Response theory for $2d$ periodically driven crystals

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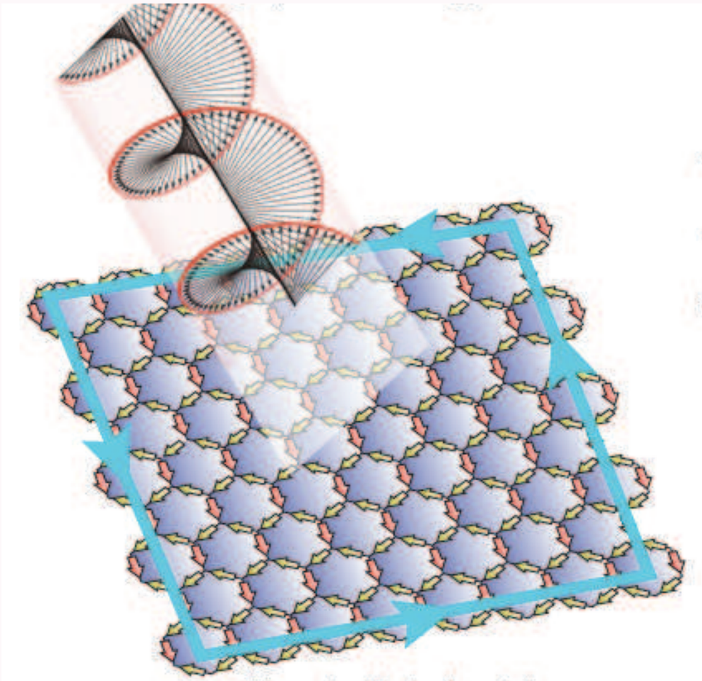
If you're not failing every now and again, it's a sign you're not doing anything very innovative

Woody Allen

General theme:

Non-trivial topological properties of certain materials may be induced by periodic driving



Our aim:

Understanding such topological properties of periodically driven crystals

- **The simplest theoretical setup:** tight-binding models in fermionic **Fock** space with the $2^{\rm nd}$-quantized time-dependent Hamiltonian

$$H(t) \;=\; \sum_{m,n\in\mathbb{Z}^d}\sum_{a,b=1}^{N}(c^a_m)^\dagger h^{ab}_{mn}(t)\, c^b_n$$

on the infinite crystalline lattice $\mathbb{Z}^d$, where $a=1,\dots,N$ enumerates the internal degrees of freedom (like spin), $(c^b_n)^\dagger$ and c^a_m create and annihilate electronic states localized at lattice sites,

$$[c^a_m,(c^b_n)^\dagger]_+ \;=\; \delta_{mn}\delta^{ab}$$

$$[c^a_m,c^b_n]_+ \;=\; 0 \;=\; [(c^a_m)^\dagger,(c^b_n)^\dagger]_+$$

and $h^{ab}_{mn}(t)=\overline{h^{ba}_{nm}(t)}$ defines the $1^{\rm st}$-quantized Hamiltonian $h(t)$ acting in $L^2(\mathbb{Z}^d,\mathbb{C}^N)$

- Many physical properties of the model may be tested coupling the system to an external electromagnetic field $A = A_\mu dx^\mu$

- The coupling is realized by the **Peierls** substitution in the 1^{st}-quantized Hamiltonian

$$h(t) \longrightarrow h_A(t)$$

where

$$h^{ab}_{A,mn}(t) = -A_0(t,m)\,\delta^{ab}\delta_{mn} + h^{ab}_{mn}\,\mathrm{e}^{-\mathrm{i}\int_m^n A_i(t,x)\mathrm{d}x^i}$$

with the corresponding 2^{nd}-quantized Hamiltonian

$$H_A(t) = \sum_{m,n\in\mathbb{Z}^d}\sum_{a,b=1}^{N}(c^a_m)^\dagger h^{ab}_{A,mn}(t)\,c^b_n$$

