Metal- Isolator oder topologische isolator für das zwei band problem.

a) Strom Operator, b) Eichinvarianz & Ladungserhaltung
c) Peierls-Phasen Faktor d) Linear Response e) Optische Leitfähigkeit

a Strom:

Klassisch. $\vec{j} = e\vec{v}$, $\vec{v} = \dot{\vec{x}}$,

E.D. $\mathcal{L} = \frac{mv^2}{2} - e\left(\phi - \frac{\vec{v}}{c}\cdot\vec{A}\right)$, $\Rightarrow$ $\vec{p} = \frac{\partial \mathcal{L}}{\partial \vec{v}} = m\vec{v} + \frac{e}{c}\vec{A}$

$\Rightarrow$ $\vec{v} = \left(p - \frac{e}{c}A\right)/m$ so dass

$$\vec{j} = \frac{e}{m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)$$

Q. M. $$\hat{\vec{j}} = \frac{e}{m}\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{x})\right)$$

Zweite Quantisierung:

$$\hat{\vec{J}} = \sum_{\sigma}\int_V d^3x\ \hat{\psi}^{+}_{\sigma}(\vec{x})\frac{e}{m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{x})\right)\hat{\psi}_{\sigma}(\vec{x}).$$

$$= \sum_{\sigma}\int_V d^3x\ \psi^{+}_{\sigma}(x)\frac{\hbar e}{mi}\vec{\nabla}\psi_{\sigma}(x) - \frac{e^2}{mc}\sum_{\sigma}\psi^{+}_{\sigma}(x)\psi_{\sigma}(x).$$

$$= \frac{e\hbar}{2mi} \sum_{\sigma} \int_V d^3x \left(\hat{\psi}^{+}_{\sigma}(x)\, \vec{\nabla}\, \hat{\psi}_{\sigma}(x) - \left(\vec{\nabla} \hat{\psi}^{+}_{\sigma}(x)\right) \hat{\psi}_{\sigma}(x) \right)$$

$$- \frac{e^2}{mc} \int_V d^3x \sum_{\sigma} \hat{\psi}^{+}_{\sigma}(x)\, \hat{\psi}_{\sigma}(x)\, \vec{A}(x) =$$

$$\boxed{\begin{aligned} &\int_V d^3x \left\{ \hat{J}^{P}(x) + \hat{J}^{D}(x) \right\} \\ &\hat{J}^{P}(x) = \frac{e\hbar}{2im} \sum_{\sigma} \left(\hat{\psi}^{+}_{\sigma}(x)\, \vec{\nabla}\, \hat{\psi}_{\sigma}(x) - \left(\vec{\nabla} \hat{\psi}^{+}_{\sigma}(x)\right) \hat{\psi}_{\sigma}(x) \right) \\ &\hat{J}^{D}(x) = -\frac{e^2}{mc} \sum_{\sigma} \hat{\psi}^{+}_{\sigma}(x)\, \hat{\psi}_{\sigma}(x)\, \vec{A}(\vec{x}) \end{aligned}}$$

Mit $\hat{H} = \int_V d^3x \sum_{\sigma} \hat{\psi}^{+}_{\sigma}(x) \left\{ \frac{1}{2m}\left(\hat{\vec{P}} - \frac{e}{c}\vec{A}\right)^2 + V_{ion}(\vec{x}) \right\} \hat{\psi}_{\sigma}(x)$

gilt: $\boxed{\hat{\vec{J}}(x) = \hat{\vec{J}}^{P}(x) + \hat{\vec{J}}^{D}(x) = -c\, \frac{\delta \hat{H}}{\delta \vec{A}(\vec{x})}}$

$$\Rightarrow \int_V d^3\vec{x} \sum_{\sigma} \hat{\psi}^{+}_{\sigma}(x) \left\{ \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}\right)^2 + V_{ion}(x) + \frac{1}{2m}\frac{e^2}{c^2}\vec{A}^2 \right.$$

$$\left. - \frac{e}{c}\frac{1}{2m}\frac{\hbar}{i}\left(\underbrace{\vec{\nabla}\cdot\vec{A}} + \vec{A}\cdot\vec{\nabla}\right) \right\} \hat{\psi}_{\sigma}(x) =$$

$$= \int_V d^3\vec{x} \sum_{\sigma} \hat{\psi}^{+}_{\sigma}(x) \left\{ \frac{P^2}{2m} + V_{ion}(x) \right\} \hat{\psi}_{\sigma}(x) +$$

$$\frac{1}{c}\left[\int_V d^3\bar{x} \sum_{r} \frac{1}{2m} \frac{e^2}{c} \vec{A}^2(x)\, \varphi^\dagger(x)\, \varphi(x)\right.$$

$$\left. - \frac{e}{2mc}\frac{\hbar}{i}\int_V d^3\bar{x} \sum_{r} \left\{ \hat{\varphi}^\dagger_r(x)\, \vec{\nabla}\, \varphi_r(x) - \left(\vec{\nabla}\, \hat{\varphi}^\dagger_r(x)\right) \hat{\varphi}_r(x)\right\} \cdot \vec{A}\right]$$

Eichtransformation:

Physik muss unter $\vec{A}'(x,t) = \vec{A}(\vec{x},t) + \vec{\nabla}\chi(x,t)$

$$\phi'(x,t) = \phi(x,t) - \frac{1}{c}\frac{\partial}{\partial t}\chi(x,t) \quad (1)$$

invariant sein:

a) Bewegungsgleichungen der Feldoperatoren.

$$\frac{\partial}{\partial t}\hat{\psi}^+_H(\vec{x},t) = \frac{\partial}{\partial t} e^{i\hat{H}t/\hbar}\,\hat{\psi}^+(\vec{x})\,e^{-i\hat{H}t/\hbar}$$

$$= \frac{i}{\hbar} e^{i\hat{H}t/\hbar}\,[\hat{H},\hat{\psi}^+(x)]\,e^{-i\hat{H}t/\hbar} =$$

$$= \ulcorner\ \hat{H} = \int d^3y \int d^3y'\,\hat{\psi}^+(\vec{y})\,\langle\vec{y}|H|y'\rangle\,\hat{\psi}(\vec{y}')\ \lrcorner$$

$$= \frac{i}{\hbar} e^{i\hat{H}t/\hbar}\int d^3y\int d^3y'\,\langle y|H|y'\rangle\,\underbrace{[\hat{\psi}^+(y)\hat{\psi}(y'),\hat{\psi}^+(x)]}_{\hat{\psi}^+(y)\,\delta^3(y-x)}\,e^{-i\hat{H}t/\hbar}$$

$$\ulcorner\ [AB,C] = ABC + ACB - ACB - CAB =$$

$$= A\{B,C\} - \{A,C\}B\ \lrcorner$$

$$= \boxed{\frac{i}{\hbar}\int d^3y\,\langle x|H|y\rangle\,\hat{\psi}^+_H(y,t) = \frac{\partial}{\partial t}\hat{\psi}^+_H(\vec{x},t)}$$

$$\Rightarrow \boxed{\underbrace{\frac{i}{\hbar}\left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 + e\,\phi(x)\right]}_{H} \hat{\psi}_H^+(\cancel{x},t) = \frac{\partial}{\partial t}\hat{\psi}_H^+(x,t) \quad (2)}$$

Unter die Eichtransformation: (1) hat man: analog.

$$\frac{i}{\hbar}\left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}A + \frac{e}{c}\vec{\nabla}\chi\right)^2 + e\,\phi(x) - \frac{e}{c}\chi(x,t)\right]\hat{\tilde{\psi}}_H^+(x,t)$$

$$= \frac{\partial}{\partial t}\hat{\tilde{\psi}}_H^+(x,t)$$

$$\Rightarrow \frac{i}{\hbar} e^{-\frac{i}{\hbar}\frac{e}{c}\chi}\left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 e^{\frac{i}{\hbar}\frac{e}{c}\chi}\hat{\tilde{\psi}}_H^+ - e\phi\, e^{\frac{i}{\hbar}\frac{e}{c}\chi}\hat{\tilde{\psi}}_H(x,t)\right]$$

$$= +\frac{i}{\hbar}\frac{e}{c}\chi(x,t)\hat{\tilde{\psi}}_H(x,t)^+ + \frac{\partial}{\partial t}\hat{\tilde{\psi}}_H^+(x,t))$$

$$\Rightarrow \frac{i}{\hbar}\left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 e^{\frac{i}{\hbar}\frac{e}{c}\chi}\hat{\tilde{\psi}}_H^+ - e\,\phi\, e^{\frac{i}{\hbar}\frac{e}{c}\chi}\hat{\tilde{\psi}}_H(x,t)\right]$$

$$= \frac{\partial}{\partial t}\left(e^{\frac{ie}{\hbar c}\chi(x,t)}\hat{\tilde{\psi}}_H^+(x,t)\right) \Rightarrow \text{Vergleich mit (2)}$$

Eichtransformation ist equivalent zu Kanonische transformation.

$$\boxed{\hat{\tilde{\psi}}_H^+(x,t) = e^{-\frac{ie}{\hbar c}\chi(x,t)}\hat{\psi}_H^+(x,t)}$$

Damit bleibt die Physik invariant. !

Eichinvarianz & Ladungserhaltung:

$$\left\langle \hat{H}\left(\vec{A} + \lambda \vec{\nabla}\chi,\ \phi - \frac{1}{c}\lambda\frac{\partial}{\partial t}\chi,\ t\right)\right\rangle - \left\langle \hat{H}\left(\vec{A}, \phi, t\right)\right\rangle = 0$$

$$\Rightarrow \int dt \ \frac{\partial}{\partial \lambda} \left\langle \hat{H}\left(\vec{A} + \lambda \vec{\nabla}\chi,\ \phi - \frac{1}{c}\lambda\frac{\partial}{\partial t}\chi,\ t\right)\right\rangle\Big|_{\lambda=0} = 0$$

$$\Rightarrow \int dt \int d^3\vec{x} \left\langle \underbrace{\frac{\delta \hat{H}}{\delta A(x,t)}}_{\equiv -\frac{1}{c}\hat{\vec{J}}(\vec{x})} \cdot \vec{\nabla}\cdot\chi(x,t) + \underbrace{\frac{\partial \hat{H}}{\delta \phi(x,t)}}_{e\underbrace{\sum_r \varphi^{+}_r(x)\varphi_r(x)}_{\hat{\varrho}}} \cdot \left(-\frac{1}{c}\frac{\partial}{\partial t}\chi\right)\right\rangle = 0$$

$$\Rightarrow \int dt \int d^3\vec{x} \left(-\frac{1}{c}\right)\left\{\langle \hat{\vec{J}}(\vec{x})\rangle(t)\, \vec{\nabla}\chi(x,t) + e\langle\hat{\varrho}(\vec{x})\rangle(t)\frac{\partial}{\partial t}\chi = 0\right\}$$

Partial integration gives

$$\int dt \int d^3\vec{x}\ \frac{1}{c}\left\{\vec{\nabla}\cdot\langle\vec{J}(x)\rangle(t) + e\frac{\partial}{\partial t}\langle\varrho(\vec{x})\rangle(t)\right\}\chi = 0$$

$\forall \chi \Rightarrow$

$$\boxed{\vec{\nabla}\cdot\langle\vec{J}(x)\rangle(t) + e\frac{\partial}{\partial t}\langle\varrho(x)\rangle(t) = 0}$$ ✓

Tight-Binding: Peierls phase factors

$$\hat{H} = \sum_{n,m} \hat{c}^{+}_{R,n}\, t_{n,m}(\vec{R}-\vec{R}')\, \hat{c}_{R',m},$$

How should we include the magnetic field?

For $$\hat{H} = \sum_{\substack{n,m\\ R,R'}} e^{\frac{2\pi i}{\phi_0}\int_{\vec{R}}^{\vec{R}'} \vec{A}(\vec{x},t)\cdot d\vec{l}}\, t_{n,m}(\bar{R}-\bar{R}')\, \hat{c}^{+}_{R,n}\, \hat{c}_{R',m}$$

$$+\ e \sum_{n,R} c^{+}_{R,n}\, c_{R,n}\, \phi(R,t) \quad , \quad \text{with } \phi_0 = \frac{hc}{e}$$

flux quanta; Gauge invariance is guaranteed.

