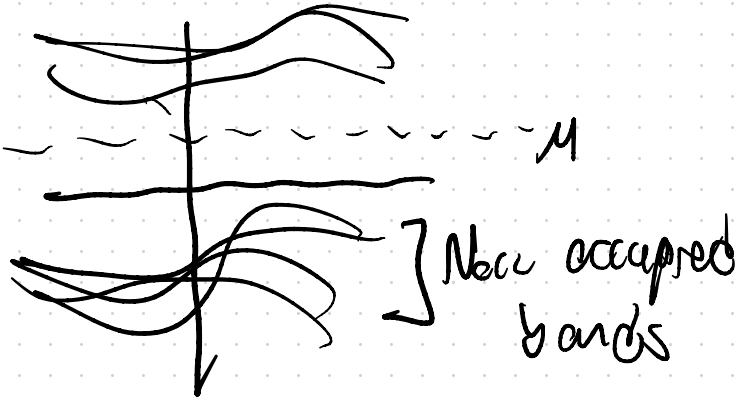
Lecture 16

Recap



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

$$|\tilde{\psi}_{ak}\rangle = \sum_{b,c=1}^{N_{occ}} |\psi_{bk}\rangle W^{(k_1)}_{k_i \leftarrow k_0} e^{-i\varphi_a(k_1)} g^c_a(k_1, k_0)$$

Wilson line $\longrightarrow$ $W^{(k_1)}_{k_i \leftarrow k_0} = \mathcal{P} e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i', \vec{k}_\perp)}$

$g^c_a(k_1, k_0)$ ← an eigenvector of

the Wilson loop $W_{2\pi\leftarrow 0}(k_2)$ w/ eigenvalue $e^{i\varphi_\alpha(k_2)}$

$$|W_{n\alpha k_2}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_1\, |\tilde{\psi}_{\alpha k}\rangle e^{-ik_1 n}$$ ← Hybrid Wannier functions

$$P x_1 P |W_{n\alpha k_2}\rangle = \left(n + \frac{\varphi_\alpha(k_2)}{2\pi}\right)|W_{n\alpha k_2}\rangle$$

(non-abelian) berry phase

displacement relative to origin

unit cell index

How to compute $W_{k_1\leftarrow k_0}(k_2) = \mathcal{P} e^{i\int_{k_0}^{k_1} dk_1' A_1(k_1', k_2)}$

Defined as solution $i\frac{\partial}{\partial k_i} W^{(k_1)}_{k_i \leftarrow k_0} = -A_i W^{(k_1)}_{k_i \leftarrow k_0}$

$W^{(k_1)}_{k_0 \leftarrow k_0} = Id = "1"$

① Dyson series: Rewrite as

$$i\int_{k_0}^{k_i} dk_i' \frac{\partial}{\partial k_i'} W^{(k_1)}_{k_i' \leftarrow k_0} = -\int_{k_0}^{k_i'} dk_i' A_i(k_i', k_1) W_{k_i' \leftarrow k_0}(k_1)$$

$$i\left[W^{(k_1)}_{k_i \leftarrow k_0} - 1\right]$$

$$W^{(k_1)}_{k_i \leftarrow k_0} = 1 + i\int_{k_0}^{k_i} dk_i' A_i(k_i', k_1) W^{(k_1)}_{k_i' \leftarrow k_0}$$

Plug into itself iteratively

$$W_{k_1 \leftarrow k_0} = \underline{1} + i\int_{k_\alpha}^{k_j} dk_j' \, A_i(k_j', k_1)(1) + (i)^2 \int_{k_\alpha}^{k_j} dk_j' \int_{k_\alpha}^{k_j'} dk_j'' \, A_i(k_j', k_1) A_i(k_j'', k_2) \cdots$$

② "Product of Projectors"

$$A_i^{ab}(k_i, k_1) = \langle u_{ak} | \frac{\partial u_{bk}}{\partial k_i} \rangle$$

$$= \lim_{\Delta \to 0} \frac{1}{\Delta} \langle u_{ak} | \left(| u_{b\, k_i + \Delta, k_1} \rangle - | u_{bk} \rangle \right)$$

$$\langle u_{ak} | u_{bk_i+\Delta, k_\perp} \rangle = \delta_{ab} - i\Delta A_i^{ab}(k) + O(\Delta^2)$$

$$\hat{=}\ e^{-i\Delta A_i(k_i)}$$

$$P e^{i\int_{k_0}^{k_i} dk A_i(k_i', k_0)} \hat{=}\ e^{i\Delta A_i(k_i-\Delta, k_\perp)} \cdots e^{i\Delta A_i(k_0+\Delta, k_\perp)\Delta i A_i(k_0, k_\perp)} \mathbb{1}$$