- The time evolution between times t_1 and t_2 are defined by the **Schrödinder** equation

$$\mathrm{i}\partial_{t_2} U(t_2, t_1) = H(t_2)\, U(t_2, t_1), \qquad U(t_1, t_1) = I$$

and similarly in the external field

$$\mathrm{i}\partial_{t_2} U_A(t_2, t_1) = H_A(t_2)\, U_A(t_2, t_1), \qquad U_A(t_1, t_1) = I$$

with the scattering matrix

$$S_A(t_2, t_1) = U(t_2, t_1)^{-1}\, U_A(t_2, t_1)$$

- If the support of A is in the interval $[t_1, t_2]$ and $t_1' < t_1 < t_2 < t_2'$ then

$$S_A(t_2', t_1') = U(t_1, t_1')^{-1} S_A(t_2, t_1)\, U(t_1, t_1')$$

- **Stationary case**

  - If $h(t) = h$ is time-independent then

$$U(t_2, t_1) \; = \; \mathrm{e}^{-\mathrm{i}(t_2 - t_1) H}$$

  - Let ω be a state invariant under the stationary evolution

$$\omega(O) \; = \; \omega\big(\mathrm{e}^{\mathrm{i}tH} O \, \mathrm{e}^{-\mathrm{i}tH}\big)$$

Then the limit

$$\boxed{\lim_{\substack{t_1 \to -\infty \\ t_2 \to +\infty}} \; \omega\big(S_A(t_2, t_1)\big) \; \equiv \; \mathrm{e}^{\mathrm{i} S^{\mathrm{eff}}_\omega (A)}}$$

(that exists trivially if the temporal support of A is compact) defines the **effective action** $S^{\mathrm{eff}}_\omega(A)$ of the electromagnetic field

- We shall consider states ω obtained in the thermodynamic limit from the periodic-boundary-conditions density matrices

$$\rho \;=\; \frac{\mathrm{e}^{-\sum\limits_{m,n}\sum\limits_{a,b}(c^a_m)^\dagger r^{ab}_{mn} c^b_n}}{\mathrm{Tr}\;\mathrm{e}^{-\sum\limits_{m,n}\sum\limits_{a,b}(c^a_m)^\dagger r^{ab}_{mn} c^b_n}}$$

where $[r, h] = 0$, e.g. in the **Gibbs** state with $r = \beta(h - \mu I)$ where β is the inverse temperature and μ the chemical potential

- Such states are characterized by the **Green** function

$$G^{ab}_{\omega,mn}(t,t') \;=\; \lim_{t_1\to-\infty}\begin{cases}\omega\big(c^a_m(t,t_1)\; c^b_n(t',t_1)^\dagger\big) & \text{if}\quad t<t'\\ -\,\omega\big(c^b_n(t',t_1)^\dagger\; c^a_m(t,t_1)\big) & \text{if}\quad t\geq t'\end{cases}$$

where

$$c^a_m(t_2,t_1) \;=\; U(t_2,t_1)^{-1} c^a_m\, U(t_2,t_1)$$

as the higher order expectations of the time-ordered products of creators and annihilators are given by the fermionic **Wick** rule

- The **Green** function satisfies the differential equation

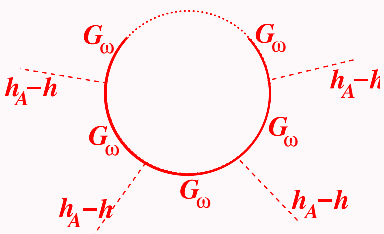
$$\big(\partial_t + \mathrm{i}h\big)G_\omega(t,t') \;=\; \delta(t-t')$$

with many different solutions

- The **effective action** defined above is given by the formula

$$S^{\mathrm{eff}}_\omega(A) \;=\; \tfrac{1}{\mathrm{i}}\,\ln\,\det\Big(I+\mathrm{i}G_\omega(h_A-h)\Big)$$

$$=\; \sum_{p=1}^{\infty}\frac{\mathrm{i}^{3p+1}}{p}\,\mathrm{Tr}\,\big(G_\omega(h_A-h)\big)^p$$



that lends itself to a perturbative calculation in A

- If h^{ab}_{mn} is translationally invariant and of finite range then it may be block-diagonalized by the discrete **Fourier-Bloch** transform

$$h^{ab}_{mn} \;=\; \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\mathrm{e}^{\mathrm{i}k\cdot(m-n)}\,\widehat{h}^{ab}(k)\,\mathrm{d}^dk$$

where $\mathbb{T}^d=\mathbb{R}^d/(2\pi\mathbb{Z}^d)$ is the **Brillouin** torus with $\widehat{h}^{ab}(k)$ smoothly dependent on the quasimomenta k, and similarly for r^{ab}_{mn}