Comments / Examples:

a) Gauge transformation $\vec{A}'(\bar{x},t) =$

$\vec{A}(\bar{x},t) + \vec{\nabla}\chi(\bar{x})$, $\phi'(x,t) = \phi(x,t)$

$$H(A',\phi') = \sum_{\substack{n,m\\ R,R'}} e^{\frac{2\pi i}{\phi_0}\int_{\bar{R}}^{\bar{R}'}(\vec{A}+\bar{\nabla}\chi)\,d\vec{l}}\, t_{n,m}(\bar{R}-\bar{R}')$$

$$\hat{c}^{+}_{R,n}\, \hat{c}_{R',m} + e\sum_{n,R} c^{+}_{R,n}\, c_{R,n}\, \phi(\bar{R},t) =$$

$$= \sum_{\substack{n,m\\ R,R'}} e^{2\pi i/\phi_0 \int_{R}^{R'} \bar{A}\cdot d\bar{l}}\, t_{n,m}(\bar{R}-\bar{R}')\, \tilde{c}^{+}_{R,n}\, \tilde{c}_{R',m} +$$

$$e\sum_{n,R} \tilde{c}^{+}_{R,n}\, \tilde{c}_{R,n}\, \phi(R,t) \quad \text{with} \quad \tilde{c}^{+}_{R,n} = e^{-2\pi i/\phi_0\, \chi(R)}\, c^{+}_{R,n}$$

b) We have implicitly assumed that the value of the hopping matrix element remains invariant $\Rightarrow$

The vector potential should vary slowly on atomic distances where the $t_{n,m}(\vec{R}-\vec{R}') \neq 0$.

c Special cases:

1. Homogeneous magnetic fields

Consider an $L\vec{a}_1 \times L\vec{a}_2$ 2d square lattice.

$\vec{B} = (0,0,B)$ so that $\vec{A} = +\frac{B}{2}(-y,+x,0)$

(symmetric gauge) $\left[\det \begin{bmatrix} e_1 & e_2 & e_3 \\ \partial_1 & \partial_2 & \partial_3 \\ -\frac{y}{2}, & \frac{x}{2}, & 0 \end{bmatrix} = \vec{e}_3 \right]$

Periodic Boundaries

$$c_i^{+} c_j \, e^{\frac{2\pi i}{\Phi_0}\int_i^j \vec{A}\,d\vec{l}} \overset{!}{=} c^{+}_{i+L\vec{a}_\#} c_{j+L\vec{a}_\#} \, e^{\frac{2\pi i}{\Phi_0}\int_{i+La_\#}^{j+La_\#} \vec{A}\cdot d\vec{l}}$$

But: $$\int_{i+La_\#}^{j+La_\#} \vec{A}\cdot(\vec{l})\,d\vec{l} = \int_i^j \vec{A}(\vec{l}'+L\vec{a}_\#)\,d\vec{l}' \qquad \vec{l}' = \vec{l} - L\vec{a}_\#$$

$$= \int_i^j \left(\vec{A}(\vec{l}') + \vec{\nabla}\chi_\#(\vec{l}')\right) d\vec{l}'$$ smooth

$$\vec{A}(\vec{x} + La\,\vec{e}_x) = \frac{B}{2}(-y, x+La, 0) = \vec{A}(\vec{x}) +$$

$$+ \vec{\nabla}\cdot\left(\frac{B}{2}La\cdot y\right) \quad \text{so that} \quad \boxed{\chi_x(\vec{x}) = \frac{B}{2}La\,y}$$

$$\vec{A}(\vec{x}+La\vec{e}_y) = +\frac{B}{2}\left(-(y+La),\ x,0\right) =$$

$$= +\frac{1}{2}(-y,x,0) + \left(-\frac{B}{2}La,0,0\right) = \vec{A}(\vec{x}) + \vec{\nabla}\chi_y(\vec{x})$$

$$\boxed{\chi_y(\vec{x}) = -\frac{B}{2}La\,x}$$

$$\Rightarrow \quad c_i^\dagger c_j \exp\left\{\frac{2\pi i}{\phi_0}\int_i^j \vec{A}\cdot d\vec{l}\right\} \overset{!}{=}$$

$$= c^\dagger_{i+La_\#}\, c_{j+La_\#} \exp\left(\frac{2\pi i}{\phi_0}\int_i^j\left(\vec{A}+\vec{\nabla}_\#\chi_\#\right)\right) =$$

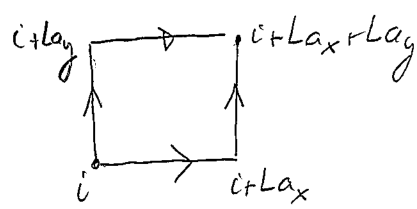
$$= c^\dagger_{i+La_\#}\, e^{-\frac{2\pi i}{\phi_0}\chi_\#(i)}\; c_{j+La_\#}\, e^{\frac{2\pi i}{\phi_0}\chi_\#(j)}$$

$\Rightarrow$ Boundary conditions:

$$\boxed{c^\dagger_{i+La_\#} = e^{\frac{2\pi i}{\phi_0}\chi_\#(\vec{i})}\, c_i^\dagger}$$

Quantization of the magnetic field: We will require the wave function to be single valued.!

$$\Rightarrow \quad T^{-1}_{La_y} T^{-1}_{La_x}\, c_i^\dagger\, T_{La_x} T_{La_y} \overset{!}{=}$$



$$T^{-1}_{La_x} T^{-1}_{La_y}\, c_i^\dagger\, T_{La_y} T_{La_x}$$

$$\Rightarrow \hat{T}^{-1}_{L\vec{a}_y}\, \hat{T}^{-1}_{L\vec{a}_x}\, c^{\dagger}_{i}\, \hat{T}_{L\vec{a}_x}\, \hat{T}_{L\vec{a}_y} =$$

$$= \hat{T}^{-1}_{La_y}\, c^{\dagger}_{i+L\vec{a}_x}\, \hat{T}_{La_y} = \exp\left(\frac{2\pi i}{\phi_0}\left(\chi_y(i+L\vec{a}_x) + \chi_x(i)\right)\right) c^{\dagger}_{i}$$

$$\overset{!}{=} \hat{T}^{-1}_{La_x}\, c^{\dagger}_{i+La_y}\, \hat{T}_{La_x} = \exp\left(\frac{2\pi i}{\phi_0}\left(\chi_x(\vec{i}+L\vec{a}_y) + \chi_y(i)\right)\right) c^{\dagger}_{i}$$

$\ulcorner\ \chi_y(\vec{x}) = -\frac{B}{2} La\, x\ ,\ \chi_x(\vec{x}) = \frac{B}{2} La\, y\ \lrcorner$

$$\Rightarrow \exp\left[\frac{2\pi i B}{\phi_0}\left(-\frac{1}{2} La\,(\cancel{i_x} + La) + \cancel{\frac{1}{2} La\, i_y}\right)\right] \overset{!}{=}$$

$$\exp\left[\frac{2\pi i B}{\phi_0}\left(\frac{1}{2} La\,(\cancel{i_y} + La) - \cancel{\frac{1}{2} La\, i_x}\right)\right]$$

$$\Rightarrow \exp\left(2\pi i \frac{BLa^2}{\phi_0}\right) = 1 \Rightarrow \boxed{\frac{BLa^2}{\phi_0} = n}$$

$\Rightarrow$ The total magnetic flux traversing the lattice has to be an integer multiple of the flux quanta.

$\rightarrow$ Hofstadter Butterfly corresponds to the spectrum of the problem as a function of $\boxed{\frac{Ba^2}{\phi_0} = \frac{n}{L^2}}$

2. Twisted Boundary conditions:

$$\vec{A}(\vec{x}) = \frac{\phi}{La} \cdot \vec{e}_x \quad , \quad c^+_{i+La_\#} = c^+_i .$$

$$\Rightarrow \quad H = \sum_{i,j} c^+_i \, t(i-j) \, c_j \exp\left(\frac{2\pi i}{\phi_0} \cdot \frac{\phi}{La}(j_x - i_x)\right)$$

$$= \sum_{i,j} \underbrace{c^+_i \exp\left(-\frac{2\pi i}{\phi_0} \frac{\phi}{La} i_x\right)}_{\equiv \tilde{c}^+_i} t(i-j) \underbrace{c_j \exp\left(\frac{2\pi i}{\phi_0} \cdot \frac{\phi}{La} j_x\right)}_{\equiv \tilde{c}_j}$$

$$= \sum_{i,j} \tilde{c}^+_i \, t(i-j) \, \tilde{c}_j$$

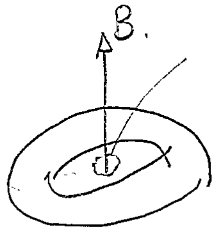
$\Rightarrow$ Magnetic field disappears from Hamiltonian but shows up in boundary condition since

$$\tilde{c}^+_{i+La_\#} = e^{-\frac{2\pi i}{\phi_0} \frac{\phi}{La} \cdot (\vec{i} + L\vec{a}_\#) \cdot \vec{e}_x} \overbrace{c^+_{i+La_\#}}^{\equiv c^+_i} =$$

$$= e^{-\frac{2\pi i}{\phi_0} \frac{\phi}{La} \cdot L\vec{a}_\# \vec{e}_x} \underbrace{c^+_i \, e^{\frac{-2\pi i}{\phi_0} \frac{\phi}{La} \cdot \vec{i} \cdot \vec{e}_x}}_{\equiv \tilde{c}^+_i}$$

$$= \exp\left(-2\pi i \frac{\phi}{\phi_0} \delta_{\#,x}\right) \tilde{c}^+_i .$$

$\vec{B}$. $\int d\vec{\Omega} \cdot \vec{B} = \Phi$.



We will see later that $\left. \frac{1}{L^{d-2}} \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \right|_{\phi=0} =$ Drude weight and acts as an "order parameter" for an insulator or metal.

Optical conductivity

L1

a) Linear response:

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t) \qquad \hat{H}_1(t\to-\infty)=0$$

Question: $\langle \hat{O}\rangle(t) = Tr\{\hat{\rho}(t)\,\hat{O}\}$ in first order in the perturbation $\hat{H}_1(t)$.

Density matrix satisfies the time evolution equation:

$$\frac{d}{dt}\rho(t) = \left[\frac{d}{dt} e^{-it\hat{H}/\hbar}|\Psi\rangle\langle\Psi| e^{+itH/\hbar}\right] = \qquad [\hbar=1]$$

$$= -\frac{i}{\hbar}[\hat{H}(t),\rho(t)] = -\frac{i}{\hbar}[\hat{H}_0+\hat{H}_1(t),\hat{\rho}(t)]$$

Density matrix of $\hat{H}_0$

Ansatz: $\hat{\rho}(t) = \hat{\rho}_0 + \hat{f}(t)$

$$\Rightarrow i\frac{d}{dt}\hat{\rho}(t) = i\frac{d}{dt}\hat{f}(t) = [H_0+H_1(t),\rho_0+\hat{f}(t)] =$$

$$= \underbrace{[H_0,\rho_0]}_{=0} + [H_1(t),\rho_0] + [H_0,f(t)] + \underbrace{[H_1(t),f(t)]}_{\sim O(H_1^2)} \Rightarrow \text{forget it.}$$

$$\Rightarrow i\frac{d}{dt}\hat{f}(t) - [H_0,f(t)] = [H_1(t),\rho_0] + O(H_1^2)$$