"Trotter decomposition"

$$P e^{i\int_{k_0}^{k_i} dk A_i(k_i', k_0)} = \lim_{\Delta \to 0} \langle u_{ak_i} | u_{bk_i-\Delta, k_\perp} \rangle \langle u_{bk_i-\Delta} | u_{ck_i-2\Delta k_\perp} \rangle \cdots \langle u_{nk_0+\Delta} | u_{mk_0} \rangle$$

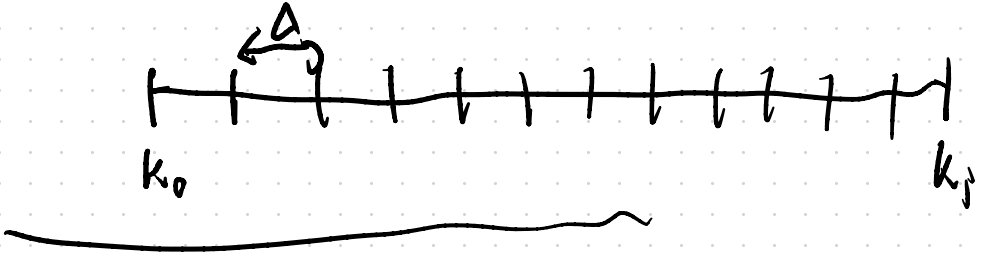
$$\tilde{P}(k) \approx \sum_{n=1}^{N_{occ}} |u_{nk}\rangle\langle u_{nk}|$$

$$= \lim_{\Delta \to 0} \langle u_{ak_1,k_2} | \tilde{P}(k_1,k_2)\tilde{P}(k_1-\Delta,k_2)\cdots\tilde{P}(k_0,k_2) | u_{bk_0,k_2}\rangle$$

$$= \langle u_{ak_1,k_2} | \prod_{k_1'}^{k_1 \leftarrow k_0} \tilde{P}(k_1',k_2) | u_{bk_0,k_2}\rangle$$

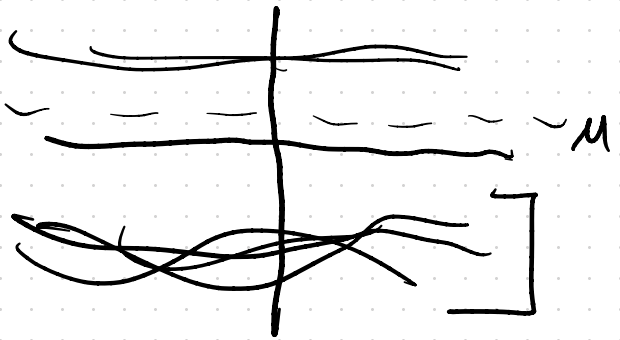
Advantages: ① No need to approximate derivates

② Converges very fast for Δ small



Connection to observables $\sum_i P x_i P \hat{t}_i = P \hat{x} P$

$P x_i \hat{t}_i P$ has eigenvalues $n t_i + \frac{\varphi_a(k_j)}{2\pi} \vec{t}_i$



ground state at $T=0$ has all N_{occ} bands filled

We can try to compute $\langle \hat{x} \rangle_0$ in this

ground state

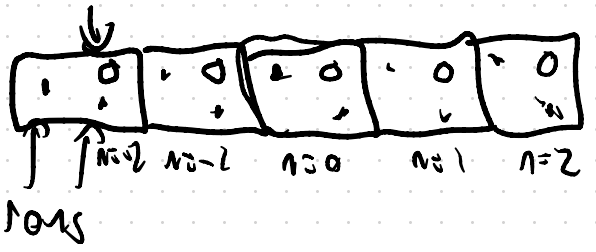
$$\langle \vec{x} \rangle_\alpha = \sum_i \langle x_i \rangle t_i = \frac{1}{(2\pi)^3} \int dk_1 dk_\perp \sum_{a=1}^{N_{occ}} \langle \psi_{ak} | x_i | \psi_{ak} \rangle t_i$$

in the Hybrid Wannier basis

$$\langle x_i \rangle = \frac{1}{(2\pi)^2} \int dk_\perp \sum_{a=1}^{N_{occ}} \sum_{n=-\infty}^{\infty} \langle W_{an k_\perp} | x_i | W_{an k_\perp} \rangle$$

$$= \frac{1}{(2\pi)^2} \int dk_\perp \sum_{a=1}^{N_{occ}} \sum_{n=-\infty}^{\infty} \left(n + \frac{\varphi_a(k_\perp)}{2\pi} \right)$$