- Locally on $\mathbb{T}^d$ one may choose a common eigenbasis $\big(\phi_a(k)\big)_{a=1}^N$ for the commuting $N\times N$ hermitian matrices $\widehat{h}(k)$ and $\widehat{r}(k)$

- To the $2^{\rm nd}$ order

$$
\begin{aligned}
S^{\rm eff}_\omega(A) \ = \ &\int {\rm d}^Dq \ Q_1^\mu(q)\,\widehat{A}_\mu(q) \\
&+ \tfrac12\int {\rm d}^Dq\int {\rm d}^Dq' \ Q_2^{\mu\nu}(q,q')\,\widehat{A}_\mu(q)\,\widehat{A}_\nu(-q') \\
&+ o(A^2)
\end{aligned}
$$

for $D=d+1$, where

$$
\widehat{A}_\mu(q) \ = \ \int {\rm d}^Dx \ \ {\rm e}^{-{\rm i}\,q_\nu x^\nu}\,A_\mu(x)
$$

is the continuum **Fourier** transform of $A_\mu(x)$

- One has

$$
\begin{aligned}
Q_1^\mu(q) \quad &= \ \delta(q_0)\Big(\prod_i \sum_{n_i\in\mathbb{Z}} \delta(q_i + 2\pi n_i)\Big)\,\Pi_1^\mu(q,n) \\
Q_2^{\mu\nu}(q,q') \ &= \ \delta(q_0 - q_0')\Big(\prod_i \sum_{n_i\in\mathbb{Z}} \delta(q_i - q_i' + 2\pi n_i)\Big)\,\Pi_2^{\mu\nu}(q,n)
\end{aligned}
$$

- The terms with $n_i \neq 0$ remembering the lattice structure give rise to oscillatory contributions to the effective action that average out on long distances and we shall drop them

- $\Pi_1^\mu(q,0)$ does not depend on q and discribes the average charge and current density in state ω (the latter vanishes)

- We shall concentrate on the quadratic contribution to $S_\omega^{\rm eff}$ in $d=2$ space dimensions describing the linear response to external electromagnetic field

- In the translation-invariant case

$$G_\omega(t,t')_{mn} \;=\; \frac{1}{(2\pi)^3}\int_{\mathbb{R}} d\omega \int_{\mathbb{T}^d} \mathrm{e}^{\mathrm{i}(\omega(t-t')+k\cdot(m-n))}\, \widehat{G}_\omega(\omega,k)$$

$$\widehat{G}_\omega(\omega,k) \;=\; \sum_{a=1}^{N}\Big(\frac{n_a(k)}{\mathrm{i}(\omega+e_a(k)+\mathrm{i}0)} + \frac{1-n_a}{\mathrm{i}(\omega+e_a(k)-\mathrm{i}0)}\Big)|\phi_a(k)\rangle\langle\phi_a(k)|$$

where $e_a(k)$ is the eigenvalue of the eigenvector $\phi_a(k)$ of $\widehat{h}(k)$ and $n_a(k)$ is its occupation number in the state ω:

$$\omega\big(c_{\phi_a}(k)^\dagger c_{\phi_a}(k')\big) \;=\; (2\pi)^d\,\delta(k-k')\,n_a(k)$$

for

$$c_{\phi_a}(k) \;=\; \sum_n\sum_b \overline{\phi_a^b(k)}\;\mathrm{e}^{-\mathrm{i}k\cdot n}\,c_n^b$$

