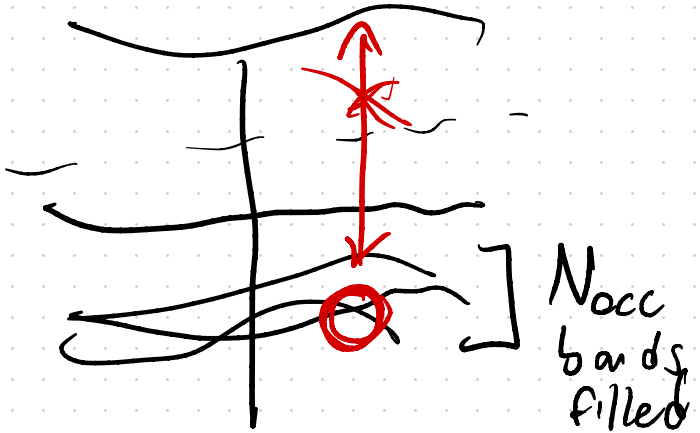
Lecture 17

Announcement: HW 2 grades returned
Solutions to be posted
HW 3 due Thursday



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

Eigenstates of $P_{x_i} P$

$$|W_{a n k_i}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_i \, |\psi_{ak}\rangle e^{-i k_i n}$$

$$|\tilde{\psi}_{ak_\perp}\rangle = \sum_{b,c=1}^{N_{occ}} |\psi_{bk_\perp}\rangle W^{bc}_{k_j \leftarrow k_a}(k_\perp) C^c_a(k_\perp, k_a) e^{-i\varphi_a(k_\perp)}$$

$$W_{k_j \leftarrow k_a}(k_\perp) = \mathcal{P} e^{i\int_{k_a}^{k_j} dk_i' A_i(k_i', k_\perp)}$$ ← Wilson line

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

basepoint $(k_a, \vec{k}_\perp)$

$e^{-i\varphi_a(k_\perp)}$ is an eigenvalue of

Wilson loop $W(k_\perp)$ $2\pi \# k_a \leftarrow k_a$

with eigenvector $\vec{C}_a(k_\perp, k_a)$

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

unit cell index

displacement relative to origin of the unit cell

Computing Wilson lines $W^{(k_\perp)}_{k_1 \leftarrow k_0}$

Defined as solns of $i \frac{\partial}{\partial k_i} W^{(k_\perp)}_{k_1 \leftarrow k_0} = -A_i(k_1, k_\perp) W^{(k_\perp)}_{k_1 \leftarrow k_0}$

$W_{k_0 \leftarrow k_0}(k_\perp) = Id = \underline{1}$

① Dyson series

$$i\int_{k_0}^{k_1} dk_1' \frac{\partial W_{k_1' \leftarrow k_0}(k_2)}{\partial k_1'} = -\int_{k_0}^{k_1} dk_1' A_1(k_1', k_2) W_{k_1' \leftarrow k_0}(k_2)$$

$$i\left(W^{(1)}_{k_1 \leftarrow k_0}(k_2) - 1\right)$$

$$W_{k_1 \leftarrow k_0}(k_2) = 1 + i\int_{k_0}^{k_1} dk_1' A_1(k_1', k_2) W_{k_1' \leftarrow k_0}(k_2)$$

Plugging in iteratively

$$W_{k_1 \leftarrow k_0}(k_2) = 1 + i\int_{k_0}^{k_1} dk_1' A_1(k_1', k_2)\left[1 + \int_{k_0}^{k_1'} dk_1'' A_1(k_1'', k_2)\left[1 + \dots\right.\right.$$

(2) "Project of projectors"