But: $$i e^{-iH_0t}\left(\frac{d}{dt} e^{iH_0t}\hat{f}(t)e^{-iH_0t}\right)e^{iH_0t} =$$

$$= i e^{-iH_0t}\left(e^{iH_0t}\, i[H_0,\hat{f}(t)]\,e^{-iH_0t} + e^{iH_0t}\left(\frac{d}{dt}\hat{f}(t)\right)e^{-itH_0t}\right)e^{+iH_0t}$$

$$= -[H_0, \hat{f}(t)] + i \frac{d}{dt} \hat{f}(t) \Rightarrow$$

$$\frac{d}{dt} e^{iH_0 t} \hat{f}(t) e^{-iH_0 t} = -i e^{iH_0 t} [H_1(t); \varrho_0] e^{-iH_0 t}$$

$$= -i [H_1^H(t), \varrho_0]$$

<u>Def</u> $H_1^H(t) = e^{iH_0 t} H_1(t) e^{-iH_0 t}$

$$\Rightarrow e^{iH_0 t} \hat{f}(t) e^{-iH_0 t} = e^{iH_0 t_0} \hat{f}(t_0) e^{-iH_0 t_0} +$$

$$+ -i \int_{t_0}^{t} dt' [H_1^H(t'), \varrho_0] \Rightarrow$$ with $\hat{f}(-\infty) = 0$ we get

$$\hat{f}(t) = -i \int_{-\infty}^{t} dt' e^{-iH_0 t} [H_1^H(t'), \varrho_0] e^{iH_0 t}$$

$$\Rightarrow \langle O \rangle(t) = Tr\{\varrho(t)\, O\} =$$

$$= \underbrace{Tr\{\varrho_0 O\}}_{= \langle O \rangle_0} + Tr\{f(t), \hat{O}\} = \langle O \rangle_0 - i$$

$$\int_{-\infty}^{t} dt' \, Tr\left[e^{-iH_0 t} [H_1^H(t'), \varrho_0] e^{iH_0 t} O\right]$$

$$= \langle O \rangle_0 - i \int_{-\infty}^{t} dt' \, Tr\left\{[H_1^H(t'), \varrho_0] \hat{O}^H(t)\right\}$$

$$= \langle O \rangle_0 - i \int_{-\infty}^{t} dt' \, Tr\left\{ [H_1^H(t') \varrho_0 - \varrho_0 H_1^H(t')] \hat{O}^H(t) \right\}$$

$$= \langle O \rangle_0 - i \int_{-\infty}^{t} dt' \; Tr \left[\hat{O}^H(t) \, H_1^H(t') \, \rho_0 - \rho_0 \, H_1^H(t') \, \hat{O}^H(t) \right]$$

$$= \langle O \rangle_0 - i \int_{-\infty}^{t} dt' \; \langle [\hat{O}^H(t), H_1^H(t')] \rangle \; = \langle O \rangle(t)$$

$= \langle O \rangle(t)$ Variable substitution: $x = t - t'$ gives:

$$\boxed{\langle O \rangle(t) = \langle O \rangle_0 - \frac{i}{\hbar} \int_0^{\infty} dx \; \langle [\hat{O}^H(t), \hat{H}_1^H(\cancel{t-x})] \rangle_0}$$

b) Linear response to electric field:

Let $\vec{A}(t) = \vec{A}(\omega)\, e^{-i(\omega + i\eta)t}$ $\quad A(t \to -\infty) = e^{+\eta t} = 0$

$$\vec{E}(t) = -\frac{1}{c}\frac{\partial}{\partial t} A(t) = +\frac{i(\omega + i\eta)}{c}\vec{A}(\omega)\, e^{-i(\omega+i\eta)t}$$

$$\equiv \vec{E}(\omega)\, e^{-i(\omega+i\eta)t} \quad \text{with} \quad A(\omega) = \frac{c\, E(\omega)}{i(\omega + i\eta)}.$$

Hamilton Operator of electrons in field $\vec{E}(t)$:

$$\hat{H} = \sum_{i,j} c_i^+ \, t(i-j)\, c_j \, e^{\frac{2\pi i}{\phi_0}\int_i^j \vec{A}(l)\, d\vec{l}}$$

$$= \sum_{i,j} c_i^+ \, t(i-j)\, c_j \left(1 + \frac{2\pi i}{\phi_0} (\bar{j} - \bar{i}) \cdot \vec{A}(t) + \mathcal{O}(E^2) \right)$$

$$= \hat{H}_0 + \hat{H}_1(t) + \mathcal{O}(E^2) \text{ with } \quad \hat{H}_0 = \sum_{i,j} c_i^+ \, t(i-j)\, c_j \quad \text{and}$$

$$\hat{H}_1(t) = \frac{2\pi}{\phi_0} \sum_{i,j} i\, (\bar{j} - \bar{i}) \cdot \vec{A}(t)\; \bar{c}_i^+ \, t(i-j)\, c_j \equiv \frac{2\pi}{\phi_0} \hat{\vec{J}}_p \cdot \vec{A}(t)$$

Current Operator

Def $\quad \hat{\vec{J}}_p = \sum_{i,j} i\,(\bar{j} - \bar{i})\; \bar{c}_i^+ \, t(i-j)\, c_j$

Current Operator:

$$H = \sum_{\substack{i,j \\ n,m}} c^{+}_{i,n}\, t_{n,m}(i-j)\, c_{j,m} \exp\left(\frac{2\pi i}{\phi_0}\int_{\vec{i}}^{\vec{j}} \vec{A}\, d\vec{l}\right)$$

$$= \sum_{i,j} c^{+}_{i}\, t(i-j)\, c_j\, e^{\frac{2\pi i}{\phi_0}\int_{\vec{i}}^{\vec{j}} \vec{A}\, d\vec{l}} \Rightarrow$$

$$\boxed{\vec{j}(\vec{r}) = -c\frac{\delta H}{\delta \vec{A}(\vec{r})}} \Rightarrow \quad j_\alpha(\vec{r}) = -c \lim_{\lambda \to 0}$$

$$\frac{H(\vec{A}(x) + \vec{e}_\alpha \lambda\, \delta(\vec{x}-r)) - H(\bar{A}(x))}{\lambda} = -c \cdot \sum_{i,j}$$

$$c^{+}_{i}\, t(i-j)\, c_j \exp\left(\frac{2\pi i}{\phi_0}\int_{i}^{j} \bar{A}\, d\vec{l}\right) \cdot \frac{2\pi i}{\phi_0}\int_{\bar{i}}^{\bar{j}} \vec{e}_\alpha \cdot \delta(\vec{l}-\vec{r})\, d\vec{l}$$

But: $\displaystyle\int_{\vec{i}}^{\vec{j}} \vec{e}_\alpha\, \delta(\bar{l}-\vec{r})\, d\vec{l} = \int_0^1 dt\, \delta(\vec{l}(t)-\vec{r})\, \frac{d\vec{l}}{dt} \cdot \vec{e}_\alpha$

$\left[\vec{l} = \vec{i} + \underline{(\vec{j}-\vec{i})}\, t\right] \quad = \displaystyle\int_0^1 dt\, \delta(\vec{l}(t)-\bar{r}) \cdot (\bar{j}-\vec{i}) \cdot \vec{e}_\alpha$

$$\Rightarrow \boxed{\vec{j}_\alpha(\vec{r}) = -c\frac{2\pi i}{\phi_0}\sum_{i,j} (\vec{j}-\vec{i}) \cdot \vec{e}_\alpha \left(\delta_{\bar{r},i} + \delta_{\bar{r},j}\right) c^{+}_{i}\, t(i-j)\, c_j\, e^{\frac{2\pi i}{\phi_0}\int_{i}^{j} \bar{A}\, d\vec{l}}}$$

$$= -c\,\frac{2\pi i}{\phi_0}\left[\sum_{j} (\bar{j}-\bar{r}) \cdot \bar{e}_\alpha\, c^{+}_{r}\, t(r-j)\, c_j\, e^{\frac{2\pi c}{\phi_0}\int_{r}^{j} \bar{A} \cdot d\vec{l}} \right.$$

$\sigma = \vec{r} - \vec{j}$

$$+ \sum_i (\vec{r}-\vec{i})\, \vec{e}_\alpha \cdot c_i^+ \, t\underbrace{(i-r)}_{\delta = i-r} c_r \, e^{\frac{2\pi i}{\phi_0} \int_i^r \vec{A} d\vec{l}} \Big]$$

$$= -c \frac{2\pi i}{\phi_0} \Big[\sum_j (\vec{j}-\vec{r})\, \vec{e}_\alpha \Big(c_r^+ t(r-j)\, c_j \, e^{\frac{2\pi i}{\phi_0} \int_r^j \vec{A} \cdot d\vec{l}} - c_j^+ t(j-r)\, c_r \, e^{\frac{2\pi i}{\phi_0} \int_j^r A d\vec{l}} \Big)$$

$\delta = j - r$ =

$$\boxed{\begin{aligned} & -c \frac{2\pi i}{\phi_0} \sum_\delta \vec{\delta} \cdot \vec{e}_\alpha \Big[c_r^+ \, t(-\vec{\delta})\, c_{r+\delta} \, e^{\frac{2\pi i}{\phi_0} \int_r^{\vec{r}+\vec{\delta}} \vec{A} \cdot d\vec{l}} \\ & \qquad - c_{r+\delta}^+ \, t(\vec{\delta})\, c_r \, e^{2\pi i \int_{\vec{r}+\vec{\delta}}^{\vec{r}} \vec{A} \cdot d\vec{l}} \Big] \\ & = \hat{j}_\alpha^{\,\omega t}(\vec{r}) \end{aligned}}$$

<u>Beispi</u>

$$H = -t \sum_{i,\, a_\#} \left(c_i^+ c_{i+a_\#} + h.c. \right)$$

$$\Rightarrow J_x(r) = +c \frac{2\pi i}{\phi_0} t \Big(a_x \left(c_r^+ c_{r+a_x} - c_{r+a_x}^+ c_r \right) - a_x \left(c_r^+ c_{r-a_x} - c_{r-a_x}^+ c_r \right) \Big)$$

$$= -c \frac{2\pi i}{\phi_0} a_x \Big(c_r^+ c_{r+a_x} - c_{r+a_x}^+ c_r + c_{r-a_x}^+ c_r - c_r^+ c_{r-a_x} \Big)$$

$\Rightarrow$ Total current $= \frac{1}{N}\sum_r \vec{j}(r) = \vec{J}^{tot} =$

$$= -2c\frac{2\pi i}{\phi_0 N}\sum_{i,j}(\vec{j}-\vec{i})\, c_i^+ t(i-j)\, c_j\, e^{\frac{2\pi i}{\phi_0}\int_i^j \vec{A}\, d\vec{l}} =$$

$$= -2c\frac{2\pi i}{\phi_0 N}\Big(\sum_{i,j} i\,(\vec{j}-\vec{i})\, c_i^+ t(i-j)\, c_j\, \Big(1 + \frac{2\pi i}{\phi_0}(\vec{j}-\vec{i})\cdot\vec{A}(t)\Big)$$

$$+ \mathcal{O}(A^2)\Big)$$

$$\boxed{\begin{aligned} \text{Let}\quad \hat{\vec{J}}_p &= i\sum_{i,j}(\vec{j}-\vec{i})\, c_i^+ t(i-j)\, c_j \\ \vec{J}_D(t) &= \sum_{i,j}(\vec{j}-\vec{i})\, c_i^+ t(i-j)\, c_j\,\big[(\vec{j}-\vec{i})\cdot\vec{A}(t)\big] \end{aligned}}$$

$$\Rightarrow \hat{\vec{J}}^{tot} = -2c\frac{2\pi}{\phi_0}\frac{1}{N}\Big(\hat{\vec{J}}_p + \vec{J}_D(t)\frac{2\pi}{\phi_0}\Big) \quad \text{and}$$

$$H_1(t) = \frac{2\pi}{\phi_0}\vec{J}_p\cdot\vec{A}(t)$$

$\Rightarrow$ Linear response:

$$\langle \hat{\vec{J}}^{tot}\rangle(t) = \langle \hat{\vec{J}}^{tot}\rangle_0(t) - \frac{i}{\hbar}\int_0^\infty dx\, \langle [\hat{\vec{J}}^{tot,H}(t),$$

$$H_1^H(t-x)]\rangle_0$$

Let $\vec{E}(t) = E(t)\cdot\vec{e}_x \Rightarrow \vec{A}(t) = A(t)\cdot\vec{e}_x$

$$\cdot \; \langle \vec{J}^{\,tot} \rangle_0 (t) = -\frac{4\pi c}{\phi_0 N} \left\{ \langle \vec{J}_p \rangle_0 + \frac{2\pi}{\phi_0} \langle \vec{J}_D(t) \rangle_0 \right]$$

$$= -\frac{4\pi c}{\phi_0 N} \Big[\underbrace{\langle \vec{J}_p \rangle_0}_{\equiv 0} - \frac{2\pi}{\phi_0} \sum_{i,j} (\vec{j}-\vec{i}) \; c_i^{+} t(i-j) c_j (j-i)_x \; A_x(t) \Big]$$