- A straightforward calculation shows that in $d=2$

$$\Pi_2^{\mu\nu}(q,0) \;=\; \frac{1}{(2\pi)^5}\,q_\lambda\,\epsilon^{\lambda\mu\nu}\int_{\mathbb{T}^d}\sum_{a=1}^{N} n_a(k)\;\big\langle \mathrm{d}\phi_a(k)\big|\mathrm{d}\phi_a(k)\big\rangle \;+\; o(q)$$

where the $o(q)$ terms are subdominant on long distances

- The singled out dominant quadratic term gives rise to the **Chern-Simons** contribution to the effective action

$$S^{\mathrm{eff}}_{\omega}(A) \;=\; -\,\tfrac{1}{2}\,\sigma^{\perp}\!\int_{\mathbb{R}^3} A\,\mathrm{d}A \;\;+\;\;\ldots$$

where (for $e = 1 = \hbar$)

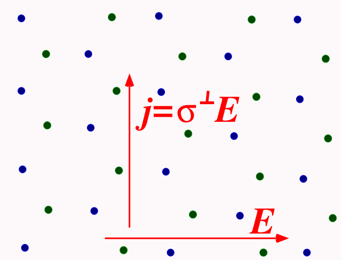
$$\boxed{\sigma^{\perp} \;=\; \frac{\mathrm{i}}{(2\pi)^2}\int_{\mathbb{T}^d}\sum_{a=1}^{M} n_a(k)\;\langle \mathrm{d}\phi_a(k)|\mathrm{d}\phi_a(k)\rangle}$$

is the **transverse conductance** (**Xiao** *et al.* Rev. Mod. Phys. **82**)
Indeed, the current expectation

$$\langle j^{\mu}(x)\rangle_A \;=\; \frac{\delta S^{\mathrm{eff}}_{\omega}(A)}{\delta A_{\mu}(x)} \;=\; -\,\sigma^{\perp}\,\epsilon^{\mu\nu\lambda}\partial_{\nu}A_{\lambda}(x) \;\;+\;\;\ldots$$

and, in particular,

$$\langle j^{i}(x)\rangle_A \;=\; \sigma^{\perp}\,\epsilon^{j\,i}\,E_j(x) \;\;+\;\;\ldots$$



- In the **Gibbs** state with $r = \beta(h - \mu n)$ the occupation numbers are given by the **Fermi** function:

$$n_a(k) = \frac{1}{\mathrm{e}^{\beta(e_a(k)-\mu)} + 1}$$

- In particular, in the insulating **ground state** obtained for $\beta \to \infty$ with the chemical potential μ placed in the spectral gap of all $\widehat{h}(k)$

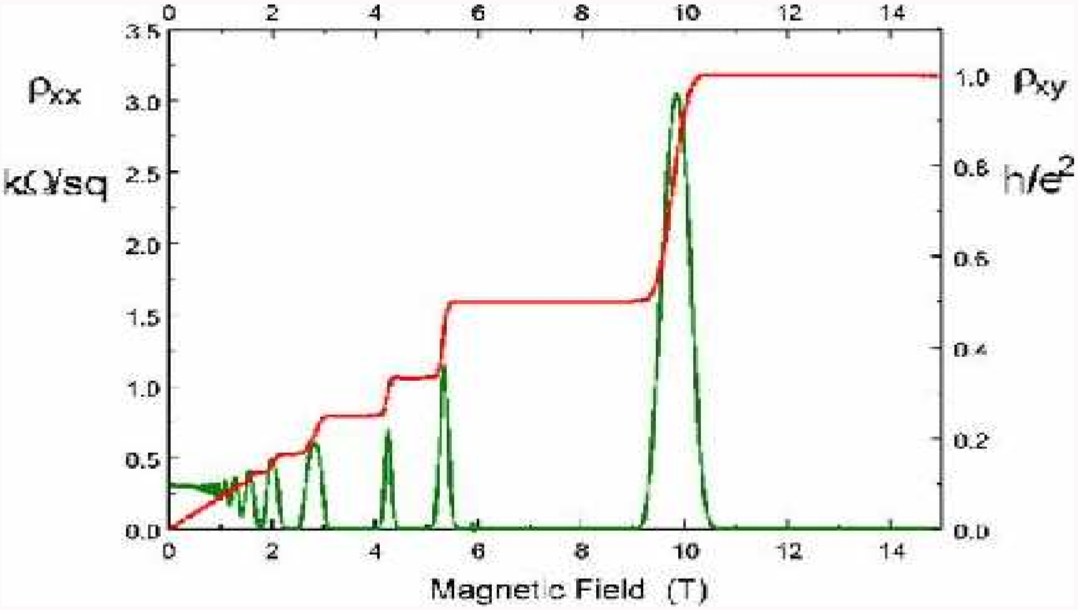
$$n_a(k) = \begin{cases} 0 & \text{if} \quad e_a(k) > \mu \\ 1 & \text{if} \quad e_a(k) < \mu \end{cases}$$

