

Lecture 18

Last time:

$$|W_{zk_1}\rangle = \frac{1}{(2\pi)} \int_0^{2\pi} dk_m |\Psi_k\rangle e^{i[S_0 k_m dk_m A_m(k'_m, k_1) - \frac{k_m \Phi}{2\pi} - k_m z]}$$

single-band Hybrid Wannier function

$$|\tilde{\Psi}_k\rangle = |\Psi_k\rangle e^{i[S_0 k_m dk_m A_m(k'_m, k_1) - \frac{k_m \Phi}{2\pi}]}$$

$|W_{zk_1}\rangle$ is the Fourier transform of $|\tilde{\Psi}_k\rangle$

$$|W_{zk_1}\rangle = \frac{1}{2\pi} \int_0^{2\pi} dk_m |\tilde{\Psi}_k\rangle e^{-ik_m z}$$

c.f. Kohn Phys Rev 1959
 Des Cloizeaux 1963, 1974

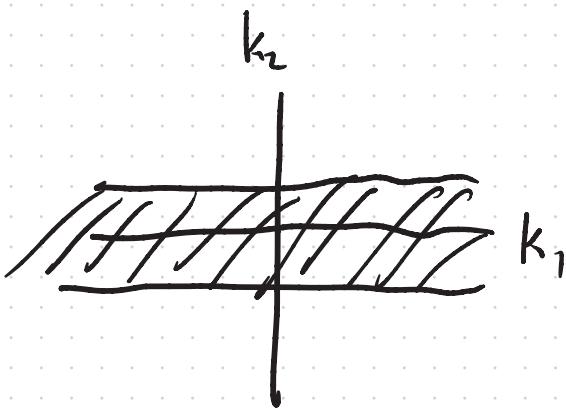
$$|\tilde{\Psi}_k\rangle = \sum_z |W_{zk_1}\rangle e^{ik_n z}$$

It can be shown that $|\tilde{\Psi}_k\rangle$ viewed as a function of k_n is complex analytic

$|\tilde{\Psi}_{k_1, k_2}\rangle$ is well-defined for

$$k_n = k_1 + i k_2 \quad k_1 \in (-\infty, \infty)$$

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



Plugging $k_m = k_1 + ik_2$ into our expression for $|\tilde{\Psi}_k\rangle$ in terms of $|W_{zk_1}\rangle$

$$|\tilde{\Psi}_{k_1+ik_2, k_1}\rangle = \sum_{z=-\infty}^{\infty} |W_{zk_1}\rangle e^{i(k_1+ik_2)z}$$

$$= \sum_{z=\infty}^{\infty} |W_{zk_1}\rangle e^{ik_1 z} e^{-k_2 z}$$

\rightarrow only well defined if $|W_{zk_1}\rangle \sim e^{-|k_2|z|}$
for large z

Payley-Wiener
theorems

Hybrid Wannier functions are exponentially localized

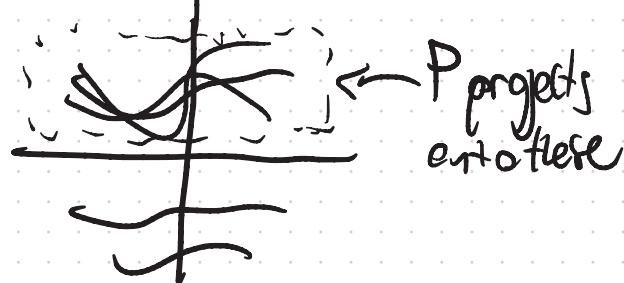
$|W_{zk_1}\rangle$ decays exponentially \rightarrow
 $|\Psi_{k_n}\rangle$ is infinitely differentiable

$$\sum_z (-iz)^N |W_{zk_1}\rangle e^{ik_n z} \\ = \partial_z^N |\Psi_{k_n, k_1}\rangle$$

Let's now go back to the general case:

\neq

$$P \left\{ \sum_{n=1}^N |\Psi_{nk}| > \langle \Psi_{nk} \rangle \left(\frac{v}{2\pi} \right)^3 d^3 k \right\}$$



$$i D_m \vec{f} = \lambda(k_1) \vec{f}$$

$$i \frac{\partial f_{nk}}{\partial k_n} + \sum_{m=1}^N A_m^{nm}(\vec{k}) f_{mk} = \lambda(k_1) f_{nk}$$

$$f_{nk} = g W$$

$$i \frac{\partial W}{\partial k_n} = - A W$$

we write $W_{k_m \rightarrow 0}(k_1) = P e^{i \int_a^{k_m} dk_n A_n(k')}$

$$f_{nk} = W_{k \in \mathbb{Z}_m}^{(n)}(k_1) g_n^a(k_1)$$

$$i \frac{\partial g}{\partial k_n} = \lambda(k_1) g$$

$$|W_{a \in \mathbb{Z}_m}\rangle = \frac{1}{2\pi} \int_0^{2\pi} dk_m |\Psi_{ek}\rangle W^{k_m}$$