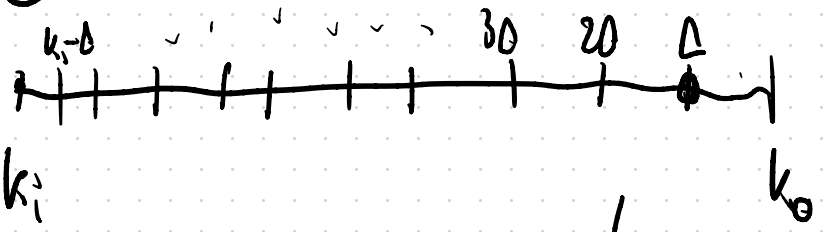
$$A_i^{ab}(k_j,k_\perp) = i\langle u_{ak} | \frac{\partial u_{bk}}{\partial k_j} \rangle_{cell}$$

$$= i \lim_{\Delta \to 0} \frac{1}{\Delta} \left(\langle u_{ak} | u_{b k_j + \Delta, k_\perp} \rangle_{cell} - \delta_{ab} \right)$$

$$\langle u_{ak} | u_{b k_j + \Delta, k_\perp} \rangle \approx \delta_{ab} - i \Delta A_j^{ab}(k_j,k_\perp) + O(\Delta^2)$$

$$\approx e^{-i \Delta A_j(k_j,k_\perp)} + O(\Delta^2)$$

$$P e^{i\int_{k_0}^{k} dk_j A_j(k_j,k_1)} \simeq e^{i\Delta A_j(k_j,k_1)} \cdots e^{-i\Delta A_j(k_0+2\Delta,k_1)} e^{-i\Delta A_j(k_0+\Delta,k_1)} \mathbb{1}$$



"Trotter decomposition" $\qquad \Delta \leq \frac{1}{2\Omega}$

$$P e^{i\int_{k_0}^{k_j} dk_j' A_j(k_j',k_1)} = \lim_{\Delta\to 0} \langle u_{q k_j k_1} | u_{q k_j-\Delta} \rangle \cdots \langle u_{q k_0+2\Delta} | u_{q k_0+\Delta} \rangle \langle u_{q k_0+\Delta,k_1} | u_{b k_0,k_1} \rangle$$

$$\hat{P}(\vec{k}) = \sum_{n=1}^{N_{occ}} |u_{n\vec{k}}\rangle\langle u_{n\vec{k}}| \qquad \vec{k} = (k_j, \vec{k}_1)$$

$$L_1 = \lim_{\Delta \to 0} \langle u_{a k_1, k_2} | \tilde{P}(k_1, k_2) \tilde{P}(k_1 - \Delta, k_2) \cdots \tilde{P}(k_0 + \Delta, k_2) \tilde{P}(k_0, k_2) | u_{b k_0, k_2} \rangle$$

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

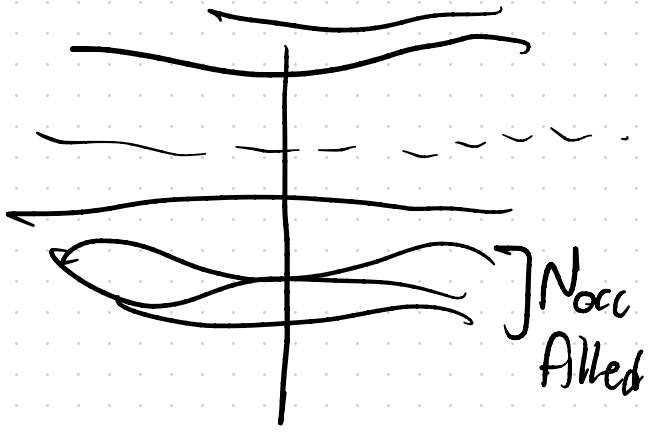
Advantages:

① No need to approximate derivatives → numerically stable

② Converges very fast for Δ small enough

Connecting eigenvalues of $P x_j P$ to observables

$P x_i \hat{t}_i P$ has eigenvalues $n \vec{t}_j + \frac{\phi_q(k_1)}{2\pi} \vec{t}_j$



