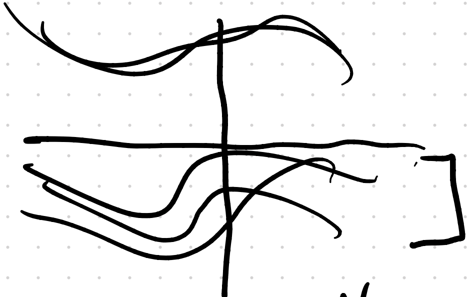
Lecture 16



N bands occupied

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

$$|\tilde{\psi}_{ak}\rangle = \sum_{b,c=1}^{N} |\psi_{bk}\rangle W^{bc}_{k_i \leftarrow k_0}(\vec{k}_\perp) e^{-i\varphi_a(k_\perp)} g^c_a(k_\perp, k_0)$$

Wilson line $\rightarrow$ $W_{k_i \leftarrow k_0}(k_\perp) = P e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i', \vec{k}_\perp)}$

depends on $k_\perp, k_0$ $\rightarrow$ $\vec{g}_a(k_\perp, k_0)$ is an eigenvector of the

Wilson loop $\quad W_{2\pi \leftarrow 0}(\vec{k}_\perp)$ w/ eigenvalue

$$e^{i\varphi_a(k_\perp)}$$

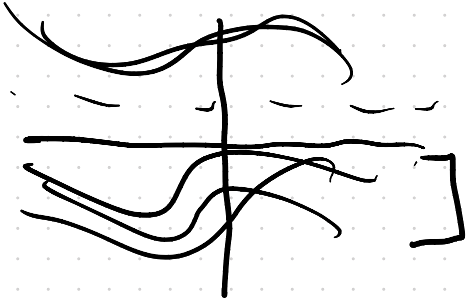
only depends on $\vec{k}_\perp$

Hybrid Wannier fns

$$|W_{an\vec{k}_\perp}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_i \, |\tilde{\psi}_{ak}\rangle e^{-ik_i n}$$

$$P x_i P |W_{an\vec{k}_\perp}\rangle = \Big(\underbrace{n}_{\text{unit cell}} + \frac{\varphi_a(k_\perp)}{2\pi}\Big) |W_{ank_\perp}\rangle$$

Berry phase - displacement relative to the origin



Observables: consider an insulator at $T=0$

We can try to compute $\langle \vec{x} \rangle_0$ in this grand State

$$\vec{x} = \sum_i x_i \vec{t}_i$$

$$\langle \vec{x} \rangle_0 = \sum_i \vec{t}_i \langle x_i \rangle_0$$

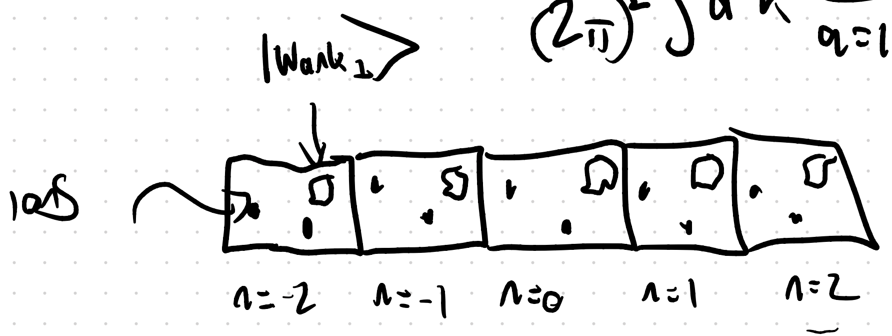
$$\langle x_i \rangle_0 = \langle P x_i P \rangle_0 = \frac{1}{(2\pi)^3} \int dk_i \, dk_\perp \sum_{a=1}^{N} \langle \psi_{ak} | x_i | \psi_{ak} \rangle$$

$$= \frac{1}{(2\pi)^3} \int dk_i \, dk_\perp \sum_{a=1}^{N} \langle \Psi_{ak} | x_i | \Psi_{ak} \rangle$$

$$= \frac{1}{(2\pi)^3}\int dk_j\, d^2k_\perp \sum_{a=1}^{N} \sum_{nm} \langle W_{ank_\perp} | x_j | W_{amk_\perp} \rangle e^{ik_j(n-m)}$$

$$= \frac{1}{(2\pi)^2}\int d^2k_\perp \sum_{a=1}^{N} \sum_{n} \langle W_{ank_\perp} | P x_j P | W_{ank_\perp} \rangle$$

