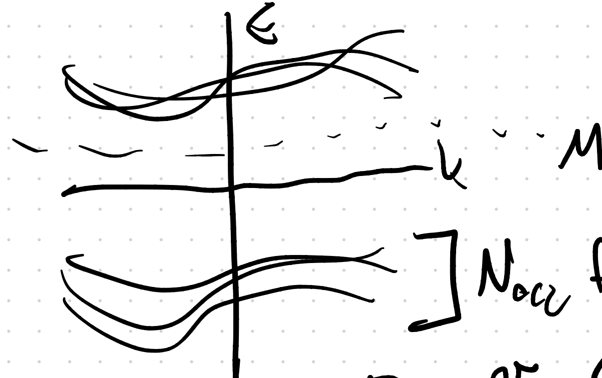
Lecture 15

Recap



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

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

$$A^{nm}_{\mu}(\vec{k}) = i\left\langle u_{nk}\middle|\frac{\partial u_{mk}}{\partial k^{\mu}}\right\rangle$$

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

$$P x^{\mu} P |f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle [iD_{\mu} f]_{nk}$$

$$[D_\mu F]_{nk} = \frac{\partial f_{nk}}{\partial k^\mu} - \sum_{m=1}^{N_{occ}} A_\mu^{nm} f_{mk}$$

want: $P x^\mu P |f\rangle = \lambda |f\rangle$ eigenstates

Coordinates $x_i = \frac{1}{2\pi} \vec{b}_i \cdot \vec{x}$ b_i - primitive reciprocal lattice vector

$(\vec{x} = x_1 \vec{t}_1 + x_2 \vec{t}_2 + x_3 \vec{t}_3)$ $\vec{t}_i$ - primitive lattice vectors

$$\vec{k} = \frac{1}{2\pi}(k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3)$$

$k_j = \vec{t}_j \cdot \vec{k}$ $k_j \in (-\pi, \pi]$

$$x_i e^{i k_i \vec{x}} = -i \frac{\partial}{\partial k_i}\left(e^{ik\cdot x}\right)$$

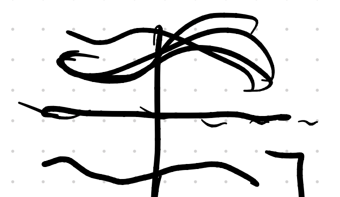
$$P x_i P |f\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle \left[i D_i f\right]_{nk}$$

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

Eigenvalue equation $\quad P x_i P|f\rangle = \lambda |f\rangle$

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

Simple case: $N_{occ} = 1$



$|\psi_k\rangle$

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

$$|f\rangle = \frac{v}{(2\pi)^3}\int d^3k\, |\psi_k\rangle f_k$$

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

$$\lambda f_k = iD_i f_k = i\frac{\partial f_{\vec{k}}}{\partial k_i} + A_i(\vec{k}) f_{\vec{k}} \qquad \vec{k} = \frac{1}{2\pi}k_i\vec{b}_i + \vec{k}_\perp$$

$$f_{\vec{k}} = f(k_i, \vec{k}_\perp)$$

$$\lambda f(k_i, \vec{k}_\perp) = i\left(\frac{\partial}{\partial k_i} - iA_i(k_i, k_\perp)\right) f(k_i, k_\perp)$$

ansatz: $f(k_j, k_\perp) = g(k_j, k_\perp) e^{i \int_{k_0}^{k_j} dk_j' A_j(k_j', k_\perp)}$

$$i \frac{\partial}{\partial k_j} g(k_j, k_\perp) = \lambda g(k_j, k_\perp)$$

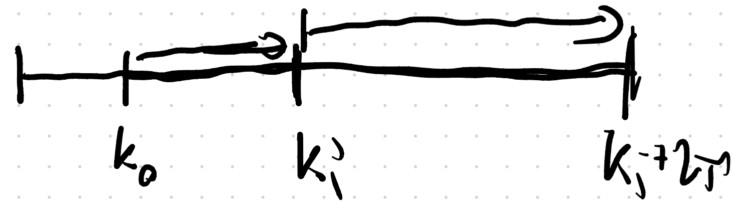
$$\Rightarrow g(k_j, k_\perp) = C(\vec{k}_\perp) e^{-i \lambda k_j}$$

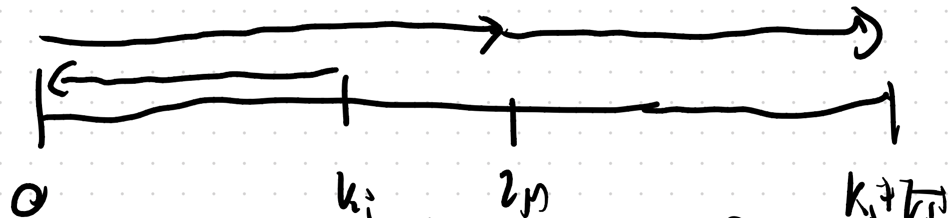
$$\boxed{f(k_j, \vec{k}_\perp) = C(\vec{k}_\perp) e^{i \int_{k_0}^{k_j} dk_j' A_j(k_j', \vec{k}_\perp) - i \lambda k_j}}$$

