Lecture 15

Recap: We want eigenstates of $P x^\mu P$

For $P = \sum_k |\psi_k\rangle\langle\psi_k|$ a projector onto one band

$$|W_{n\vec{k}_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_\mu\, |\psi_k\rangle\, e^{i\left[\int_{k_0}^{k_\mu} dk'_\mu A_\mu(k'_\mu, k_\perp) - \frac{k_\mu}{2\pi}\varphi(k_\perp) - k_\mu n\right]}$$

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

integer index for unit cells in the e_μ direction

$$\varphi(k_\perp) = \int_0^{2\pi} dk_\mu A_\mu(k_\mu, k_\perp)$$

Define:

$$|\tilde{\Psi}_k\rangle = |\Psi_{k}\rangle e^{i\left[\int_{k_0}^{k_\mu} dk_\mu' A_\mu(k_\mu', k_\perp) - \frac{k_\mu}{2\pi}\varphi(k_\perp)\right]}$$

$|\tilde{\Psi}_{k+\vec{G}}\rangle = |\tilde{\Psi}_k\rangle$ for reciprocal lattice vectors $\vec{G}$

$$|W_{nk_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_\mu \, |\tilde{\Psi}_k\rangle e^{-ik_\mu n}$$

$|W_{nk_\perp}\rangle$ is the fourier transform of $|\tilde{\Psi}_{\vec{k}}\rangle$

$$|\tilde{\Psi}_k\rangle = \sum_n |W_{n k_\perp}\rangle e^{i k_\mu n}$$

It can be shown that $|\tilde{\Psi}_{\vec{k}}\rangle$ can be viewed as a function of $\vec{k}_\perp$ and complex $k_\mu = k_1 + i k_2$

$|\tilde{\Psi}_{k_\mu, k_\perp}\rangle$ will be analytic in k_μ for

$k_1 = (0, 2\pi]$

$k_2 \in [-\varkappa, \varkappa]$ $\quad \varkappa > 0 \sim$ energy gap

$\boxed{\text{Kohn, Phys. Rev 1959} \quad \text{des Cloizeaux 1963, 1964}}$

Using this

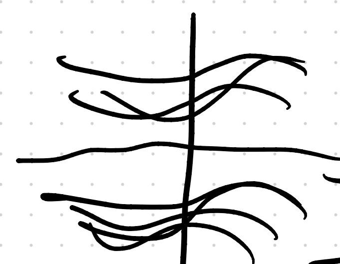
$$|\tilde{\psi}_{k_1+ik_2,k_\perp}\rangle = \sum_{n=-\infty}^{\infty} |W_{nk_\perp}\rangle e^{i(k_1+ik_2)n}$$

$$= \sum_{n=-\infty}^{\infty} |W_{nk_\perp}\rangle e^{ik_1 n} e^{-k_2 n}$$

Converges only if $|W_{nk_\perp}\rangle \to e^{-\varkappa|n|}$

$\to$ Hybrid Wannier functions are exponentially localized

Next: General case



P

$$P = \frac{V}{(2\pi)^3}\int d^3k \sum_{a=1}^{N} |\psi_{ak}\rangle\langle\psi_{ak}| \qquad |W_{ank_\perp}\rangle = \int dk_\mu \sum_{b=1}^{N} |\psi_{bk}\rangle f_b^a(k)$$

$$iD_\mu \vec{f} = \lambda(k_\perp)\vec{f}$$

$$i\frac{\partial f_{bk}}{\partial k_\mu} + \sum_{c=1}^{N} A_\mu^{bc}(k_\mu, k_\perp) f_{c\vec{k}} = \lambda(k_\perp) f_{b\vec{k}}$$

Lets introduce a matrix W that solves

$$i\frac{\partial W}{\partial k_\mu} = -A_\mu W \qquad W_{k_\mu \leftarrow 0}(k_\perp) = P e^{i\int_0^{k_\mu} dk'_\mu A_\mu(k'_\mu, k_\perp)}$$

$$W_{0\leftarrow 0}(k_\perp) = \mathbb{1}$$

define $f_{b\vec{k}} = \sum_{c=1}^{N} W^{bc}_{k_\parallel \leftarrow 0}(k_\perp)\, g_c(k_\perp)$

then $i \dfrac{\partial g_c(k_\parallel, k_\perp)}{\partial k_\parallel} = \lambda(k_\perp)\, g_c(k_\parallel, k_\perp)$

Periodicity: $f_{b\, k_\parallel + 2\pi, k_\perp} = f_{b\, k_\parallel, k_\perp}$

$$\vec{F}_{k_\parallel + 2\pi, k_\perp} = W_{k_\parallel \leftarrow 0}(k_\perp)\, W_{2\pi \leftarrow 0}(k_\perp)\, \vec{g}(k_\parallel + 2\pi, k_\perp) = f_{k_\parallel, k_\perp} = W_{k_\parallel \leftarrow 0}(k_\perp)\, g(k_\perp$$

$\Rightarrow$ $\vec{g}(k_\perp)$ is an eigenvector of $W_{2\pi \leftarrow 0}(k_\perp)$