Parity

$$\Rightarrow \langle \vec{J}^{\,tot}_{\alpha} \rangle_0 = + \frac{4\pi c}{\phi_0 N} \Big[\frac{2\pi}{\phi_0} \underbrace{\langle \sum_{i,j} (j-i)_x^2 \; c_i^{+} t(i-j) c_j \rangle}_{\equiv \hat{K}_x} \Big] A_x(t) \, \delta_{\alpha,x}$$

$$= + \frac{4\pi c}{\phi_0} \; \frac{2\pi}{\phi_0 N} \langle \hat{K}_x \rangle \cdot A_x(t) \, \delta_{\alpha,x} \quad \Rightarrow$$

Retaining only terms of order $A_x(t)$ we obtain:

$$\langle J^{tot}_{\alpha} \rangle (t) = - \frac{4\pi c}{\phi_0 N} \left\{ \frac{2\pi}{\phi_0} \langle \hat{K}_x \rangle A_x(t) \, \delta_{x,\alpha} \right.$$

$$\left. - i \frac{1}{N} \int_0^\infty dx \; \langle \Big[-\frac{4\pi c}{\phi_0} j^{H}_{p,\alpha}(t) \, , \, \frac{2\pi}{\phi_0} j^{H}_{p,x}(t-x) \; A_x(t-x) \Big) \Big] \rangle_0 \right]$$

$$= + \frac{4\pi c}{\phi_0} \cdot \frac{2\pi}{\phi_0 N} \Big[+ \langle K_x \rangle \delta_{x,\alpha} + i \int_0^\infty dx \; \underbrace{\langle [j^{H}_{p,\alpha}(t) , j^{H}_{p,x}(t-x)] \rangle_0}_{t \text{ independent}}$$

$$\cdot \, e^{+ix(\omega + i\eta)} \Big] \; A_x(\omega) \, e^{-it(\omega + i\eta)}$$

$$\Rightarrow \langle J^{tot}_{\alpha} \rangle (\omega) = \frac{4\pi^2 c}{\phi_0^2 N} \Big[+ \langle K_x \rangle \delta_{x\alpha} + i \int_0^\infty dx \; \langle [j_{p,\alpha} , j^{H}_{p,x}(-x)] \rangle_0 \, e^{ix(\omega+i\eta)} \Big] A_x(\omega)$$

$$J_{\alpha}^{tot}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2} \cdot \frac{1}{N\, i(\omega+i\eta)} \left[+ \langle K_x \rangle \delta_{x,\alpha} + i \int_0^\infty dt\, e^{ix(\omega+i\eta)} \right.$$

$$\left. \langle [j_{p,\alpha}, j_{p,x}(-x)] \rangle_0 \right] E_x(\omega)$$

$$\Rightarrow \boxed{\sigma_{\alpha,\gamma}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2} \frac{1}{i(\omega+i\eta)} \frac{1}{N} \left[+ \langle K_\alpha \rangle \delta_{\alpha,\gamma} + \frac{i}{\hbar} \int_0^\infty dt\, e^{it(\omega+i\eta)} \langle [j_{p,\alpha}, j^H_{p,\gamma}(-t)] \rangle_0 \right]}$$

with
$$\hat{H}_0 = \sum_{i,j} \vec{c}_i^{\dagger}\, t(i-j)\, \vec{c}_j$$

$$\vec{j}_p = \sum_{i,j} i(\vec{j}-\vec{i})\; c_i^{\dagger}\, t(i-j)\, c_j$$

$$K_\alpha = \sum_{i,j} (\vec{j}-\vec{i})_\alpha^2\; c_i^{\dagger}\, t(i-j)\, c_j$$

Explicit calculation of $\Gamma_{\alpha,\beta}(\omega)$ for n-band model.

$$H_0 = \sum_{i,j} c_i^+ \, t(i-j) \, c_j = \qquad \ulcorner c_i^+ = \frac{1}{\sqrt{N}} \sum_k e^{-iki} c_k^+$$

$$= \sum_{i,j} \frac{1}{N} \sum_{k,p} e^{-i\vec{k}\cdot\vec{i}} \, c_k^+ \, t(i-j) \, e^{i\vec{p}\vec{j}} \, c_p$$

$$= \sum_{k,p} c_k^+ \left[\frac{1}{N} \sum_{i,j} e^{-i\vec{k}(i-j)} \, t(i-j) \, e^{+i(p-k)j} \right] c_p$$

$$= \boxed{\sum_k c_k^+ \, H_0(k) \, c_k = \hat{H}_0} \quad \text{with} \quad H(k) = \sum_r e^{-i\vec{k}\vec{r}} \, t(r)$$

$$\boxed{\vec{j}_P = -\sum_k c_k^+ \frac{\partial H_0(\vec{k})}{\partial \vec{k}} c_k} = da$$

$$\sum_k c_{\vec{k}}^+ \left(\frac{\partial}{\partial \vec{k}} \frac{1}{N} \sum_{i,j} e^{-i k (\vec{i}-\vec{j})} \, t(i-j) = \right) c_{\vec{k}}$$

$$= \sum_{i,j} i(\vec{j}-\vec{i}) \frac{1}{N} \sum_k e^{-i\vec{k}(\vec{i}-\vec{j})} \, c_k^+ \, t(i-j) \, c_k$$

$$= \sum_{\vec{i},\vec{j}} i(\vec{j}-\vec{i}) \frac{1}{N} \sum_k \frac{1}{N} \sum_{p,r} e^{ir(k-p)} \, e^{-ik(i-j)} \, c_k^+ \, t(i-j) \, c_k$$

$$= \sum_{\vec{i},\vec{j}} i(\vec{j}-\vec{i}) \frac{1}{N^2} \sum_r \sum_{k,p} e^{-ik(i-r)} \, c_k^+ \, t(i-j) \, e^{+ip(j-\vec{r})} \, c_p$$

$$= \sum_{\vec{i},\vec{j}} i(\vec{j}-\vec{i}) \frac{1}{N} \sum_r c_{i-r}^+ \, t(i-r-(j-r)) \, c_{j-r} =$$

$$= \frac{1}{N} \sum_{\bar r} \sum_{i,j} i(\bar j - \bar r - (\bar i - \bar r))\; c^{+}_{\bar i - \bar r}\; t(\bar i - \bar r - (\bar j - \bar r))\; c_{\bar j - \bar r} =$$

$$= \sum_{i,j} i(\bar j - \bar i)\; c^{+}_{\bar i}\; t(\bar i - \bar j)\; c_{\bar j} = \vec{J}_P .$$

Computing the Current-Current correlations:

$$H_0 = \sum_k \vec{c}^{\,+}_k \cdot H(k)\, \vec{c}_k = \sum_k \vec{c}^{\,+}_k U_k\, U^{+}_k H_0(k)\, U_k\, U^{+}_k \vec{c}_k$$

$$= \sum_{k,n} \gamma^{+}_{k,n}\, \gamma_{k,n}\, E_n(k) \quad \text{with:} \quad \boxed{\begin{aligned} \vec{\gamma}^{+}_k &= \vec{c}^{\,+}_k U_k \\ \vec{\gamma}_k &= U^{+}_k \vec{c}_k \end{aligned}}$$

$$\vec{c}^{\,+}_k(t) = e^{itH_0}\, \vec{c}^{\,+}_k\, e^{-itH_0} \Rightarrow$$

$$\Rightarrow \frac{\partial}{\partial t} \vec{c}^{\,+}_{k,n}(t) = i\, e^{itH_0} \left[H_0 , \vec{c}^{\,+}_{k,n} \right] e^{-itH_0} =$$

$$= i\, e^{itH_0} \sum_{m,m'} H(k)_{m,m'} \left[\overset{A}{c^{+}_{k,m}}\, \overset{B}{c_{k,m'}} , \overset{C}{c^{+}_{k,n}} \right] e^{-itH_0} =$$

$$\left\ulcorner [AB, C] = ABC + ACB - ACB - CAB = A\{B,C\} - \{A,C\}B \right\lrcorner$$

$$= i\, e^{itH_0} \sum_{m,m'} H_{m,m'}(k)\; c^{+}_{k,m}\; \delta_{m',n}\; e^{-itH_0}$$

$$= i \left[\vec{c}^{\,+}_k(t)\, H(k) \right]_n \Rightarrow \boxed{\vec{c}^{\,+}_k(t) = \vec{c}^{\,+}_k\, e^{itH(k)}}$$

Analog: $\boxed{c_k(t) = e^{-itH(k)}\, c_k}$

$$\Lambda_{\alpha,\beta}(\omega) \equiv i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \langle [J_{p,\alpha} , J_{p,\beta}(-t)] \rangle_0 =$$

$$= i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_{\substack{k,p\\ n,m\\ n',m'}} \frac{\partial}{\partial k_\alpha} H(k)_{n,m} \frac{\partial}{\partial p_\beta} H_{n',m'}(p) \cdot \langle [c^\dagger_{k,n} c_{k,m} ,$$

$$c^\dagger_{p,n'}(-t)\, c_{p,m'}(-t)] \rangle_0 =$$

$$i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_{\substack{k,p\\ n,m\\ n',m'}} \frac{\partial}{\partial k_\alpha} H_{n,m}(k) \frac{\partial}{\partial p_\beta} H_{n',m'}(\bar p) \cdot\cdot \sum_{r,s} \left(e^{-itH(p)}\right)_{r,n'}$$

$$\left(e^{itH(p)}\right)_{m',s} \underbrace{\langle [\overset{A}{c^\dagger_{k,n}} \overset{B}{c_{k,m}} , \overset{C}{c^\dagger_{p,r}} \overset{D}{c_{p,s}}] \rangle_0}_{\equiv I}$$

$$[AB, \overset{X}{CD}] = ABX - AXB + AXB - XAB =$$

$$= A[B,X] + [A,X]B = A[B,CD] + [A,CD]B =$$

$$= A\{ BCD + CBD - CBD - CDB \} + [ACD + CAD - CAD - CDA]B =$$

$$= A[\{B,C\}D - C\{B,D\}] + [\{A,C\}D - C\{A,D\}]B =$$

$$= A\{B,C\}D - AC\{B,D\} + \{A,C\}DB - C\{A,D\}B \quad \Rightarrow$$

$$I = \delta_{\vec k,\vec p} \{ \delta_{m,r} \langle c^\dagger_{k,n} c_{k,s} \rangle - \delta_{n,s} \langle c^\dagger_{k,r} c_{k,m} \rangle \} =$$

$$= \delta_{\vec k,\vec p} \{ \delta_{m,r} \sum_{x,y} \langle \gamma^\dagger_{k,x} U^\dagger_{x,n}(k) U_{s,y}(k) \gamma_{k,y} \rangle - \delta_{n,s} \sum_{x,y} \langle \gamma^\dagger_{k,x} U^\dagger_{x,r}(k) U_{m,y}(k) \gamma_{k,y} \rangle \}$$

$$=$$

$$= \delta_{\vec{k},\vec{p}} \Big\{ \delta_{m,r} \sum_{x} U_{s,x}(k)\, f(E_{k,x})\, U^{+}_{x,n}$$

$$- \delta_{n,s} \sum_{x} U_{m,x}(k)\, f(E_{k,x})\, U^{+}_{x,r} \Big\} =$$

$$= \delta_{k,p} \left\{ \delta_{m,r}\, G_{s,n}(k) - \delta_{n,s}\, G_{m,r}(k) \right\} \quad \text{with}$$

$$\boxed{G_{s,n}(\vec{k}) = - \langle T\, c^{(0^-)}_{s,k}\, c^{+}_{n,k} \rangle = \langle c^{+}_{n,k}\, c_{s,k} \rangle \equiv \sum_{x} U_{s,x}(k)\, f(E_{k,x})\, U^{+}_{x,n}}$$