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

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

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





$$e^{2\pi i\lambda} = e^{i\left[\cancel{\int_{k_0}^{0} dk_j' A_j(k_j',k_\perp)} + \int_0^{2\pi} dk_j' A_j(k_j',k_\perp) + \cancel{\int_{2\pi}^{k_j+2\pi} dk_j' A_j(k_j,k_\perp)}\right]}$$

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

$$e^{2\pi i\lambda} = e^{i\int_0^{2\pi} dk_j A_j(k_j',\vec{k}_\perp)}$$

$$\lambda_n(k_\perp) = n + \underbrace{\int_0^{2\pi} dk_i A_i(k_i, k_\perp)}_{\varphi(k_\perp) \text{ - Berry phase}}$$

Px_iP eigenvalues are integers + the Berry phase

$P(x_i t_i)P$ has eigenvalues

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

The Berry phase gives the fractional part of the Px_iP spectrum

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

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

(Hybrid Wannier functions

$$\underline{|W_{nk_\perp}\rangle} = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_j\, e^{-ink_i}\left[\boxed{|\psi_k\rangle} e^{i\left[\int_{k_0}^{k_i} dk_j'\, A_j(k_i,\vec{k}_\perp) - \frac{k_j\varphi(k_\perp)}{2\pi}\right]}\right]$$

$$\equiv \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_j\, e^{-ink_j}\, |\tilde{\psi}_k\rangle$$

$$\langle W_{nk_\perp} | x_i | W_{nk_\perp} \rangle = \left(n + \frac{\varphi(k_\perp)}{2\pi} \right)$$

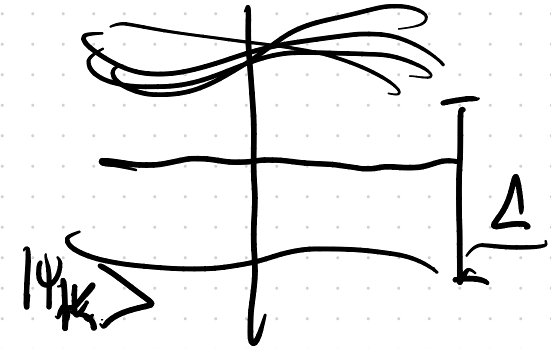
Localisation $$\langle W_{nk_\perp} | x_i^2 | W_{nk_\perp} \rangle - \left| \langle W_{nk_\perp} | x_i | W_{nk_\perp} \rangle \right|^2 = \Omega$$

$$x_i^2 = x_i P x_i + x_i Q x_i \qquad Q = 1 - P$$

$$\Omega = \langle W_{nk} | P x_i P x_i P | W_{nk} \rangle + \langle W_{nk} | P x_i Q x_i P | W_{nk} \rangle - \left| \langle W_{nk} | P x_i P | W_{nk} \rangle \right|^2$$

0 for $P x_i P$ eigenstates

$$|W_{nk_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_i\, |\tilde{\Psi}_{k}\rangle e^{-ink_i}$$



if we have a gap, we can

view $|\tilde{\Psi}_{k_i,k_\perp}\rangle$ as a function of $k_i = k_1 + ik_2$

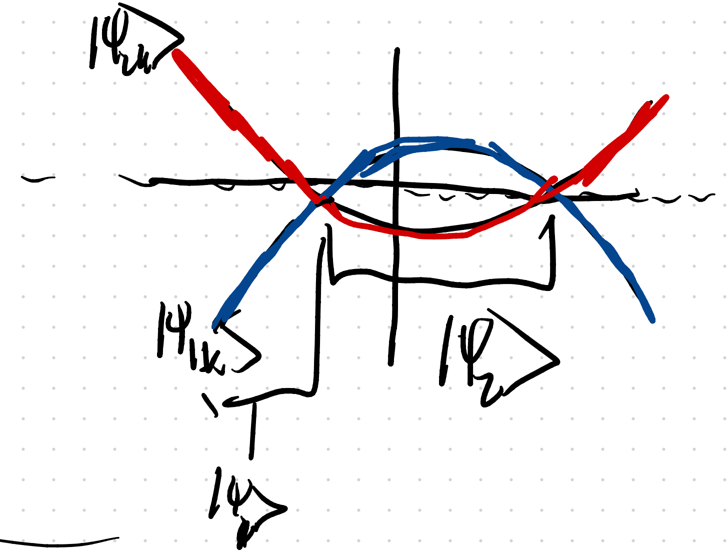
is a complex analytic function for $k_2 \in [-\tilde{\kappa}, \tilde{\kappa}]$