$W_{2\pi\leftarrow 0}(k_\perp)$ has eigenvalues $e^{i\varphi_a(k_\perp)}$ w/ eigenvector $\vec{g}_a(k_\perp)$

$$\boxed{\lambda_a = \varphi_a(k_\perp)/2\pi + n}$$

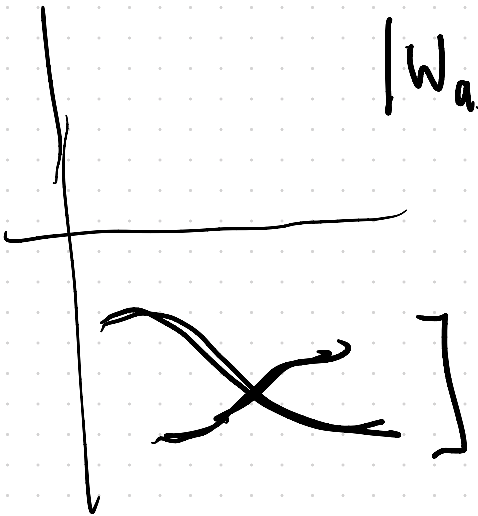
$$\boxed{g = \vec{g}_a(k_\perp)\, e^{-i[\varphi_a(k_\perp)+n]k_\parallel/2\pi}}$$

Putting it all together:

$$|W_{ank_\perp}\rangle = \frac{1}{2\pi}\sum_{b,c=1}^{N}\int_0^{2\pi} dk_\parallel\, |\psi_{bk}\rangle \underbrace{W^{bc}_{k_\parallel\leftarrow 0}(k_\perp)\, e^{-i\left[\frac{\varphi_a(k_\perp)+n}{2\pi}\right]k_\parallel}\, g^c_a(k_\perp)}$$

$$|\tilde{\psi}_{a\vec{k}}\rangle = \sum_{bc} |\psi_{b\vec{k}}\rangle W^{bc}_{k_\mu \leftarrow 0}\, e^{-i\frac{\varphi_a(k_\perp)}{2\pi}k_\mu}\, g^c_a(k_\perp)$$

$$|W_{an k_\perp}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_\mu\, |\tilde{\psi}_{a\vec{k}}\rangle e^{-ink_\mu}$$



$(k_\mu = 0, k_\perp)$ - base point

$(k_\mu, k_\perp)$ - endpoint

$W_{k_\mu \leftarrow 0}(k_\perp)$ - "Wilson line"

$W_{2\pi \leftarrow 0}(k_\perp)$ - "Wilson loop"

Two ways to compute $W_{k_\mu \leftarrow 0}(k_\perp)$

$$i\frac{\partial}{\partial k_\mu} W_{k_\mu\leftarrow 0}(k_\perp) = -A_\mu(k_\mu, k_\perp) W_{k_\mu \leftarrow 0}(k_\perp) \qquad W_{0\leftarrow 0}(k_\perp) = 1$$

① Dyson Series: $$W_{k_\mu\leftarrow 0}(k_\mu) = W_{0\leftarrow 0}(k_\perp) + i\int_0^{k_\mu} dk_\mu' \, A_\mu(k_\mu', k_\perp) W_{k_\mu'\leftarrow 0}(k_\perp)$$

$$W_{k_\mu\leftarrow 0}(k_\mu) = 1 + i\int_0^{k_\mu} dk_\mu' \, A_\mu(k_\mu', k_\perp) + (i)^2 \int_0^{k_\mu} dk_\mu' \int_0^{k_\mu'} dk_\mu'' \, \overline{A_\mu(k_\mu', k_\perp) A_\mu(k_\mu'', k_\perp)}$$

$$+ \ldots$$

$$A_\mu = \left\langle u_{nk} \middle| \frac{\partial u_{nk}}{\partial k_\mu} \right\rangle_{\text{cell}}$$

② Product of projectors $\quad \tilde{P}(k) = \sum_{n=1}^{N} |u_{nk}\rangle\langle u_{nk}|$

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

$$\left[P e^{i\int_0^{k_\mu} dk'_\mu A_\mu(k')} \right]^{nm} = \lim_{\Delta\to 0} \langle u_{nk_\mu,k_1}| \tilde{P}(k_\mu,\vec{k}_1)\tilde{P}(k_\mu-\Delta,\vec{k}_1)\tilde{P}(k_\mu-2\Delta,k_1) \cdots \tilde{P}(\Delta,k_1)\tilde{P}(0,k_1)|u_{m0,k_1}\rangle$$

$$= \langle u_{nk_\mu,k_1}| \prod_{k'_\mu}^{k_\mu\leftarrow 0} \tilde{P}(k'_\mu,k_1)|u_{m0,k_1}\rangle$$

$$\left[W_{k_\mu\leftarrow 0}(k_1) \right]^{nm}$$

Properties of Wilson loops/lines

periodic unitary matrix

① Gauge transformations $|u_{nk}\rangle \to |u'_{nk}\rangle = \sum_{m=1}^{N} |u_{mk}\rangle U_{mn}(k)$

$$\hat{P}'(k) = \sum_{n=1}^{N} |u'_{nk}\rangle\langle u'_{nk}| = \hat{P}(k)$$ projector invariant

$$\left[W'_{k_\mu \leftarrow 0}\right]^{nm} = \langle u'_{n k_\mu, k_1}| \prod_{k_\mu}^{k \leftarrow 0} \hat{P}'(k) |u'_{m 0 k_1}\rangle$$

$$= \left[U^\dagger(k_\mu, k_1) W_{k_\mu \leftarrow 0}(k_1) U(0, k_1)\right]^{nm}$$

Not gauge covariant

For wilson loops : $k_n = 2\pi$ $\quad U^\dagger(2\pi, k_\perp) = U^\dagger(0, k_\perp)$

$$W'_{2\pi\leftarrow 0}(k_\perp) = U^\dagger(0, k_\perp) W_{2\pi\leftarrow 0} U(0, k_\perp)$$

$\Rightarrow$ the eigenvalues $e^{i\varphi_a(k_\perp)}$ of $W_{2\pi\leftarrow 0}(k_\perp)$

are gauge invariant

$$P x_n P |W_{an k_\perp}\rangle \quad \left(n + \frac{\varphi_a(k_\perp)}{2\pi}\right)|W_{an k_\perp}\rangle$$