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

We can try to compute $\langle \vec{t}_i x_j \rangle_0$ in the ground

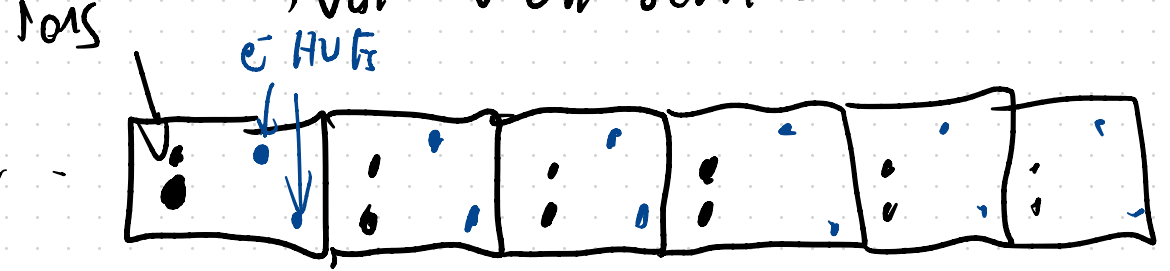
state

$$\langle \vec{t}_i x_i \rangle = \langle x_i \rangle_0 \vec{t}_i = \frac{1}{(2\pi)^2} \int dk_\perp \sum_{a=1}^{N_{occ}} \sum_{n=-\infty}^{\infty} \langle W_{ank_\perp} | x_i | W_{ank_\perp} \rangle$$

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

HWF = Hybrid Wannier functions

Not well behaved



Charge per unit cell: $\sum_{\alpha \in \text{ions}} q_\alpha = N_{occ} e$

q_α Charge of ion α

Electric dipole moment

$$\vec{d}_j = -e\langle x_j \rangle_\alpha + \sum_{ions} q_\alpha R_{\alpha,j}$$

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

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

Charge neutrality

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

electric dipole moment per unit cell

$$\sum_\alpha q_\alpha r_\alpha = x_{0i} \, q_{tot}$$

x_{0i}: center of charge in the unit cell

$$d_i = N \rho_i$$

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

$e^{i\varphi_a(k_2)}$ eigenvalues of Wilson loop $W_{2\pi>0}(k_2)$

$$\sum_{a=1}^{N_{occ}} \varphi_a(k_2) = \mathrm{Im}\log\left(e^{i\sum_{a=1}^{N_{occ}}\varphi_a(k_2)}\right)$$

$$= \mathrm{Im}\log\prod_{a=1}^{N_{occ}} e^{i\varphi_a(k_2)}$$

$$= \mathrm{Im}\log\det W_{2\pi>0}(k_2)$$

$$= \mathrm{Im}\log e^{i\int_0^{2\pi} dk_j \,\mathrm{tr}\, A_j(k_j,k_2)}$$

$$= \int_0^{2\pi} dk_j \,\mathrm{tr}\, A_j(k_j,k_2)$$

$$\vec{P} = N_{occ} e \vec{X}_a - \frac{e}{(2\pi)^3} \int d^3k \; tr \vec{A}(k_1, k_2)$$

dipole moment/ unitcell

Ionic part

electronic part

What about gauge transformations (change of basis)

$$\vec{A} \rightarrow U^\dagger A U + i U^\dagger \nabla_k U \qquad U \; N_{occ} \times N_{occ} \text{ unitary matrix}$$