Wannier functions



Average dipole moment

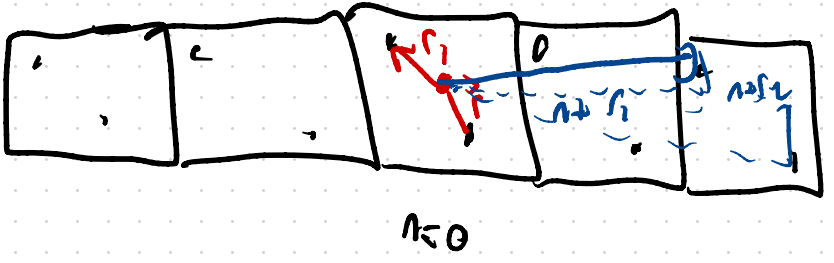
$$d_i = -e\langle x_i \rangle_0 + \sum_{\text{ions}} q_\alpha R_{\alpha,i}$$

↑ indexes ions in the unit cell

N_{occ} electrons/unit cell

Charge neutrality $\sum_\alpha q_\alpha = N_{occ} e$

$$R_{\alpha,i} = n + r_\alpha$$



$$d_i = -e\langle x_i \rangle + \sum_{\text{ions}} q_\alpha R_{\alpha,i}$$

$$= \sum_{n=-\infty}^{\infty} \left(\frac{-e}{(2\pi)^2} \int dk_\perp \sum_{\alpha=1}^{N_{occ}} \left(n + \frac{\varphi_\alpha(k_\perp)}{2\pi} \right) + \sum_{\substack{\alpha \\ \text{unitcell}}} q_\alpha (n + r_\alpha) \right)$$

n- dependent terms:

$$\sum_{n=-\infty}^{\infty}\left(-eN_{bg}n+\sum_{\alpha}q_{\alpha}n\right)=\sum_{n=-\infty}^{\infty}\left(-eN_{occ}n+eN_{occ}n\right)$$

$$=0$$

the rest

$$\sum_{n=-\infty}^{\infty}\left[\left(\frac{-e}{(2\pi)^2}\sum_{a=1}^{N_{occ}}\int dk_{\perp}\,\frac{\varphi_a(k_{\perp})}{2\pi}+\sum_{\alpha}q_{\alpha}r_{\alpha}\right)\right]$$

ρ_i - electric dipole moment density per unit cell

$d_i = N \rho_i$

$\frac{1}{q_{tot}} \sum_\alpha q_\alpha r_\alpha = X_{0i}$ - center of ionic charge in the unit cell

$q_{tot} = N_{occ} e$

$$\rho_i = N_{occ} e X_{0i} - e \sum_{a=1}^{N_{occ}} \int d^2 k_\perp \frac{1}{(2\pi)^3} \varphi_a(k_\perp)$$

Remember - $e^{i\varphi_a(k_\perp)}$ eigenvalue of Wilson loop $W_{z=0}(k_\perp)$

$$\sum_{a=1}^{N_{occ}} \varphi_a(k_\perp) = \mathrm{Im}\log\left(e^{i\sum_{a=1}^{N_{occ}}\varphi_a(k_\perp)}\right)$$

$$= \mathrm{Im}\log\prod_{a=1}^{N_{occ}} e^{i\varphi_a(k_\perp)}$$

$$= \mathrm{Im}\log\det W_{\Sigma_{IJ}=0}(k_\perp)$$

$$= \mathrm{Im}\log\; e^{i\int_0^{2\pi} dk_i\, \mathrm{tr}\, A_i(k_i,k_\perp)}$$

$$= \int_0^{2\pi} dk_i\, \mathrm{tr}\, A_i(k_i,k_\perp)$$

$$\rho_i = N_{occ} e X_{oi} - \frac{e}{(2\pi)^3} \int d^3k \, \mathrm{tr}\, A_i(k_1, k_1)$$

$$\vec{\rho} = N_{occ} e \vec{X}_o - \frac{e}{(2\pi)^3} \int d^3k \, \mathrm{tr}\, \vec{A}(k_1, k_1)$$