$\Rightarrow$ All in All you have:

$$\Lambda_{\alpha,\beta}(\omega) = i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_{\substack{k \\ n,m \\ n',m' \\ r,s}} \left(\frac{\partial}{\partial k_\alpha} H(k)_{n,m} \right) \left(\frac{\partial}{\partial k_\beta} H_{n',m'}(k) \right) \cdot$$

$$\left(e^{-it H(k)} \right)_{r,n'} \left(e^{it H(\bar{k})} \right)_{m',s} \cdot \left[\delta_{m,r}\, G_{s,n}(k) - \delta_{n,s}\, G_{m,r}(k) \right]$$

$$= i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_{\substack{k \\ n,m \\ r,s}} \left(\frac{\partial}{\partial k_\alpha} H(k) \right)_{n,m} \left[e^{-itH(k)} \left[\frac{\partial}{\partial k_\beta} H(k) \right] e^{itH(k)} \right]_{r,s}$$

$$\cdot \left\{ \delta_{m,r}\, G_{s,n}(k) - \delta_{n,s}\, G_{m,r}(k) \right\} =$$

$$= i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_{k} \mathrm{Tr} \left[e^{-itH(k)} \left[\frac{\partial}{\partial k_\beta} H(k) \right] e^{itH(k)}\, G(k) \left(\frac{\partial}{\partial k_\alpha} H(k) \right) \right]$$

$$- \mathrm{Tr} \left[\frac{\partial}{\partial k_\alpha} H(k)\, G(k)\, e^{-itH(k)} \left[\frac{\partial}{\partial k_\beta} H(k) \right] e^{itH(k)} \right]$$

$$= i \int_0^\infty dt \, e^{i(\omega + i\eta)t} \sum_{\vec{k}} \mathrm{Tr}\left[G(\vec{k}) \left[j_\alpha(\vec{k}) \, , \, e^{-itH_0(k)} \left[j_\beta(k) \right] e^{itH_0(\vec{k})} \right] \right] = \Lambda_{\alpha,\beta}(\omega).$$

$$J_\alpha(k) = \frac{\partial}{\partial k_\alpha} H_0(k)$$

$\Rightarrow$ Consequence. For any single band model the commutator vanishes and hence $\Lambda_{\alpha,\beta}(\omega) = 0$

The Kinetic Energy:

$$K_\alpha = \sum_{i,j} (j-i)^2_\alpha \, c^+_i \, t(i-j) \, c_j =$$

$$= \sum_{k,p} c^+_k \left[\frac{1}{N} \sum_{i,j} e^{-i\bar{k}\cdot(\bar{i}-\bar{j})} \, t(i-j) \, (\bar{i}-\bar{j})^2_\alpha \, e^{i(\bar{p}-\bar{k})j} \right] c_p$$

$$= \sum_{k,p} c^+_k \sum_r e^{-i\bar{k}\bar{r}} \, t(\bar{r}) \, r^2_\alpha \frac{1}{N} \sum_j e^{i(\bar{p}-\bar{k})j} \, c_p$$

$$= \sum_k c^+_k - \left(\frac{\partial}{\partial k_\alpha} \right)^2 \sum_r e^{i\bar{k}\bar{r}} \, t(r) \, c_k$$

$$= \sum_k c^+_k \left[-\left(\frac{\partial}{\partial k_\alpha} \right)^2 H_0(k) \right] c_k \Rightarrow$$

$$\langle K_\alpha \rangle = \sum_k \left[-\left(\frac{\partial}{\partial k_\alpha} \right)^2 H_{0,n,m}(k) \right] G_{m,n}(k) =$$

$$= -\sum_k \mathrm{Tr}\left[\left[\left(\frac{\partial}{\partial k_\alpha} \right)^2 H_0(k) \right] G(k) \right]$$

$\Rightarrow$ All in all:

$$\boxed{\sigma_{\alpha,\beta}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2} \frac{1}{N} \frac{1}{i(\omega+i\eta)} \cdot \Big[+ \sum_k \mathrm{Tr}\left[K_\alpha(\vec{k})\, G(k)\right] \delta_{\alpha,\beta} + \Lambda_{\alpha,\beta}(\omega) \Big] \quad , \quad K_\alpha(\vec{k}) = -\left(\frac{\partial}{\partial k_\alpha}\right)^2 H_0(\vec{k})}$$

Explicit evaluation of $\Lambda_{\alpha,\beta}(\omega)$; Time integration

Let $H_0(k) = \sum_n \underset{\text{scal}}{E_n} \underset{\text{matrix}}{P_n} \rightarrow$ Note

$P_n^2 = P_n \qquad P_n P_m = 0$ for $n \neq m$ P_n: orthogonal projectors.

$$\Rightarrow e^{-it H_0(k)} = \sum_n e^{-it E_n(k)} P_n \Rightarrow$$

$$\Lambda_{\alpha,\beta}(\omega) = i \int_0^\infty dt\, e^{i(\omega+i\eta)t} \sum_k \mathrm{Tr}\Big\{ G(k) \Big[J_\alpha(k), \sum_n e^{-itE_n} P_n\, J_\beta(k) \sum_m e^{itE_m} P_m \Big] \Big\} =$$

$$= \frac{i}{\hbar} \sum_{k,m,n} \int_0^\infty dt\, e^{i(\hbar\omega + i\eta + E_m - E_n)t/\hbar}\, \mathrm{Tr}\Big\{ G(k) \cdot \big[J_\alpha(k), P_n J_\beta(k) P_m$$

$$= i \sum_{k,m,n} \frac{1 \cdot (-1)}{i(\hbar\omega + i\eta + E_m - E_n)} \mathrm{Tr}\{ G [J_\alpha, P_n J_\beta P_m] \}$$

$$= -\sum_{k,m,n} \frac{1}{\hbar\omega + i\eta + E_m - E_n} \sum_x f(E_x) \mathrm{Tr}[P_x J_\alpha P_n J_\beta P_m - P_x P_n J_\beta P_m J_\alpha \} =$$

$$= -\sum_{k,m,n} \frac{1}{\hbar\omega + i\eta + E_m - E_n} \Big\{ f(E_m) \mathrm{Tr}[J_\alpha P_n J_\beta P_m \} - f(E_n) \mathrm{Tr}\{ J_\alpha P_n J_\beta P_m \} =$$

$$= -\sum_{k,m,n} \frac{f(E_m) - f(E_n)}{\hbar\omega + i\eta + E_m - E_n} \mathrm{Tr}\{ J_\alpha P_n J_\beta P_m \} \equiv \Lambda_{\alpha,\beta}(\omega)$$

with Kinetic Energy

$$\sum_k \mathrm{Tr}\left\{K_\alpha(k)\; G(k)\right\} = \sum_k \sum_n \mathrm{Tr}\left\{K_\alpha(k)\, P_n\right\} f(E_n) \Rightarrow$$

we have all in all:

$$\boxed{\Gamma_{\alpha,\beta}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2}\,\frac{1}{N}\,\frac{1}{i(\omega+i\eta)}\left[+\delta_{\alpha\beta}\sum_{k,n} f(E_n(k))\,\mathrm{Tr}\left\{K_\alpha(k) P_n\right\} - \sum_{k\, n,m}\frac{f(E_m)-f(E_n)}{\omega+i\eta+E_m-E_n}\,\mathrm{Tr}\left\{J_\alpha P_n J_\beta P_m\right\}\right]}$$

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We are interested in the response to a real field

$$\overset{\leftarrow \text{Real}}{E_\beta(\omega)}\cos(\omega t) = E_\beta(\omega)\,\frac{1}{2}\left(e^{i\omega t}+e^{-i\omega t}\right)$$

$$\Rightarrow j_\alpha(\omega) = \frac{1}{2}\left(\Gamma_{\alpha,\beta}(\omega)+\Gamma_{\alpha,\beta}(-\omega)\right)E_\beta(\omega)$$

But:

$$\sigma_{\alpha,\beta}(-\omega) = \frac{4\pi^2 e^2}{\phi_0^2} \frac{1}{N} \frac{1}{i(-\omega+i\eta)} \left[-\langle K_\alpha \rangle \delta_{\alpha,\beta} \right.$$

$$\left. + \Lambda_{\alpha,\beta}(-\omega) \right] = \sigma^*_{\alpha,\beta}(\omega)$$

since a) $$\left[\frac{1}{i(\omega+i\eta)}\right]^* = \frac{1}{-i(\omega-i\eta)} = \frac{1}{i(-\omega+i\eta)}$$

and $$\Lambda_{\alpha,\beta}(\omega)^* = -i\int_0^\infty dt\, e^{-i(\omega+i\eta)t} \langle [J_\alpha(0), J_\beta(-t)]^* \rangle$$

$$= -i\int_0^\infty dt\, e^{i(-\omega+i\eta)t} \langle [J_\beta(-t), J_\alpha(0)] \rangle =$$

$$= \Lambda_{\alpha,\beta}(-\omega) \quad \Rightarrow$$

$$\frac{1}{2}\left(\sigma_{\alpha,\beta}(\omega) + \sigma_{\alpha,\beta}(-\omega)\right) = \mathrm{Re}\, \sigma_{\alpha,\beta}(\omega) \quad \Rightarrow$$ We are interested in the real part of the optical conductivity:

Hence:

$$\mathrm{Re}\left[\sigma_{\alpha,\beta}(\omega)\right] = \frac{4\pi^2 e^2}{\phi_0^2} \frac{1}{N} \left[\mathrm{Re}\left[\frac{1}{i(\omega+i\eta)}\right] \cdot \mathrm{Re}\left[+\langle K_\alpha \rangle \delta_{\alpha\beta} \right.\right.$$

$$\left. + \Lambda_{\alpha\beta}(\omega) \right]$$

$$- \frac{4\pi^2 c^2}{\phi_0^2} \frac{1}{N} \left[\text{Im}\left[\frac{1}{i(\omega + i\eta)} \right] \cdot \text{Im}\left\{ + \langle K_\alpha \rangle \delta_{\alpha,\beta} + \Lambda_{\alpha,\beta}(\omega) \right\} \cdot \right]$$

Now:

$$\frac{1}{i} \frac{1}{\omega + i\eta} = -i \left[P \frac{1}{\omega} - i\pi \delta(\omega) \right] =$$

$$-i P \frac{1}{\omega} - \pi \delta(\omega) = -\pi \delta(\omega) + i \left(- P\frac{1}{\omega} \right)$$

$$\Rightarrow \boxed{\begin{aligned} \Gamma'_{\alpha,\beta}(\omega) &= \frac{4\pi^2 c^2}{\phi_0^2} (-\pi) \delta(\omega) \frac{1}{N} \left[+ \langle K_\alpha \rangle \delta_{\alpha,\beta} + \text{Re}\, \Lambda_{\alpha,\beta}(\omega) \right] \\ &+ \frac{4\pi^2 c^2}{\phi_0^2} P \frac{1}{\omega} \frac{1}{N} \left[\text{Im}\, \Lambda_{\alpha,\beta}(\omega) \right] \end{aligned}}$$

The first term corresponds to the Drude weight [Perfect conductor]

Example: a Two band model:

