp) = f_b^{na}(k_i, \vec{k}_\perp)$$

$$\Rightarrow W^{(k_\perp)}_{k_i+2\pi \leftarrow k_0} \vec{g}^{an}(k_\perp, k_0) e^{-2\pi i \lambda_{an}(k_\perp)} = W_{k_i \leftarrow k_0} \vec{g}^{an}(\vec{k}_\perp, k_0)$$

$$\boxed{\cancel{W^{(k_\perp)}_{k_i+2\pi \leftarrow k_0+2\pi}}} W^{(k_\perp)}_{k_0+2\pi \leftarrow k_0} \vec{g}^{an}(k_\perp, k_0) e^{-2\pi i \lambda_{an}(k_\perp)} = \boxed{\cancel{W_{k_i \leftarrow k_0}}} \vec{g}^{an}(\vec{k}_\perp, k_0)$$

$$\boxed{W^{(k_\perp)}_{\underline{k_0+2\pi \leftarrow k_0}} \vec{g}^{an}(k_\perp, k_0) = e^{2\pi i \lambda_{an}(k_\perp)} \vec{g}^{an}(k_\perp, k_0)}$$

$\vec{g}^{an}$ is an eigenvector of $W^{(k_\perp)}_{k_0+2\pi \leftarrow k_0}$ w/ eigenvalue $e^{i\lambda_{an}(k_\perp)2\pi}$

let $W^{(k_\perp)}_{k_0+2\pi \leftarrow k_0}$ have eigenvalues $e^{i\varphi_a(k_\perp)}$

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

$$\vec{f}^{an}(\vec{k}) = W_{k_i \leftarrow k_0} \vec{g}^{a}(k_0, k_\perp) e^{-i\left[\frac{\varphi_a(k_\perp)}{2\pi}+n\right]k_i}$$

where $W^{(k_\perp)}_{k_0+2\pi \leftarrow k_0} \vec{g}^{a}(k_0, k_\perp) = e^{-i\varphi_a(k_\perp)} \vec{g}^{a}_{(k_0,k_\perp)}$

$$\Rightarrow \boxed{|W_{ank_\perp}\rangle = \frac{1}{2\pi} \sum_{b,c=1}^{N} \int_{k_0}^{k_0+2\pi} dk_i \, |\psi_{b\vec{k}}\rangle W^{bc\,(k_\perp)}_{k_i \leftarrow k_0} e^{-i\left[\frac{\varphi_a(k_\perp)}{2\pi}+n\right]k_i} g^{a}_{c}(k_0, k_\perp)}$$

$$P x_i P |W_{an\vec{k}}\rangle = \left(\frac{\varphi_a(k_\perp)}{2\pi} + n\right) |W_{an k_\perp}\rangle$$

$W_{k_j \leftarrow k_0}(k_\perp)$ - "Wilson line" $(k_0, \vec{k}_\perp)$ - basepoint

$(k_j, \vec{k}_\perp)$ - endpoint

$W_{k_0+2\pi \leftarrow k_0}(k_\perp)$ - "Wilson loop"

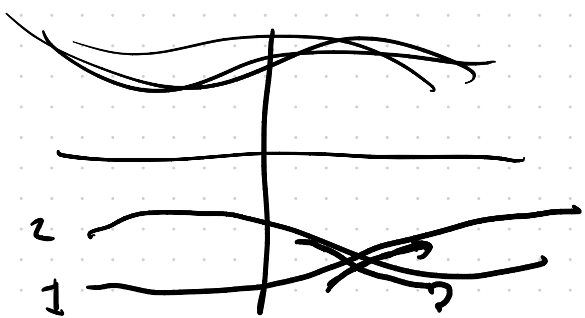
Note: $W_{k_0+2\pi \leftarrow k_0} = \underline{W_{k_0+2\pi \leftarrow 2\pi}} \, W_{2\pi \leftarrow 0} \, W_{0 \leftarrow k_0}$

$= W_{k_0 \leftarrow 0} \, W_{2\pi \leftarrow 0} \, W_{0 \leftarrow k_0}$ from the defining diffeq

$$= W_{k_0 \leftarrow 0}\, W_{2\pi \leftarrow 0} \left(W_{k_0 \leftarrow 0}\right)^{-1}$$

$\Rightarrow$ eigenvalues of $W^{(k_1)}_{k_0+2\pi \leftarrow k_0}$ and $W^{(k_1)}_{2\pi \leftarrow 0}$ are the same

Define $$|\tilde{\psi}_{a\vec{k}}\rangle = \sum_{b,c=1}^{N} |\psi_{b\vec{k}}\rangle\, W^{bc}_{k_i \leftarrow k_0}(k_1)\, e^{-i\frac{\theta_a(k_1)}{2\pi} k_i} \cdot g^a_c(k_0, k_1)$$



Computing path-ordered exponentials

$$i \frac{\partial}{\partial k_i} W_{k_i \leftarrow k_0} = -A_i W_{k_i \leftarrow k_0}$$

$$W_{k_0 \leftarrow k_0} = \mathrm{Id} = "1"$$

① Dyson series

$$W_{k_i \leftarrow k_0} = 1 + i \int_{k_0}^{k_i} dk_i' A_i(k_i', k_\perp) W_{k_i' \leftarrow k_0}$$

$$= 1 + i \int_{k_0}^{k_i} dk_i' A_i(k_i', k_\perp) + (i)^2 \int_{k_0}^{k_i} dk_i' \int_{k_0}^{k_i'} dk_i'' A_i(k_i', k_\perp) A_i(k_i'', k_\perp) + \cdots$$

② "Product of projectors"

$$\tilde{P}(k) = \sum_{a=1}^{N} |u_{ak}\rangle\langle u_{ak}|$$

$$\langle u_{ak} | u_{bk+\Delta_i}\rangle$$

$$\simeq \delta_{ab} + \Delta \langle u_{ak} | \frac{\partial u_{bk}}{\partial k_i}\rangle$$

$$\simeq \delta_{ab} - i\Delta A_i^{ab}$$

$$\langle u_{ak} | u_{bk'}\rangle = \int_{\text{cell}} d^3y\, u^*_{ak}(y) u_{bk'}(y)$$

$$W^{ab}_{k_j \leftarrow k_0} = \lim_{\Delta \to 0} \langle u_{ak_j,k_\perp} | \tilde{P}(k_i,k_\perp)\tilde{P}(k_i-\Delta,k_\perp)\cdots\tilde{P}(k_0+\Delta,k_\perp)\tilde{P}(k_0,k_\perp)|u_{bk_0,k_\perp}\rangle$$

$$\equiv \langle u_{ak_i,k_\perp}| \prod_{k_i'}^{k_j \leftarrow k_0} \tilde{P}(k_i',k_\perp)|u_{bk_0,k_\perp}\rangle$$

$$\mathcal{P} e^{\int_{k_0}^{k_j} dk_j A_j(k_j')} \simeq e^{i\Delta A(k_j-\Delta, k_\perp)} \cdots e^{i\Delta A(k_0+k_\perp)} e^{i\Delta A(k_0, k_\perp)}$$