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



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

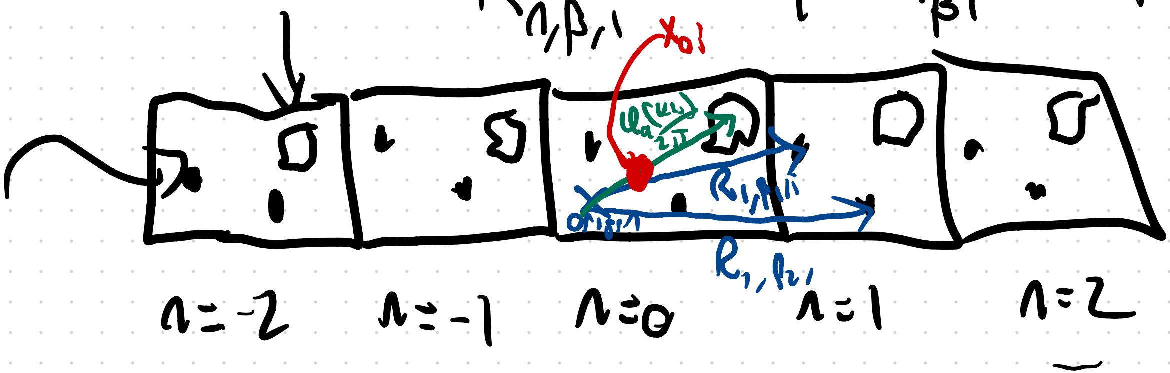
Two observations: total charge in each unit cell is zero

N electrons / unit cell $\Rightarrow$

α indexes ions (n, β)

$$R_{n,\beta,i} = n_i + r_{\beta i}$$

β – ions in one unit cell



x_{0i} – center of ionic charge

$$x_{0i} = \frac{1}{q_{tot}} \sum_\beta q_\beta r_{\beta i}$$

$$q_{tot} = \sum_\beta q_\beta$$

$$d_i = -e\langle x_i \rangle + \sum_{\substack{\text{ions} \\ \alpha}} q_\alpha R_{\alpha i} \qquad \langle e^{\frac{2\pi i}{L} x} \rangle$$

$$= \sum_{n=-\infty}^{\infty} \left[\left(-e \frac{1}{(2\pi)^2} \int d^2 k_\perp \sum_{a=1}^{N} \left(n + \frac{\varphi_a(k_\perp)}{2\pi} \right) + q_{tot}(n + x_{0i}) \right) \right]$$

$$= \sum_{n=-\infty}^{\infty} \left[\cancel{\left(q_{tot} n - eNn \right)} + -e \sum_{a=1}^{N} \varphi_a(k_\perp)/2\pi + q_{tot} x_{0i} \right]$$

Charge neutrality $q_{tot} = +Ne$

$$d_i = e \sum_{n=-\infty}^{\infty} \frac{1}{(2\pi)^2} \int d^2 k \left(x_{0i} - \frac{\varphi_a(k_\perp)}{2\pi} \right)$$

P_i - dipole moment per unit cell

$$P_i = \frac{e}{(2\pi)^2} \sum_{a=1}^{N} \int d^2 k_\perp \left(x_{0i} - \frac{\varphi_a(k_\perp)}{2\pi} \right) \quad \leftarrow \text{"polarization density"}$$

$$d_i = \sum_n P_i$$

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

$$\sum_{a=1}^{N} \varphi_a(k_\perp) = \mathrm{Im} \ln e^{i\sum_{a=1}^{N} \varphi_a(k_\perp)}$$

$$= \mathrm{Im} \ln \prod_{a=1}^{N} e^{i\varphi_a(k_\perp)}$$

$$= \mathrm{Im}\ln\det W$$

$$\det \mathcal{P} e^{i\int_0^{2\pi} dk_i A_i(k_i, k_\perp)} = e^{i\int_0^{2\pi} dk_i \,\mathrm{tr} A_i(k_i, k_\perp)}$$

$$\sum_{a=1}^{N} \varphi_a(k_\perp) = \int_0^{2\pi} dk_i \,\mathrm{tr}\, A_i(k_i, k_\perp)$$

$$p_i = \frac{e}{(2\pi)^3}\int d^3k \left[\left(N x_{0i} - \mathrm{tr}(A_i(\vec{k})\right)\right]$$

putting back units

$$\boxed{\vec{p} = Ne\vec{x}_0 - \frac{e}{(2\pi)^3}\int d^3k \,\mathrm{tr}\left(\vec{A}(\vec{k})\right)}$$

dipole moment per unit cell

What about gauge transformations?