PRB 74, 085308, (06) X. L. Qi, Y.S. Wu & S.C. Zhang

Let $\mathbb{H}_0(k) = \varepsilon(k) + V d_\alpha(\vec{k})\, \Gamma^\alpha(k)$ with

$$\Gamma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \Gamma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \Gamma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mathbb{H}_0 \doteq \begin{bmatrix} \varepsilon + Vd_3 & +Vd_1 - iVd_2 \\ Vd_1 + iVd_2 & \varepsilon - Vd_3 \end{bmatrix} \Rightarrow$$

$$\det(\mathbb{H}_0 - E) \doteq ([\varepsilon + Vd_3] - E)([\varepsilon - Vd_3] - E) - |Vd_1 - iVd_2|^2 = 0$$

$$\Rightarrow (\varepsilon + Vd_3)(\varepsilon - Vd_3) + E^2 - E(\varepsilon + Vd_3) - E(\varepsilon - Vd_3) - V^2(d_1^2 + d_2^2) = 0$$

$$\Rightarrow E^2 - 2\varepsilon E + \varepsilon^2 - V^2 |\vec{d}|^2 = 0$$

$$\Rightarrow E = \frac{2\varepsilon \pm \sqrt{4\varepsilon^2 - 4\varepsilon^2 + 4V^2|d|^2}}{2} =$$

$$= \varepsilon \pm V|\vec{d}| \Rightarrow$$

$$\boxed{E_\pm(\vec{k}) = \varepsilon(k) \pm V|\vec{d}(\vec{k})|}$$

Looking for: $U(\cdot)$, $U^\dagger(\cdot)U(\cdot)=1$ with:

$$U^\dagger(\cdot)\, H_0(k)\, U(\cdot) = \varepsilon(k) + V|d(k)|\,\tau^z$$

$$U(\cdot) \equiv e^{-i\vec{e}\cdot\theta\frac{\vec{\tau}}{2}} \Rightarrow U^\dagger\vec{\tau}\,U = R(\vec{e},\theta)\,\vec{\tau}$$

with $R(\vec{e},\theta) = \ldots$, $SO(3)$ Rotation, angle θ, axis $\vec{e}$

Note: $R(\vec{e},\theta)\vec{x} = \vec{e}\cdot(\vec{e}\cdot\vec{x}) - \cos(\theta)\,\vec{e}\times(\vec{e}\times\vec{x}) + \sin(\theta)(\vec{e}\times\vec{x})$

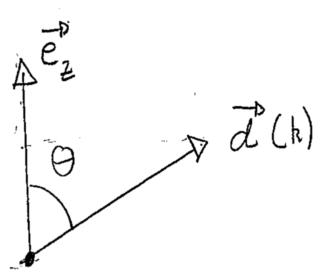
$$\Rightarrow U^\dagger H_0(k)\, U = U^\dagger\left[\varepsilon(k) + V d_\alpha(k)\,\tau^\alpha\right]U =$$

$$= \varepsilon(k) + V d_\alpha(k)\left(U^\dagger\tau^\alpha U\right) =$$

$$= \varepsilon(k) + V d_\alpha(k)\left(R(e,\theta)\vec{\tau}\right)^\alpha =$$

$$= \varepsilon(k) + V\left(R^T(\vec{e},\theta)\,\vec{d}(k)\right)_\alpha\cdot\tau^\alpha$$

$$\Rightarrow R^T(\vec{e},\theta)\,\vec{d} \overset{!}{\equiv} |\vec{d}|\,\vec{e}_z\,,\quad \vec{d} = |d|\,R(\vec{e},\theta)\,\vec{e}_z$$



plane

axis $\vec{e} = \dfrac{\vec{e}_z\times\vec{d}(\vec{k})}{|\vec{e}_z\times\vec{d}(k)|}$, $\quad\vec{e}_z\cdot\vec{d}(k) = |\vec{d}(k)|\cos(\theta)$

$$\Rightarrow \quad U^{+} H_0(k)\, U = \mathcal{E}(k) + V|d|\, \Gamma^z$$

$$= E_+ \; \tfrac{1}{2}(1+\Gamma^z) + E_- \; \tfrac{1}{2}(1-\Gamma^z)$$

$$\Rightarrow \quad H_0(k) = E_+(k) \; \tfrac{1}{2}\left(1 + U\Gamma^z U^{+}\right) + E_-(k)\, \tfrac{1}{2}(1 - U\Gamma^z U^{+})$$

Now $\quad U\Gamma^z U^{+} = \vec{e}_z \cdot U\vec{\Gamma}U^{+} =$

$$= \vec{e}_z \cdot R^T(e,\theta)\,\vec{\Gamma} = R(e,\theta)\,\vec{e}_z \cdot \vec{\Gamma} = \hat{\vec{d}}\,\vec{\Gamma}$$

with $\quad \hat{d} = \dfrac{\vec{d}}{|\vec{d}|}$

$$\Rightarrow \quad H_0(k) = E_+(k)\; P_+ + E_-(k)\; P_- \qquad \text{with}$$

$$P_+ = \tfrac{1}{2}(1 + \hat{d}\cdot\vec{\Gamma}), \qquad P_- = \tfrac{1}{2}(1 - \hat{d}\cdot\vec{\Gamma})$$, Stop today;

P_+, P_- are orthogonal projectors: $\quad P^{+\,2} = U\, \tfrac{1}{2}(1+\Gamma^z)\,\tfrac{1}{2}(1+\Gamma^z)\,U^{+}$

$$= U\,\tfrac{1}{4}\,(1 + 1 + 2\Gamma^z)\,U^{+} = U\,\tfrac{1}{2}(1+\Gamma^z)\,U^{+} = P^{+}$$

$$P_+ P_- = U\,\tfrac{1}{2}(1+\Gamma^z)\,\tfrac{1}{2}(1-\Gamma^z)\,U^{+} =$$

$$U\,\tfrac{1}{4}\left(1 - \Gamma^z + \Gamma^z - \Gamma^{z\,2}\right) U^{+} = 0 = P_- P_+$$

$$\Rightarrow \quad \boxed{e^{itH_0(k)} = \sum_{n=\pm} e^{itE_n(k)} P_n}$$

$$P_\pm = \frac{1}{2}\left(1 \pm \hat{d}\cdot\vec{\Gamma}\right) \Rightarrow$$

Optical conductivity (Drude weight) $\sigma_{xx}(\omega)$

a) $$\sigma_{x,x}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2}\left[(-\pi)\,\delta(\omega)\,D_{xx}\right.$$

$$\left. + P\frac{1}{\omega}\,\frac{1}{N}\,\mathrm{Im}\,\Lambda_{x,x}(\omega)\right]$$

with $$D_{x,x} = +\frac{1}{N}\sum_{k,n} f(E_n(k))\,\mathrm{Tr}\left[K_x(\vec{k})\,P_n\right]$$

$$+ \frac{1}{N}\,\mathrm{Re}\,\Lambda_{xx}(\omega \to 0)$$

We need to compute $\frac{1}{N}\mathrm{Re}\,\Lambda_{xx}(\omega \to 0) =$

$$= -\frac{1}{N}\sum_{k,n,m}\frac{f(E_m) - f(E_n)}{E_m - E_n}\,\mathrm{Tr}\left\{J_x P_n J_x P_m\right\}$$

$$= -\frac{1}{N}\sum_{k}\left[\frac{f(E_-) - f(E_+)}{E_- - E_+}\,\mathrm{Tr}\left[J_x P_+ J_x P_-\right] + \right.$$

$$m=+$$

$$-+- \quad \frac{f(E_+)-f(E_-)}{E_+(k)-E_-(k)} \cdot \mathrm{Tr}\left[J_x P_- J_x P_+\right] \Big] =$$

$$= + \frac{1}{N} \sum_k \left[\frac{f(E_-)-f(E_+)}{E_+ - E_-} \quad \mathrm{Tr}\left\{ J_x P_+ J_x P_- + J_x P_- J_x P_+ \right\}\right.$$

$$= \frac{2}{N} \sum_k \frac{f(E_-)-f(E_+)}{E_+ - E_-} \quad \mathrm{Tr}\left\{ J_x P_+ J_x P_- \right\}$$

Now: $\boxed{E_+ - E_- = 2V|\vec{d}|}$

Assume that $E_+ - E_- > 0 \ \forall k$ and let the chemical potential be between both bands $\Rightarrow$

$$f(E_-) = 1 \quad f(E_+) = 0 \quad \Rightarrow$$

$$\frac{1}{N} \mathrm{Re}\, \Lambda_{xx}(\omega=0) = \frac{2}{N} \sum_k \frac{1}{2V|d(k)|} \mathrm{Tr}\left[(\partial_x H_0(k))\, P_+ (\partial_x H_0(k))\, P_- \right]$$

$$= \frac{1}{(2\pi)^2} \int_{BZ} d\vec{k} \, \frac{1}{V|d(k)|} \cdot \underbrace{\mathrm{Tr}\left\{P_- \left[\partial_x H_0(k)\right] P_+ \left[\partial_x H_0(k)\right]\right\}}_{=I}$$

Calculating I:

$$J_x = \partial_x H_0(k) = \partial_x \varepsilon(k) + V \underbrace{(\partial_x \vec{d})}_{\equiv \vec{c}} \cdot \vec{\sigma} \equiv$$

$$\Rightarrow \mathrm{Tr}\left[P_- J_x P_+ J_x \right] =$$

$$= \mathrm{Tr}\left[P_- (\partial_x \varepsilon + V \vec{c} \cdot \vec{\sigma}) P_+ (\partial_x \varepsilon + V \vec{c} \cdot \vec{\sigma}) \right]$$

$$= \mathrm{Tr}\left[\underbrace{P_- \partial_x \varepsilon P_+}_{\equiv 0} J_x \right] + V \mathrm{Tr}\left[P_- \vec{c} \cdot \vec{\sigma} P_+ J \right]$$

$$= V^2 \mathrm{Tr}\left[P_- \vec{c} \cdot \vec{\sigma} P_+ \vec{c} \cdot \vec{\sigma} \right] + V \mathrm{Tr}\left[\underbrace{P_- (\partial_x \vec{d}) \cdot \vec{\sigma} P_+ \partial_x \varepsilon}_{\equiv 0} \right]$$

$$\Rightarrow I = \frac{V^2}{4} \mathrm{Tr}\left[(1 - \hat{d} \cdot \vec{\sigma}) (\vec{c} \cdot \vec{\sigma}) (1 + \hat{d} \cdot \vec{\sigma}) (\vec{c} \cdot \vec{\sigma}) \right]$$

$$= \frac{V^2}{4} \mathrm{Tr}\left[\left[(\vec{c} \cdot \vec{\sigma}) - (\hat{d} \cdot \vec{\sigma})(\vec{c} \cdot \vec{\sigma}) \right] \left[(\vec{c} \cdot \vec{\sigma}) + (\hat{d} \cdot \vec{\sigma}) \cdot (\vec{c} \cdot \vec{\sigma}) \right] \right] =$$

$$= \frac{V^2}{4} \mathrm{Tr}\left\{ \underbrace{(\vec{c} \cdot \vec{\sigma})^2}_{\sigma_0 (\vec{c} \cdot \vec{c})} - \underbrace{(\hat{d} \cdot \vec{\sigma})(\vec{c} \cdot \vec{\sigma})}(\hat{d} \cdot \vec{\sigma}) \cdot (\vec{c} \cdot \vec{\sigma}) \right]$$

$$= \frac{V^2}{4} \mathrm{Tr}\left\{ \sigma_0 (\vec{c} \cdot \vec{c}) - \left(\sigma_0 (\hat{d} \cdot \vec{c}) + i \vec{\sigma} (\hat{d} \times \vec{c}) \right) \left(\sigma_0 (\hat{d} \cdot \vec{c}) + i \vec{\sigma} (\hat{d} \times \hat{c}) \right.\right.$$

since $(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \sigma_0 \cdot (\vec{a} \cdot \vec{b}) + i \vec{\sigma} (\vec{a} \times \vec{b})$ $\leftarrow$

$$= \frac{V^2}{4}\left[2\,(\vec{c}\cdot\vec{c}) - 2(\hat{\vec{d}}\cdot\vec{c})^2 + \mathrm{Tr}\left[(\vec{\Gamma}\cdot(\hat{d}\times\vec{c}))\,(\vec{\Gamma}\cdot(\hat{d}\times\vec{c}))\right]\right] =$$

$$= \frac{V^2}{2}\left[(\vec{c}\cdot\vec{c}) - (\hat{\vec{d}}\cdot\vec{c})^2 + (\underset{a}{\hat{d}}\times\underset{b}{\vec{c}})\cdot(\underset{c}{\hat{\vec{d}}}\times\underset{d}{\vec{c}})\right]$$

$$= \Gamma \quad (\overset{\hat{d}}{\underset{e_x}{a}}\times\underset{e_y}{\bar{b}})\cdot(\overset{\hat{d}}{\underset{e_y}{\bar{c}}}\times\underset{e_x}{\vec{d}}) = (a\cdot c)(b\cdot d) - (b\cdot c)(a\cdot d) \leftarrow$$

$$= \frac{V^2}{2}\left\{(\vec{c}\cdot\vec{c}) - (\hat{d}\cdot\vec{c})^2 + (\vec{c}\cdot\vec{c}) - (\vec{c}\,\hat{d})\cdot(\vec{c}\,\hat{d})\right]$$

$$= V^2\left\{(\vec{c}\cdot\vec{c}) - (\hat{d}\cdot\vec{c})^2\right]$$

$$= V^2\left[(\hat{d}\cdot\hat{d})(\vec{c}\cdot\vec{c}) - (\hat{d}\cdot\vec{c})(\hat{d}\cdot\vec{c})\right]$$

$$= V^2\,(\hat{d}\times\vec{c})^2 \quad \Rightarrow \quad \frac{1}{N}\,\mathrm{Re}\,\Lambda_{xx}(\omega=0)$$

$$= \frac{1}{(2\pi)^2}\int_{BZ} d\vec{k}\;\frac{1}{\cancel{V}\,|d(k)|}\cdot V^2\,(\hat{d}\times\partial_x\vec{d})^2$$

$$= \frac{V}{(2\pi)^2}\int_{BZ} d\vec{k}\;\frac{1}{|d(k)|}\,(\hat{\vec{d}}\times\partial_x\vec{d})^2 \,..$$