dipole moment density per unit volume

$$\vec{\rho}_v = \vec{\rho}/v$$

But what about gauge transformation

$$\vec{A} \to U^\dagger \vec{A} U + i U^\dagger \nabla_k U$$

$$\mathrm{tr}A \to \mathrm{tr}A + i\,\mathrm{tr}(U^\dagger \nabla_k U)$$

$$\mathrm{tr}A \to \mathrm{tr}A - \nabla_k \theta(k)$$

U - $N_{occ} \times N_{occ}$ unitary matrix

eigenvalues of U: $e^{i\theta_i(k)}$

$$\theta(k) = \sum_i \theta_i(k)$$

$$\vec{P} \to \vec{P} - \frac{e}{(2\pi)^3}\int d^3k\, \nabla_k \theta(k)$$

$$\downarrow$$

$$\vec{P} - \sum_i e M_i \vec{b}_i$$

$\det U$ is periodic

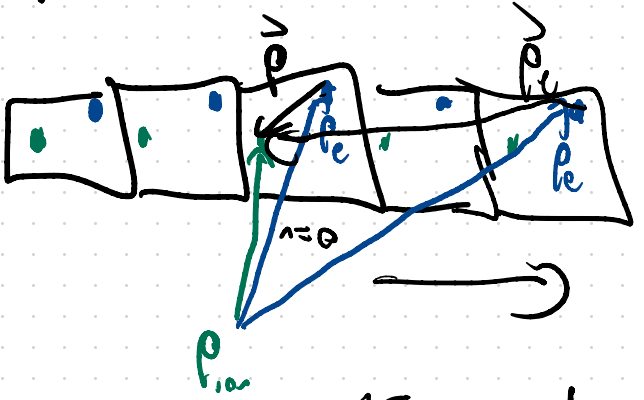
$$\det U(k+G) = e^{i\theta(k+G)} = e^{i\theta(k)}$$

$$\Rightarrow \theta(k+b_i) = \theta(k) + 2\pi M_j$$

$\vec{p}$ is not gauge invariant

$\vec{p}$ is only well defined mod bravais lattice translations

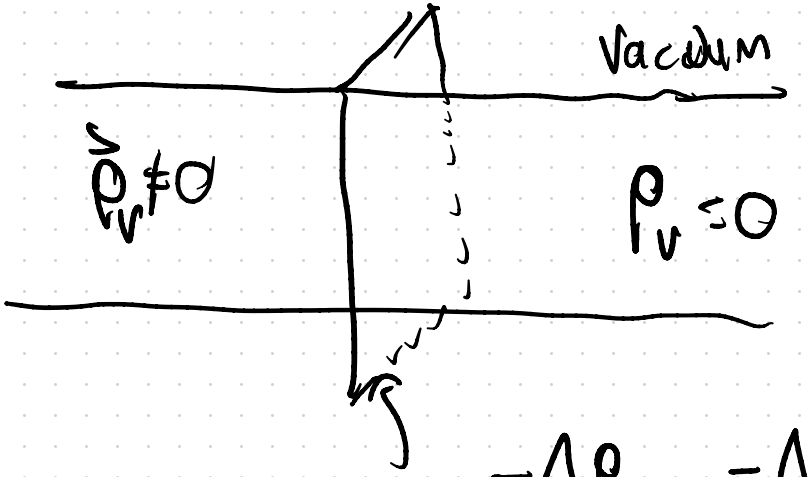
- ρ_{ion} - center of ionic charge
- ρ_e center of electronic charge



$$|W_{ank}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_i \, e^{-ik_i n} |\psi_{ak}\rangle \times e^{-ik_i M_i}$$

How do we detect any of this

Maxwell's equations: $\rho_b = -\nabla \cdot \vec{P}_v$



$$\sigma_b = -\Delta P_v = -\frac{\Delta p}{v} = \frac{\vec{p} \cdot \hat{n}}{v}$$

$$\vec{p} = \frac{-e}{(2\pi)^3}\int d^3k\, \mathrm{tr}\,\vec{A}(k) + e\vec{t}$$

$\mathrm{tr}\,\vec{A}(k)$: contributes to a fractional σ_6/e

$e\vec{t}$: corresponds to adding electrons on the boundary

Summary

$$\vec{p} = -e\vec{t}N - \frac{e}{(2\pi)^3}\int d^3k\, \mathrm{tr}\,\vec{A}_j(k) + N_{occ}\,e\,x_0$$

can choose origin @ x_0 to get rid of this

- $\vec{p}$ mod $e\vec{t}$ is intrinsic
- contributes a fractional # of e/unit cell to σ_b
- cannot be changed by adding e^- to the boundary