$$|\psi_{ak}\rangle \to \sum_b |\psi_{bk}\rangle U_{ba}(k) \qquad U(k) - N\times N$$

unitary matrix

$$U(k+\vec{G}) = U(\vec{k})$$

$$\vec{A}(k) \to U^{\dagger}(k)\vec{A}\,U(k) + i\,U^{\dagger}\nabla_k U$$

$$\mathrm{tr}(\vec{A}(k)) \to \mathrm{tr}(\vec{A}(k)) + i\,\mathrm{tr}[U^{\dagger}\nabla_k U] \quad \Big\{ \quad \mathrm{tr}[U^{\dagger}\nabla_k U] = \nabla_k[\mathrm{tr}\log U]$$

$$\to \mathrm{tr}(\vec{A}(k)) + i\,\nabla_k(\mathrm{tr}\log U)$$

$$\to \mathrm{tr}(\vec{A}(k)) + i\,\nabla_k \log\det U$$

$$U \text{ unitary} \to \det U(k) = e^{i\theta(k)} +$$

U periodic $\quad e^{i\theta(k+\vec{G})} = e^{i\theta(k) + 2\pi i n_{\vec{G}}}$

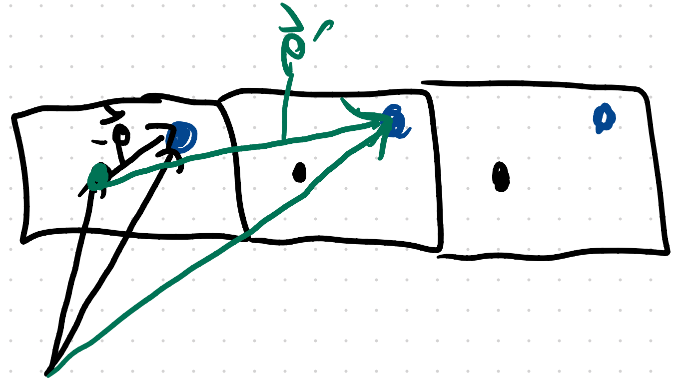
$$\vec{p} \to \vec{p} - \frac{ie}{(2\pi)^3}\int d^3k\, \nabla_k \log\det U$$

$$= \vec{p} + \frac{e}{(2\pi)^3}\int d^3k\, \nabla_{\vec{k}}\theta(k)$$

$$= \vec{p} + e\vec{t} \qquad \vec{t} \in T \quad \text{that is the winding of } \theta(k)$$

$\vec{p}$ is only well-defined modulo $e\vec{t}$ for $\vec{t} \in$ the Bravais lattice

$|W_{a n k_1}\rangle$



• - center of ionic charge

o - center of electronic charge

$$\vec{p}' = \vec{p} - e\vec{t}$$

$$e^{i\frac{n k_j}{2\pi}} \qquad \Theta(k) = n_i k_i$$

$$\nabla_k \Theta = \vec{n}$$

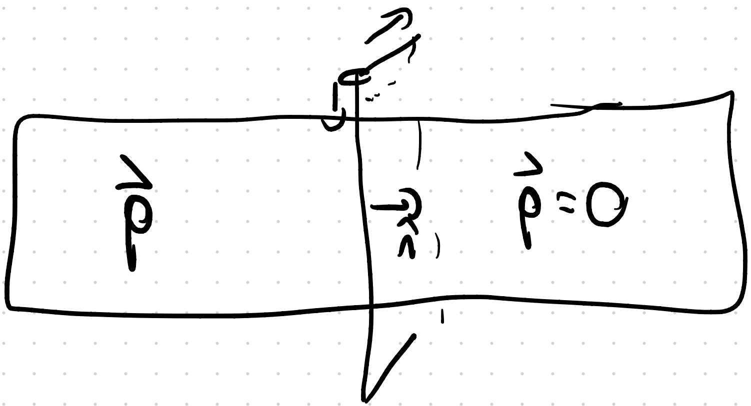
$$\int \nabla_k \Theta = \boxed{2\pi \vec{n}}$$

How do we detect any of this

Maxwell's eqns

$$\rho_b = -\frac{1}{v}\nabla\cdot\vec{p}$$

unit cell volume



$\frac{\vec{p}}{v}$ - dipole moment per unit volume

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

$$\vec{P} = e\vec{t}N - \frac{e}{(2\pi)^3}\int d^3k \; \mathrm{tr}(\vec{A}(k))$$

ionic contribution
+ gauge ambiguity

- $\vec{P} \bmod e\vec{t}$ is intrinsic
- contributes fractional # of electrons/unit cell to σ_b
- cannot be changed by adding e's to the boundary