The Kinetic energy:

$$+\frac{\langle K_x\rangle}{N} = +\frac{1}{N}\sum_k \mathrm{Tr}\{K_x(\vec{k})\, P_-\}$$

$$= -\frac{1}{(2\pi)^2}\int_{BZ} d\vec{k}\; \mathrm{Tr}\left[\left[\partial_x^2 \varepsilon + V\left(\partial_x^2 \vec{d}\right)\cdot\vec{\Gamma}\right] P_-\right]$$

$$= -\frac{1}{(2\pi)^2}\underbrace{\int_{B.Z} d\vec{k}\; \mathrm{Tr}\left[\partial_x^2 \varepsilon(k)\, P_-\right]}_{\equiv\, 0 \quad (*)} - \frac{V}{(2\pi)^2}\int_{B.Z} d\vec{k}\, \mathrm{Tr}\left[\left((\partial_x^2\vec{d})\,\vec{\Gamma}\right)\frac{1}{2}\left(1-\hat{d}\,\vec{\Gamma}\right)\right]$$

$$= \frac{V}{2(2\pi)^2}\int_{B.Z.} d\vec{k}\; \mathrm{Tr}\left[\left[(\partial_x^2\vec{d}).\vec{\Gamma}\right](\hat{d}.\vec{\Gamma})\right] =$$

$$= \frac{V}{2(2\pi)^2}\int_{B.Z.} d\vec{k}\; \mathrm{Tr}\; \Gamma_0\left[(\partial_x^2.\vec{d}).\,\hat{d}\right] =$$

$$= \frac{V}{(2\pi)^2}\int_{B.Z} d\vec{k}\; \left(\hat{\vec{d}}\cdot(\partial_x^2\vec{d})\right) = -\frac{V}{(2\pi)^2}\int_{B.Z.} d\vec{k}\; \left(\partial_x\frac{\vec{d}}{|d|}\,,\,\partial_x\vec{d}\right) =$$

$$\Big[\; \text{But } \partial_x\frac{\vec{d}}{|\vec{d}|} = \frac{(\partial_x\vec{d})}{|d|} + \vec{d}\,\partial_x\left(\sum_i d_i^2\right)^{-\frac{1}{2}} = \frac{\partial_x\vec{d}}{|\vec{d}|} - \frac{1}{2}\frac{\vec{d}}{|d|^3}.2(\vec{d}.\partial_x\vec{d}) \;\Big]$$

$$-\frac{V}{(2\pi)^2}\int_{B.Z} d\vec{k}\; \frac{1}{|d|}\left[(\partial_x\vec{d},\partial_x\vec{d}) - (\hat{\vec{d}}\cdot\partial_x\vec{d})(\hat{d}\cdot\partial_x\vec{d})\right]$$

$$= -\frac{V}{(2\pi)^2}\int_{BZ} d\vec{k}\; \frac{1}{|d|}\left(\hat{\vec{d}}\times\partial_x\vec{d}\right)^2 = -\frac{\Lambda_{xx}(\omega_0)}{N}$$

$$\Rightarrow \boxed{\left[+\frac{\langle K_x\rangle}{N} + \frac{\Lambda_{xx}(\omega_0)}{N}\right] = D_{xx} = 0} \Rightarrow \text{Drude}$$

weight vanishes for band insulator.

✓ e.g. square.

(*) $$\int_{B.Z} d\bar{k}\; \mathrm{Tr}\left\{\partial_x^2 \varepsilon(k)\, P_-\right\} = \int_{BZ} dk_y\, dk_x\, \partial_x^2 \varepsilon(k) =$$

$$= \int_{-\pi}^{\pi} dk_y\; \partial_x \varepsilon(k_x,k_y)\Big|_{-\pi}^{\pi} = \int_{-\pi}^{\pi} dk_y \Big[\partial_x \varepsilon(k_x,k_y)\Big|_{\bar{k}=(\pi,k_y)}$$

$$- \partial_x \varepsilon(k_x,k_y)\Big|_{k=(\pi,k_y)-\vec{b}_x}\Big] \qquad \bar{b}_x = (2\pi, 0)$$

$(\partial_x \varepsilon(\bar{k}))$ is a periodic function in $\vec{b}_x, \vec{b}_y$.

<u>Regular part.</u> $$\sigma_{xx}(\omega) = \frac{4\pi^2 c^2}{\phi_0^2}\Big[(-\pi)\,\delta(\omega)\, D_{xx}$$

$$+ \underbrace{P\frac{1}{\omega}\,\frac{1}{N}\,\mathrm{Im}\,\Lambda_{xx}(\omega)}_{\sigma_{reg,xx}(\omega)}\Big]$$

$$\sigma_{reg,xx}(\omega) = \frac{1}{\omega}\,\frac{\pi}{N}\sum_{k,n,m} \delta(\omega + E_m - E_n)\,\big(f(E_m) - f(E_n)\big)\,\mathrm{Tr}\left[J_x P_n J_x P_m\right]$$

$$= \frac{\pi}{N}\sum_{k,n,m} \delta(\omega + E_m - E_n)\,\frac{f(E_m) - f(E_n)}{E_n - E_m}\,\mathrm{Tr}\left\{J_x P_n J_x P_m\right\}$$

Interband transitions:

$\sigma_{xy}(\omega)$

$$\Lambda_{xy}(\omega) = -\sum_{k,m,n}^{m\neq t} \frac{f(E_m)-f(E_n)}{\omega+i\eta+E_m-E_n} \, Tr\{J_x P_n J_y P_m\}$$

$$= -\sum_k \Bigg[\frac{f(E_+)-f(E_-)}{\omega+i\eta+E_+-E_-} \, Tr\{J_x P_- J_y P_+\} +$$

$$\frac{f(E_-)-f(E_+)}{\omega+i\eta+E_--E_+} \, Tr\{J_x P_+ J_y P_-\} \Bigg]$$

$$= -\sum_k \big(f(E_-)-f(E_+)\big) \left[\frac{Tr\{J_x P_- J_y P_+\}}{\omega+i\eta+2V|d|} - \frac{Tr\{J_x P_+ J_y P_-\}}{\omega+i\eta-2V|d|} \right]$$

- Matrix element:

$$Z_k = Tr\{J_x P_- J_y P_+\}$$

$$Z_k^* = Tr\{P_+ J_y P_- J_x\} = Tr\{J_x P_+ J_y P_-\}$$

$$\Rightarrow \quad \sigma_{x,y}(\omega) = \underbrace{\frac{4\pi^2 c^2}{\phi_0^2}}_{=\alpha} \frac{1}{i(\omega+i\eta)} \frac{1}{N} \sum_k \big(f(E_-)-f(E_+)\big) \left[\frac{Z_k}{\omega+i\eta+2V|d|} - \frac{Z_k^*}{\omega+i\eta-2V|d|} \right]$$

Consider the insulating case: $f(E_-) = 1$, $f(E_+) = 0$ $\quad 2V|d| > 0$

and the limit $\omega \to 0$ i.e. $|\omega| \ll 2V|d|$.

$$\Rightarrow \quad \frac{1}{\omega + i\eta \pm 2V|d|} = \frac{1}{\omega \pm 2V|d|}$$ since the δ-function

contribution vanishes $\Rightarrow$

$$\Pi_{x,y}(\omega) = \underbrace{\frac{4\pi^2 c^2}{\phi_0^2}}_{\equiv \alpha} \frac{1}{i(\omega+i\eta)} \frac{1}{N} \sum_k \left(f(E_-) - f(E_+)\right)\left[\frac{z_k}{\omega + 2V|d|} - \frac{z_k^*}{\omega - 2V|d|}\right]$$

$$= \alpha \frac{1}{i(\omega+i\eta)} \frac{1}{N} \sum_k \left(f(E_-) - f(E_+)\right) \frac{z(\omega - 2V|d|) - z^*(\omega + 2V|d|)}{\omega^2 - 4V^2|d|^2}$$

$$= \alpha \frac{1}{i(\omega+i\eta)} \frac{1}{N} \sum_k \left[f(E_-) - f(E_+)\right] \frac{\overset{\text{Im}}{(z - z^*)}\,\omega - \overset{\text{Re}}{(z + z^*)}\,2V|d|}{\omega^2 - 4V^2|d|^2}$$

$$\Rightarrow \text{Re}\, \Pi_{x,y}(\omega) = $$

$$\left\ulcorner \frac{1}{i} \frac{1}{\omega + i\eta} = \frac{1}{i}\left(P\frac{1}{\omega} - i\pi\delta(\omega)\right) = \frac{1}{i} P\frac{1}{\omega} - \pi\delta(\omega) \right\lrcorner$$

$$\boxed{= \alpha \frac{1}{N} \sum_k \left[f(E_-) - f(E_+)\right]\left[\frac{1}{i} \frac{(z - z^*)}{(\omega^2 - 4V^2|d|^2)} - \frac{\pi(z + z^*)\,\delta(\omega)}{2V|d|}\right]}$$

$$= \text{Re}\, \Pi_{x,y}(\omega)$$

We now have to compute the matrix element

$$Z_k = Tr\{ J_x P_- J_y P_+ \} =$$

$$= Tr \{ [(\partial_x \varepsilon) + V\underbrace{(\partial_x \vec{\alpha})}_{\vec{x}} \cdot \vec{\sigma}] P_- (\partial_y \varepsilon + V\underbrace{(\partial_y \vec{\alpha})}_{\vec{y}} \vec{\sigma}) P_+ \} =$$

$$= \frac{V^2}{4} Tr [(\vec{x}\cdot\vec{\sigma}) (1 - \hat{\alpha}\cdot\vec{\sigma}) (\vec{y}\cdot\vec{\sigma}) (1 + \hat{\alpha}\vec{\sigma})]$$

$$= \frac{V^2}{4} Tr [[(\vec{x}\cdot\vec{\sigma}) - (\vec{x}\cdot\vec{\sigma})(\hat{\alpha}\cdot\vec{\sigma})] [(\vec{y}\cdot\vec{\sigma}) + (\vec{y}\cdot\vec{\sigma})(\hat{\alpha}\cdot\vec{\sigma})]$$

$$\Gamma (\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = \sigma_0 (\vec{a}\cdot\vec{b}) + i \vec{\sigma}\cdot(\vec{a}\times\vec{b}) \lrcorner$$

$$= \frac{V^2}{4} Tr [[(\vec{x}\cdot\vec{\sigma}) - \sigma_0 (\vec{x}\cdot\hat{\alpha}) - i \vec{\sigma}\cdot(\vec{x}\times\hat{\alpha})]$$
$$[(\vec{y}\cdot\vec{\sigma}) + \sigma_0 (\vec{y}\cdot\hat{\alpha}) + i\vec{\sigma}\cdot(\vec{y}\times\hat{\alpha})] \} =$$

$$= \frac{V^2}{4} \cdot Tr [(\vec{x}\cdot\vec{\sigma})(\vec{y}\cdot\vec{\sigma}) + i (x\cdot\vec{\sigma}) [(\vec{y}\times\hat{\alpha})\cdot\vec{\sigma}]^{①}$$
$$- (\vec{x}\cdot\hat{\alpha})(\vec{y}\cdot\hat{\alpha}) - i [(\vec{x}\times\hat{\alpha})\cdot\vec{\sigma}]^{②}(\vec{y}\cdot\vec{\sigma})$$
$$+ [\vec{\sigma}\cdot(\vec{x}\times\hat{\alpha})][\vec{\sigma}\cdot(\vec{y}\times\hat{\alpha})]] =$$

$$= i \frac{V^2}{4} \overset{Tr}{2} [+ \overset{①}{\vec{x}\cdot(\vec{y}\times\hat{\alpha})} - \underbrace{\overset{②}{(\vec{x}\times\hat{\alpha})\cdot\vec{y}}}_{\vec{y}\cdot(\vec{x}\times\hat{\alpha}) = \vec{x}\cdot(\hat{\alpha}\times\vec{y}) = -\vec{x}\cdot(\vec{y}\times\hat{\alpha})}]$$

$$+ \frac{V^2}{4} \overset{Tr}{2} [\underbrace{(\vec{x}\cdot\vec{y}) - (\vec{x}\cdot\hat{\alpha})(\vec{y}\cdot\hat{\alpha})}_{\equiv + (\overset{a}{\vec{x}}\times\overset{b}{\hat{\alpha}})\cdot(\overset{c}{\vec{y}}\times\overset{d}{\hat{\alpha}})} + (\vec{x}\times\hat{\alpha})\cdot(\vec{y}\times\hat{\alpha})] =$$

$$= i V^2 \; \hat{\alpha}\cdot(\partial_x\vec{\alpha}\times\partial_y\vec{\alpha}) + V^2 (\vec{x}\times\hat{\alpha})(\vec{y}\times\hat{\alpha})$$