$$tr\vec{A} \rightarrow tr\vec{A} + i \, tr\, U^\dagger \nabla_k U$$

$\rightarrow tr\vec{A} - \nabla_k \theta(k)$

U has eigenvalues $e^{i\theta_j(k)}$

$\sum_j \theta_j(k) = \theta(k)$

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

$\hookrightarrow \vec{P} - \sum_j e\, m_j \vec{t}_j$

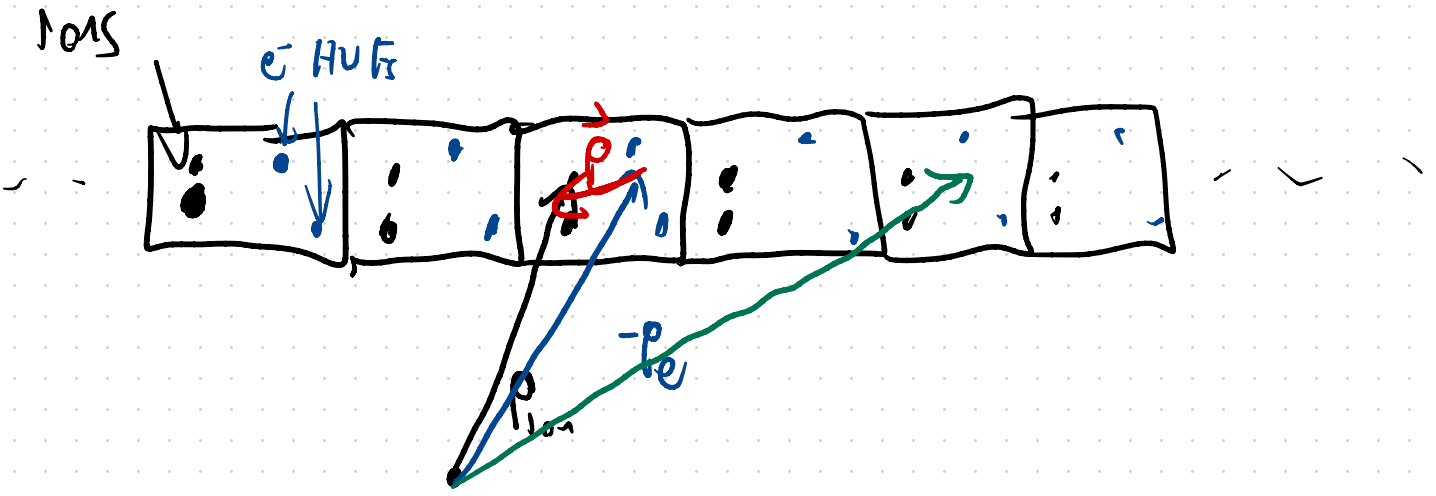
$\det U$ is periodic

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

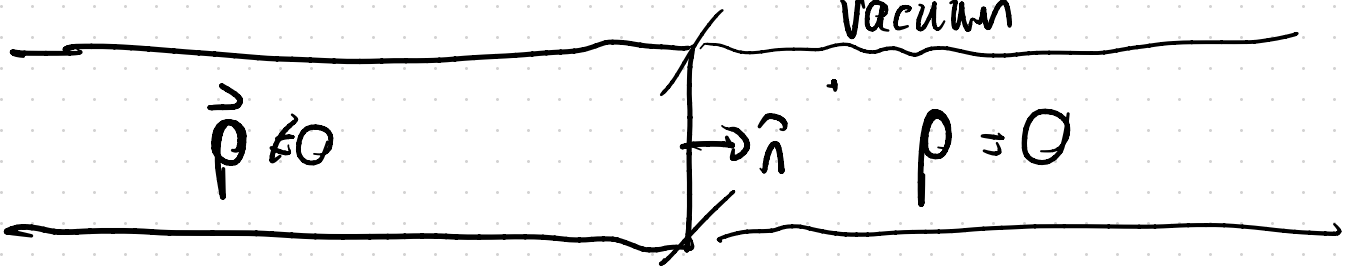
$\theta(k+\vec{b}_j) = \theta(k) + 2\pi m_j$

dipole moment per unit cell is not gauge invariant

$\vec{P}$ is only well defined Bravais lattice translations



What is physical is $\vec{p}_i$ mod $e\vec{t}_j$



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

Surface charge $\sigma_b = -\Delta \vec{P} = \vec{P} \cdot \hat{n}$

we can always add an e^- to the interface to change $\sigma_b \to \sigma_b + e$

$$\vec{P} = -\frac{e}{(2\pi)^3} \int d^3k \, \hbar \vec{A}(k) + e\vec{t}\,m$$

integer ← can change

contributes a fractional $\sigma_{b/e}$

this by adding e^-'s

- $\vec{p}$ mod $e\vec{t}$ is an intrinsic property related to Berry phase
- contributes fractional # of e^-s/unit cell to σ_b