Periodicity:

g_n^a should be

an eigenvector of

$W_{k \in \mathbb{Z}_m}(k_1)$ with eigenvalue
 $e^{i\varphi_n^a(k_1)}$

$$|W_{azk_L}\rangle = \frac{1}{2\pi} \int_0^{2\pi} dk_n |\Psi_{ek}\rangle W_{k_n=0}(k_L) e^{-i(\frac{\varphi_a}{2\pi} + z) k_n} g_n^a(k_L)$$

$$P \times_P |W_{azk_L}\rangle = \left(z + \frac{\varphi_a(k_L)}{2\pi} \right) |W_{azk_L}\rangle$$

$e^{i\varphi_a(k_L)}$ is the eigenvalue of $W(k_L)$
 (w/ eigenvector $\vec{g}^a(k_L)$)

"Wilson loop"

$W_{k_n=0}(k_L)$ is called a "Wilson line"

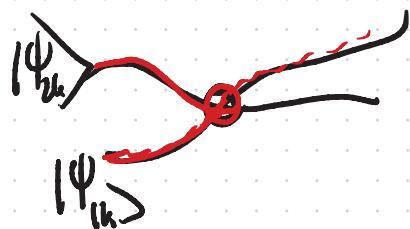
$(k_m=0, k_{\perp})$ is the base point

(k_m, k_{\perp}) is the endpoint

$a=1, \dots, N$

$$|\tilde{\Psi}_{ak}\rangle = |\Psi_{ek}\rangle W_{k_m=0}^{lm}(k_{\perp}) g_m^a(k_{\perp}) e^{-i\varphi_{ak} k_m / 2\pi}$$

$$|W_{ak} k_{\perp}\rangle = \frac{1}{2\pi} \int_0^{2\pi} dk_m |\tilde{\Psi}_{ak}\rangle e^{-i k_m}$$



$$W_{k_m=0}^{lm} g_m^a e^{-i\varphi_{ak} k_m / 2\pi}$$

ensures that we label our Bloch

functions smoothly (analytically) through degeneracies

Two ways of computing $W_{k_m \leftarrow 0}(k_1)$:

$$i \frac{\partial}{\partial k_m} W_{k_m \leftarrow 0} = -A W_{k_m \leftarrow 0}$$

① Dyson Series

$$W_{k_m \leftarrow 0} = i \int_0^{k_m} dk'_m A(k'_m, k_1) W_{k'_m \leftarrow 0} + W^0$$

Look for a solution perturbatively in A

$$W_{k_m=0} = W^0 + W^1 + \dots \quad \text{Initial conditions:}$$

$$W^0 = 1$$

$$W_{0=0} = I$$

$$1 + W^1 + W^2 + \dots = +i \int_0^{k_m} dk_m' A(k_m') (1 + W^1 + W^2 + \dots)$$

$$W^1 = +i \int_0^{k_m} dk_m' A(k_m')$$

$$W^2 = -i \int_0^{k_m} dk_m' A(k_m') W^1 = (-i)^2 \int_0^{k_m} dk_m' A(k_m') \int_0^{k_m'} dk_m'' A(k_m'')$$

$$W^n = (+i)^n \int_0^{k_n} dk_1 \int_0^{k_1} dk_2 \int_0^{k_2} dk_3 \cdots \int_0^{k_{n-1}} dk_n A(k_1) A(k_2) A(k_3) \cdots A(k_n)$$

Path ordered product

$$W = \sum_{\substack{k_m > 0 \\ k_0 < 0}}^{\infty} W^n = P e^{+i \int_0^{k_m} dk_m A(k_m)}$$

(2)