But $\quad \partial_x \vec{d} = |d|\, \partial_x \hat{\vec{d}} + \frac{\vec{d}}{|d|^2} \cdot (\vec{d} \cdot \partial_x \vec{d})$

$$\Rightarrow \quad \hat{\vec{d}} \cdot \left((\partial_x \vec{d}) \times (\partial_y \vec{d}) \right) =$$

$$= \hat{\vec{d}} \cdot \left[\left(|d| (\partial_x \hat{\vec{d}}) + \frac{\vec{d}}{|d|^2} (\vec{d} \cdot \partial_x \vec{d}) \right) \times \left(|d| (\partial_y \hat{\vec{d}}) + \frac{\vec{d}}{|d|^2} \cdot (\vec{d} \cdot \partial_y \vec{d}) \right) \right]$$

$$= |d|^2 \; \hat{\vec{d}} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}})$$

$$+ \underbrace{\frac{1}{|d|} \hat{\vec{d}} \cdot \left[\left((\partial_x \hat{\vec{d}}) \times \vec{d} \right) \cdot (\vec{d} \cdot \partial_y \vec{d}) + \left(\vec{d} \times (\partial_y \hat{\vec{d}}) \right) \cdot (\vec{d} \cdot \partial_x \vec{d}) \right]}_{= 0}$$

$$= |d|^2 \; \hat{\vec{d}} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}}) \quad \Rightarrow$$

$$Z(k) = i V^2 |d|^2 \; \hat{\vec{d}} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}}) \quad + \cancel{V}^2 ((\partial_x \vec{d}) \times \vec{d}) \cdot ((\partial_y \vec{d}) \times \vec{d}$$

$$\lim_{\omega \to 0} \mathrm{Re}\, \sigma_{xy}(\omega) = \frac{4\pi^2 c}{\phi_0^2} \, .$$

$$\frac{1}{N} \sum_k \left[f(E_-) - f(E_+) \right] \cdot \frac{2 \cancel{V^2} \cancel{|d|^2} \; \hat{d} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}})}{(-) 4 \cancel{V^2} \cancel{|d|^2}}$$

$$= - \frac{2\pi^2 c}{\phi_0^2} \frac{1}{(2\pi)^2} \int_{BZ} d\vec{k} \left[f(E_-) - f(E_+) \right] \; \hat{\vec{d}} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}})$$

For the insulator, $f(E_-) - f(E_+) = 1$

$$\Rightarrow \boxed{\lim_{\omega\to 0} \sigma_{xy}(\omega) = -\frac{(2\pi)^2 c^2}{\phi_0^2} \frac{1}{8\pi^2} \int_{BZ} d\vec{k}\; \hat{\vec{d}} \cdot \left(\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}}\right)}$$

Topological quantity: Depends only on # of times $\hat{\vec{d}}$ covers the unit sphere.

Mapping $\vec{k} \in B.Z \rightarrow \hat{\vec{d}}(\vec{k}) \in S^2$.

Jacobian of the mapping: $\hat{\vec{d}} \cdot (\partial_x \hat{\vec{d}} \times \partial_y \hat{\vec{d}}) \rightarrow$ PPt

Let $n =$ # of times $\hat{\vec{d}}(k)$ covers the unit sphere.

$$\Rightarrow \lim_{\omega\to 0} \sigma_{x,y}(\omega) = -\frac{(2\pi)^2 c^2}{\phi_0^2} \frac{1}{8\pi^2} 4\pi \cdot n \quad \text{is Quantized.}$$

S.C. Zhang $= \dfrac{e^2 c^2}{\frac{h^2}{(2\pi)^2} c^2} = \dfrac{e^2}{\hbar^2} = 1$

$\Rightarrow$ Topological insulator: $D_{x,x} = 0 \quad \lim_{\omega\to 0} \sigma_{xy}(\omega) \neq 0$

Explict example.

$$\varepsilon(k) = -2t(\cos(k_x) + \cos(k_y))$$

$$\sum_{k,\sigma} \varepsilon(k)\, c^{\dagger}_{k,\sigma} c_{k,\sigma}$$

$$V \quad j_y S_x - j_x S_y$$

$$\hat{H}_0 = V \sum_k \sin(k_y)\, c^{\dagger}_{k\sigma} \sigma^x_{\sigma\sigma'} c_{k\sigma'} - \sin(k_x)\, c^{\dagger}_{k,\sigma} \sigma^y_{\sigma\sigma'} c_{k,\sigma'}$$

Spin orbit interaction Rashba

$$+ Vc \sum_{\sigma, k} \Big(2 - \cos(k_x) - \cos(k_y)\Big)\, \sigma\, c^{\dagger}_{k,\sigma} c_{k,\sigma}$$

spin dep. effective mass

$$- V e_s c \sum_{k,\sigma} c^{\dagger}_{k,\sigma} c_{k,\sigma}\, \sigma$$

Magnetic field.

$$\Rightarrow \quad \varepsilon(k) = 0 \qquad d_x(k) = \sin(k_y), \quad d_y(k) = -\sin(k_x)$$

$$d_z(k) = c\,(2 - \cos(k_x) - \cos(k_y) - e_s)$$

$$\Rightarrow \quad E_{\pm}(k) = \pm V\, |\vec{d}(k)|$$

Southpole $\quad$ z-component of $\vec{d}\,\vec{e}_z > 0$ Northpole

$$\lim_{\omega \to 0} \sigma_{x,y}(\omega) = \begin{cases} 0 & e_s > 4 \quad e_s < 0 \\ \frac{1}{2\pi} & 2 > e_s > 0 \\ -\frac{1}{2\pi} & 4 > e_s > 2 \end{cases}$$

Properties of topological insulators: edge states:

Consider a topology with open boundary conditions in the x-direction and periodic boundaries in the y-direction.

$\Rightarrow$ k_y is still a good quantum number.

$$\hat{H}(\alpha) = -t \sum_{i,\#,\Gamma} \left(c^{+}_{i,\Gamma} c_{i+a_{\#},\Gamma} + h.c. \right) \quad + \quad \alpha \sum_{i} \delta_{i_x,L} c^{+}_{i,\Gamma} c_{i,\Gamma}$$

$$- \frac{V_c}{2} \sum_{i,\#,\Gamma,\Gamma'} i \left(c^{+}_{i,\Gamma} c_{i+a_x,\Gamma'} - c^{+}_{i+a_x,\Gamma} c_{i,\Gamma'} \right) \Gamma^{y}_{\Gamma,\Gamma'}$$

$$+ \frac{V_c}{2} \sum_{i,\Gamma,\Gamma'} i \left(c^{+}_{i,\Gamma} c_{i+a_y,\Gamma'} - c^{+}_{i+a_y,\Gamma} c_{i,\Gamma'} \right) \Gamma^{x}_{\Gamma,\Gamma'}$$

$$+ V_c \sum_{i,\Gamma,\Gamma'} \left(2 - e_s \right) c^{+}_{i,\Gamma} c_{i,\Gamma'} \Gamma^{z}_{\Gamma,\Gamma'}$$

$$- \frac{V_c}{2} \sum_{i,\Gamma,\Gamma',\#} \left(c^{+}_{i,\Gamma} c_{i+a_{\#},\Gamma'} + c^{+}_{i+a_{\#},\Gamma} c_{i,\Gamma'} \right) \Gamma^{z}_{\Gamma,\Gamma'}$$

Partial Fourier transform.

$$c^{+}_{i_x,i_y} = \frac{1}{\sqrt{L}} \sum_{k_y} e^{+ i k_y i_y} c^{+}_{i_x,k_y}$$ gives Hamiltonian:

$$\hat{H}(\alpha) = \sum_{\sigma,\sigma',i_x,k_y} \Big[c^{+}_{i_x,k_y,\sigma} \Big[\sum_{\sigma,\sigma'} -2t\cos(k_y)\,\sigma^0 + V_c \sin(k_y)\,\sigma^x$$

$$+ V_c\,(2-\cos(k_y) - e_s)\,\sigma^z$$

$$+ \alpha\, \delta_{i_x,L}\, \sigma^0 \Big]_{\sigma,\sigma'} c^{+}_{i_x,k_y,\sigma'}$$

$$-t\left(c^{+}_{i_x,k_y,\sigma}\, c_{i_x+a_x,k_y,\sigma'} + h.c.\right)\sigma^0_{\sigma,\sigma'}$$

$$-\frac{V_c}{2}\, i\left(c^{+}_{i_x,k_y,\sigma}\, c_{i_x+a_x,k_y,\sigma'} - h.c.\right)\sigma^y_{\sigma,\sigma'}$$

$$-\frac{V_c}{2}\left(c^{+}_{i_x,k_y,\sigma}\, c_{i_x+a_x,k_y,\sigma'} + h.c.\right)\sigma^z_{\sigma,\sigma'} \Big] =$$

$2L \times 2L$ matrix $\quad (i_x, \sigma)$

$$= \sum_{k_y} \vec{c}^{\,+}_{k_y}\, H(k_y)\, \vec{c}_{k_y}$$

$\Rightarrow$ For each k_y we have $2L$ bands.

In the limit $\alpha \to \infty$ the wave function vanishes at $i_x = L$ thereby producing open boundary condition.

$\to$ ppt. $\to$ the topological insulator with open boundary conditions in the x-direction has gapless excitations

(one dimensional L and R movers).

To understand where those gapless excitations are located, it is instructive to consider the k_y and i_x resolved density of states:

$$N_{i_x k_y}(\omega) \overset{T=0}{=} \frac{1}{Z_{\text{out}}} \sum_{n,m,\sigma} e^{-\beta E_m^{\text{out}}} \left| \langle n | c^+_{i_x, k_y, \sigma} | 0 \rangle^N \right|^2 \delta\left(\omega - \left(E_n^{N+1} - E_0^{N+1}\right)\right)$$

$$\equiv -\frac{1}{\pi} \sum_\sigma \operatorname{Im} G^{\text{ret}}_{i_x k_y, \sigma}(\omega)$$

The quantity $\frac{2}{L} \sum_{k_y > 0} N_{i_x, k_y}(\omega = 0) \equiv N^+_{i_x}(\omega = 0)$

will tell us where the gapless excitations with $k_y > 0$ are located.

In the same way $N^-_{i_x}(\omega=0) = \frac{2}{L} \sum_{k_y < 0} N_{i_x, k_y}(\omega = 0)$

will tell us where the gapless excitations with $k_y < 0$ are located.

~~ppt.~~ → Gapless excitations are located on the edges of the sample. → Correspond to chiral Luttinger liquids since only one velocity is represented.