so that

$$\sigma^{\perp} = \frac{\mathrm{i}}{(2\pi)^2} \int_{\mathbb{T}^d} \overbrace{\sum_{\substack{a \\ e_a(k)<\mu}} \big\langle \mathrm{d}\phi_a(k) \big| \mathrm{d}\phi_a(k) \big\rangle}^{\textbf{Berry curvature of } \mathcal{E}} = \frac{c_1(\mathcal{E})}{2\pi}$$

where $c_1(\mathcal{E}) \in \mathbb{Z}$ is the 1^{st} **Chern** number of the vector bundle $\mathcal{E}$ over $\mathbb{T}^2$ spanned by the **valence states** $\phi_a(k)$ with $e_a(k) < \mu$

- Such a topological quantization of $\sigma^\perp$ was first obtained by **Thouless-Kohmoto-Nightingale-den Nijs** in 1982 (via the **Green-Kubo** formula) providing a (partial) explanation of the **integer quantum Hall effect**



$$= \frac{1}{2\pi\sigma^\perp}$$

- $c_1(\mathcal{E})$ counts with chirality the massless modes localized near each edge of a finite sample of the $2d$ insulator having their energies in the bulk gap (the **bulk-edge** correspondence)

- **Periodically-driven (Floquet) case**

  - If $h(t+T) = h(t)$ is periodic in time then $U(t) \equiv U(t,0)$ satisfies

  $$U(t+T) \;=\; U(t)\,U(T)$$

  For integers $p'_1 < p_1 < p_2 < p'_2$ sufficiently large in absolute value the scattering matrix satisfies now the relation

  $$S_A(p'_2T, p'_1T) \;=\; U(T)^{p'_1 - p_1}\, S_A(p_2T, p_1T)\, U(T)^{p_1 - p'_1}$$

  - If the state ω is invariant under the evolution over one period of time

  $$\omega\big(O\big) \;=\; \omega\big(U(T)^{-1} O\, U(T)\big)$$

  then the limit

  $$\boxed{\lim_{\substack{t_1 = p_1 T \to -\infty \\ t_2 = p_2 T \to +\infty}} \omega\big(S_A(t_1, t_2)\big) \;\equiv\; \mathrm{e}^{\mathrm{i} S^{\mathrm{eff}}_\omega (A)}}$$

  defines the **effective action** $S^{\mathrm{eff}}_\omega(A)$ as in the stationary case

- We shall again consider states ω obtained from the periodic boundary conditions density matrices

$$\rho \;=\; \frac{\mathrm{e}^{-\sum\limits_{m,n}\sum\limits_{a,b}(c^a_m)^\dagger r^{ab}_{mn}\, c^b_n}}{\mathrm{Tr}\;\mathrm{e}^{-\sum\limits_{m,n}\sum\limits_{a,b}(c^a_m)^\dagger r^{ab}_{mn}\, c^b_n}}$$

demanding now that $[r, u(T)] = 0$ where $u(t)$ is the 1^{st}-quantized version of the evolution $U(t)$:

$$\mathrm{i}\partial_t u(t) \;=\; h(t)\, u(t), \qquad\qquad u(0) = I$$

- Again such states are characterized by the **Green** function

$$G^{ab}_{\omega,mn}(t,t') \;=\; \lim_{t_1 = p_1 T \to -\infty} \begin{cases} \omega\big(c^a_m(t,t_1)\; c^b_n(t',t_1)^\dagger\big) & \text{if} \quad t < t' \\ -\,\omega\big(c^b_n(t',t_1)^\dagger\; c^a_m(t,t_1)\big) & \text{if} \quad t \geq t' \end{cases}$$

satisfying the equation $\big(\partial_t + \mathrm{i}\,h(t)\big)G_\omega(t,t') \;=\; \delta(t-t')$ and again

$$S^{\mathrm{eff}}_\omega(A) \;=\; \tfrac{1}{\mathrm{i}}\,\ln\,\det\Big(I + \mathrm{i}G_\omega(h_A - h)\Big)$$

- The diagonalization of the evolution operator $u(T)$ is the essence of the **Floquet** theory of periodically driven systems

- In the translation-invariant case we may choose locally on $\mathbb{T}^d$ a common eigenbasis $\big(\phi_a(k)\big)_{a=1}^N$ for the commuting $N \times N$ matrices $\widehat{u}(T,k)$ and $\widehat{r}(k)$

- Let $\mathrm{e}^{-\mathrm{i}Te_a(k)}$ be the eigenvalues of $\widehat{u}(T,k)$ corresponding to $\phi_a(k)$. The reals $e_a(k)$ defined modulo $\frac{2\pi}{T} \equiv \Omega$ are called **quasienergies**

- The **Green** function takes in the **Fourier** representation the form

$$G_\omega(t,t')_{mn} \;=\; \frac{1}{(2\pi)^2\Omega}\int_0^\Omega d\omega \int_{\mathbb{T}^d} \mathrm{e}^{\mathrm{i}k\cdot(m-n)}\,\widehat{G}_\omega(t,t';\omega,k)$$

where

$$\begin{aligned}\widehat{G}_\omega(t,t';\omega,k) \;&=\; \mathrm{e}^{-\mathrm{i}\omega T}\,\widehat{G}_\omega(t+T,t';\omega,k)\\ &=\; \mathrm{e}^{\mathrm{i}\omega T}\,\widehat{G}_\omega(t,t'+T;\omega,k) \;=\; \widehat{G}_\omega(t,t';\omega+\Omega,k)\end{aligned}$$

$$\widehat{G}_\omega(t,t';\omega,k) \;=\; \begin{cases} \sum_a \Big(\frac{n_a(k)}{1-\mathrm{e}^{-\mathrm{i}(\omega+e_a(k)+\mathrm{i}0)T}} + \frac{1-n_a(k)}{1-\mathrm{e}^{-\mathrm{i}(\omega+e_a(k)-\mathrm{i}0)T}}\Big) & \\ \times\; \widehat{u}(t,k)|\phi_a(k)\rangle\langle\phi_a(k)|\widehat{u}(t',k)^{-1} \quad \text{for} \quad 0\le t'<t\le T & \\ & \\ -\sum_a \Big(\frac{n_a(k)}{1-\mathrm{e}^{\mathrm{i}(\omega+e_a(k)+\mathrm{i}0)T}} + \frac{1-n_a(k)}{1-\mathrm{e}^{\mathrm{i}(\omega+e_a(k)-\mathrm{i}0)T}}\Big) & \\ \times\; \widehat{u}(t,k)|\phi_a(k)\rangle\langle\phi_a(k)|\widehat{u}(t',k)^{-1} \quad \text{for} \quad 0\le t\le t'\le T & \end{cases}$$

($n_a(k)$ are still the occupation numbers of $\phi_a(k)$ in the state ω)