Product of projectors

$$\tilde{P}(k) = \sum_{n=1}^N |U_{nk} \times U_{nk}|$$

$$\langle U_{nk} | U_{nk'} \rangle = \sum_{\text{cell}} \langle U_{nk}^+(v) U_{nk'}(v) \rangle$$

$$Pe^{i \int_0^{k_m} dk' A(k')} = \lim_{\Delta \rightarrow 0} \langle u_{nk_m} | \tilde{P}(k_m) \tilde{P}(k_m - \Delta) \tilde{P}(k_m - 2\Delta) \dots \tilde{P}(\Delta) \tilde{P}_0 | u_{n0} \rangle$$

$$= \langle u_{nk_m} | \prod_{k_m}^{k_m=0} \tilde{P}(k'_m) | u_{n0} \rangle$$

$$W_{k_m=0}^{nm}(k_1) = \langle u_{nk_m k_1} | \prod_{k'_m}^{k_m=0} \tilde{P}(k'_m, k_1) | u_{n0 k_1} \rangle$$

Some properties of Wilson loops/lines

① Gauge transformation $|u_{nk}\rangle \rightarrow |u'_{nk}\rangle = |u_{nk}\rangle U(k)$

$$\tilde{P}'(k) = \sum_{n=1}^N |u'_{nk}\rangle \langle u'_{nk}| = \sum_{n=1}^N |u_{nk}\rangle \langle u_{nk}| U(k) U^*(k)$$

$$= \tilde{P}(k)$$

$$(W'_{k_n=0})^{nm} = \langle u'_{nk_1 k_2} | \prod \tilde{P}(k) | u'_{nk_1} \rangle$$

$$= U_{ln}^*(k_n, k_1) \langle u_{lk_1 k_2} | \prod \tilde{P}(k) | u_{pk_1} \rangle U_{pn}(k)$$

$$= [U^*(k_n, k_1) W_{k_n=0} U(0, k_1)]^{nm}$$

$$W'_{k_m=0} = U^t(k_m, k_\perp) W_{k_m=0} U(0, k_\perp)$$

Not gauge covariant

If we look at a Wilson loop : $k_m = 2\pi$

gauge transformations must be periodic (so $|\Psi'_{k+G}\rangle = |\Psi_k\rangle$)

$$\begin{aligned} W'_{2\pi=0}(k_\perp) &= U^t(2\pi, k_\perp) W_{2\pi=0} U(0, k_\perp) \\ &= U^t(0, k_\perp) W_{2\pi=0} U(0, k_\perp) \end{aligned}$$

$W'_{2\pi \sim 0}$ and $W_{2\pi \sim 0}$ are related by similarity transformation

→ eigenvalues of $W_{2\pi \sim 0}^{(k_1)}$ are gauge invariant

$$\underbrace{e^{i\varphi^q(k_1)}}$$

$P_{X_\mu} P$ eigenvalues are $\left(\frac{\varphi^q(k_1)}{2\pi} + z\right)$

What about symmetries: Assume we have symmetries of some space group G_s .

P is a projector onto eigenstates of H isolated from others $[U_g, H] = 0 \Rightarrow [U_g, P] = 0$

for $g \in G$

$$\text{if } g = \{\bar{g} | \vec{d}\} \quad U_g^+ P \vec{x} P U_g = P U_g^+ \vec{x} U_g P \\ = P(\bar{g} x + \vec{d})P$$

This has implications for our HWFs (hybrid Wannier functions)

$$\textcircled{1} \quad P|W_{azk_1}\rangle = |W_{azk_1}\rangle$$

$$\textcircled{2} \quad f \quad P X_m P |W_{azk_1}\rangle = \left(\frac{1}{2\pi} \varphi^a + z \right) |W_{azk_1}\rangle$$

then $U_g P (\bar{g}x + d) P U_g^\dagger |W_{azk_1}\rangle = \left(\frac{1}{2\pi} \varphi^a + z \right) |W_{azk_1}\rangle$

$U_g^\dagger |W_{azk_1}\rangle$ is an eigenstate of $P (\bar{g}x + d) P$
with eigenvalue $\left(\frac{1}{2\pi} \varphi^a + z \right)$