$\tilde{\kappa} \propto \sqrt{\Delta}$

$$\Rightarrow |\tilde{\Psi}_k\rangle = \sum_n |W_{nk}\rangle e^{i(k_1+ik_2)n} \Rightarrow |W_{nk}\rangle \text{ is exponentially localized } |W_{nk_\perp}\rangle \propto e^{-\kappa|n|}$$

Kohn, Phys Rev 1959

des Cloizeaux 1963, 1964



Now: General case

] 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 $|W_{an k_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{k_0+2\pi} dk_j \sum_{b=1}^{N_{occ}} |\psi_{bk}\rangle \underbrace{f_b^{an}(k_j, \vec{k}_\perp)}$

band index

unit cell index

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

$$\left[iD_j f^{an}\right]_{bk_j} = \lambda_{an}(k_\perp) f_b^{an} = i\left(\frac{\partial f_b^{an}}{\partial k_j} - i\sum_{c=1}^{N_{occ}} A_j^{bc} f_c^{an}\right)$$

To solve this, introduce a matrix

$$W^{(k_\perp)}_{k_i \leftarrow k_0}$$

$$i \frac{\partial W^{(k_\perp)}_{k_i \leftarrow k_0}}{\partial k_i} = - A_i(k_i, \vec{k}_\perp) W^{(k_\perp)}_{k_i \leftarrow k_0}$$

$$W^{(k_\perp)}_{k_0 \leftarrow k_0} = \mathrm{Id}$$

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

$$W_{k_2 \leftarrow k_0}(k_\perp) = W^{(k_\perp)}_{k_2 \leftarrow k_1} W^{(k_\perp)}_{k_1 \leftarrow k_0}$$

Ansatz: $$f^{a1}_b(k_i, k_\perp) = \sum_{c=1}^{N} W^{bc\,(k_\perp)}_{k_i \leftarrow k_0} g^{a1}_c(\vec{k}, k_0)$$

$$\Rightarrow i \frac{\partial}{\partial k_i} g_c^{a1}(\vec{k}, k_0) = \lambda_{a1}(k_\perp)\, g_c^{a1}(\vec{k}, k_0)$$

$$\vec{g}^{a1} = \vec{C}(k_\perp, k_0)\, e^{-i \lambda_{a1}(k_\perp) k_i}$$

$$f_b^{1a}(k_i, \vec{k}_\perp) = \sum_{c=1}^{N} W^{bc}_{k_i \leftarrow k_0}(k_\perp)\, \vec{C}_{1a}(k_\perp, k_0)\, e^{-i \lambda_{a1}(k_\perp) k_i}$$

$$f_b^{1a}(k_i + 2\pi, k_\perp) = f_b^{1a}(k_i, k_\perp)$$

$$\Rightarrow \quad W_{k_0+2\pi \leftarrow k_0}(k_\perp)\, \vec{C}_{1a}(k_\perp, k_0) = e^{2\pi i \lambda_{a1}(k_\perp)}\, \vec{C}_{1a}(k_\perp, k_0)$$

Choose $\vec{C}_{na}(k_\perp, k_0)$ to be an eigenvector of $W^{(k_\perp)}_{2\pi+k_0 \leftarrow k_0}$

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

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

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

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

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

eigenvalue $e^{i\varphi_a(k_\perp)}$ ← non-abelian Berry phases

$$W_{k_i \leftarrow k_0}(k_\perp) = P e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i', k_\perp)}$$ - Wilson line; $(k_0, \vec{k}_\perp)$ base point, $(k_i, k_\perp)$: endpoint

$$W_{2\pi + k_0 \leftarrow k_0}(k_\perp) = P e^{i\int_{k_0}^{k_0+2\pi} dk_i A_i(k_i, k_\perp)}$$ - Wilson loop

Note $W_{k_0+2\pi \leftarrow k_0}(k_\perp) = W_{k_0+2\pi \leftarrow 2\pi}(k_\perp) W_{2\pi \leftarrow 0}(k_\perp) W_{0 \leftarrow k_0}(k_\perp)$

$$= W^{\dagger(k_\perp)}_{0\leftarrow k_0} W^{(k_\perp)}_{2\pi\leftarrow 0} W^{(k_\perp)}_{0\leftarrow k_0}$$

Eigenvalues $e^{i\varphi_a(k_\perp)}$ are independent of k_0

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

$$|\tilde{\psi}_{a\vec{k}}\rangle \equiv \sum_{b,c=1}^{N_{occ}} |\psi_{b k_i}\rangle W^{bc}_{k_i\leftarrow k_0}(k_\perp) e^{-i\frac{\varphi_a(k_\perp)}{2\pi}k_i} C^{c}_{a}(k_\perp, k_0)$$

$$|W_{a n k_\perp}\rangle = \frac{1}{2\pi}\int dk_i\, e^{-i n k_i} |\tilde{\psi}_{a\vec{k}}\rangle$$