We can get even stronger constraints when

$$(\bar{g}X + d) \propto X_m$$

Ex1 Time-reversal symmetry $TXT^{-1} = X$

$$TPX_mP T^{-1} = P X_m P$$

$|W_{q2k_1}\rangle$ and $T|W_{q2k_1}\rangle$ have the same PX_mP eigenvalue

Lets act with a lattice translation on $|W_{q2k_1}\rangle$

$$\vec{t}_\perp \cdot \vec{b}_m = 0$$

$$\begin{aligned}
 U_{\vec{t}_\perp} |W_{azk_\perp}\rangle &= \frac{1}{(2\pi)} \int_0^{k_m} dk_m U_{\vec{t}_\perp} |\tilde{\Psi}_{ak}\rangle e^{+ik_m z} \\
 &= \frac{1}{2\pi} \int_0^{k_m} dk_m e^{-ik_\perp \cdot \vec{t}_\perp} |\tilde{\Psi}_{ak}\rangle e^{ik_m z} \\
 &= e^{-ik_\perp \cdot \vec{t}_\perp} |W_{azk_\perp}\rangle
 \end{aligned}$$

$$U_{\vec{t}_\perp} T |W_{azk_\perp}\rangle = T U_{\vec{t}_\perp} |W_{azk_\perp}\rangle$$

$$= T e^{-i \vec{k}_1 \cdot \vec{t}_L} |W_{a\vec{z}\vec{k}_1}\rangle$$

$$= e^{i \vec{k}_1 \cdot \vec{t}_L} T |W_{a\vec{z}\vec{k}_1}\rangle$$

$T |W_{a\vec{z}\vec{k}_1}\rangle$ is a bWF with $\vec{k}'_1 = -\vec{k}_1$

and the same $P_{X_n} P$ eigenvalue as $|W_{a\vec{z}\vec{k}_1}\rangle$

$\{\varphi^a(\vec{k}_1), a=1, \dots N\}$ determine centers of $|W_{a\vec{z}\vec{k}_1}\rangle$

$\{\varphi^a(-\vec{k}_1), a=1, \dots N\}$ determine centers of $T |W_{a\vec{z}\vec{k}_1}\rangle$

$$\{\varphi^a(k_\perp)\} = \{\varphi^a(-k_\perp)\} \pmod{2\pi}$$

$e^{i\varphi^a(k_\perp)}$ is the eigenvalue of $W_{2\pi t=0}(k_\perp)$

With time-reversal symmetry $W_{2\pi t=0}(k_\perp)$ and

$W_{2\pi t=0}(-k_\perp)$ have the same spectrum

If $k_\perp \equiv -k_\perp$ modulo a reciprocal lattice vector, then something interesting happens

then $\{|W_{azk_1}\rangle, T|W_{azk_1}\rangle\}$ have to have k_1

if $T^2 = -1$ this implies $|W_{azk_1}\rangle, T|W_{azk_1}\rangle$ are linearly independent from Kramers' theorem:

Then if T is antiunitary and $T^2 = -1$

then $|\Psi\rangle$ and $T|\Psi\rangle$ are orthogonal

$$\begin{aligned} \langle \Psi | T \Psi \rangle &= \langle T T \Psi | T \Psi \rangle \\ &= \langle T^2 \Psi | T \Psi \rangle = -\langle \Psi | T \Psi \rangle \\ \Rightarrow \langle \Psi | T \Psi \rangle &= 0 \end{aligned}$$

$$\langle T\psi|T\psi\rangle = \langle \psi|\psi\rangle = 1$$

at TRIMs k_1^* if $T=1$ our hybrid Wannier fns come in pairs $\{ |W_{a3k_1^*}\rangle, T|W_{a3k_1^*}\rangle \}$ with the same centers $\varphi^a(k_1^*)$

→ Wilson loop eigenvalues are twofold degenerate

Ex: Inversion Symmetry $\{ I | 0 \}$

$$U_I^\dagger P \chi_m P U_I = -P \chi_m P \quad U_I^\dagger U_I = U_I U_I^\dagger$$

If $|W_{\alpha \beta k_1}\rangle$ has $P \times P$ eigenvalue $\mathcal{E} + \frac{\varphi^\alpha(k_1)}{2\pi}$

then $U_I |W_{\alpha \beta k_1}\rangle$ has $P \times P$ eigenvalue $-\mathcal{E} - \frac{\varphi^\alpha(-k_1)}{2\pi}$
with momentum $-k_1$

Inversion Symmetry: $\{\varphi^\alpha(k_1)\} = \{-\varphi^\alpha(-k_1)\}$
modulo 2π

(we say that the eigenvalue
 $\mathcal{E} + \frac{\varphi^\alpha(k_1)}{2\pi}$ is the (hybrid Wannier) center)

(of $|W_{azk_1}\rangle$)

$$\langle W_{azk_1} | X_n | W_{azk_1} \rangle = e^+ \frac{\phi(\vec{k}_1)}{2\pi}$$