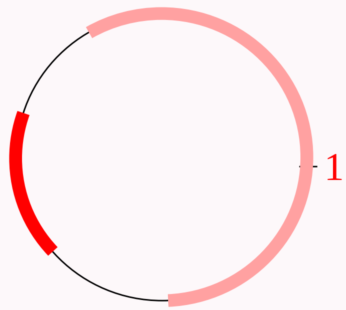
- A (rather tedious) perturbative calculation obscured by the appearance of further non-relativistic terms gives in the 2^{nd} order in $2d$ the **Chern-Simons** contribution:

$$S^{\text{eff}}_\omega(A) \;=\; -\,\tfrac{1}{2}\,\sigma^\perp\!\int_{\mathbb{R}^3} A\,\mathrm{d}A \;+\; \dots$$

where now

$$\sigma^\perp \;=\; \frac{\mathrm{i}}{(2\pi)^2}\int_{\mathbb{T}^d}\sum_{a=1}^{M} n_a(k)\,\Big(\big\langle \mathrm{d}\phi_a(k)\big|\mathrm{d}\phi_a(k)\big\rangle \\ \qquad\qquad + \,\mathrm{d}\int_0^T \frac{dt}{T}\,\big\langle\phi_a(k)\big|(\widehat{u}^{-1}\mathrm{d}\widehat{u})(t,k)\big|\phi_a(k)\big\rangle\Big)$$

- Suppose that the spectrum of the unitary $u(T)$ has two distinct gaps:



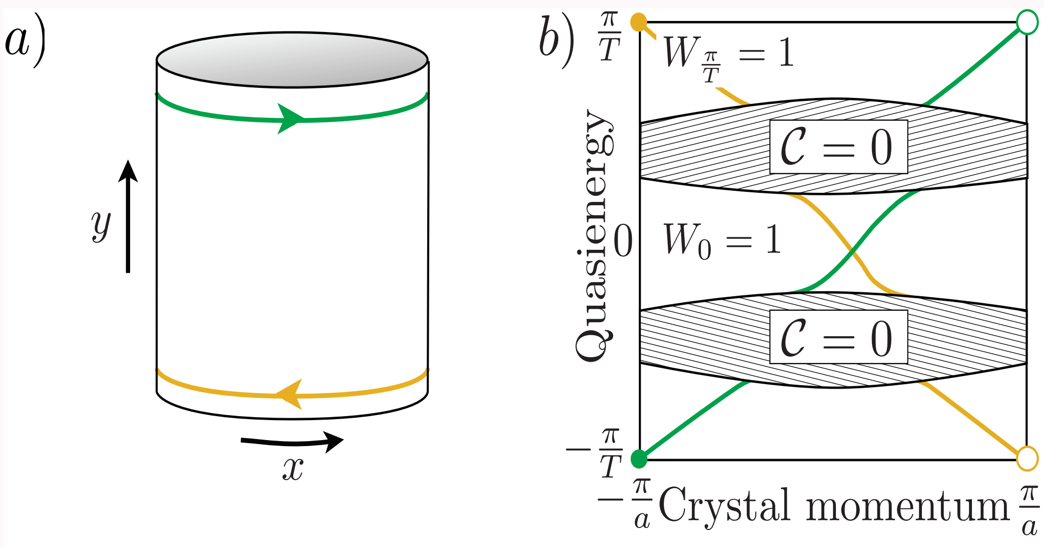
In the state ω with the bands between the gaps filled on one side (e.g. the deep-red ones) and empty on the other side (the light-red ones)

$$\sigma^{\perp} = \frac{c_1(\mathcal{E}_{\mathrm{dr}})}{2\pi}$$

where $\mathcal{E}_{\mathrm{dr}}$ is the vector bundle over $\mathbb{T}^2$ spanned by the eigenstates of $\widehat{u}(T,k)$ with eigenvalues in the deep-red part of the spectrum. The transverse conductance is quantized in such a state.

- In finite geometry, $c_1(\mathcal{E}_{dr})$ counts with chirality the difference of the massless edge states with energies in the two bulk gaps surrounding the deep-red part of the spectrum

- **Rudner-Lindner-Berg-Levin** (2013) defined a dynamical topological invariant W counting with chirality the number of edge states with energies in a fixed bulk gap



- Suppose that $\mathrm{e}^{-\mathrm{i}T\mu}$ lies in the spectral gap of $u(T)$. We may then choose the quasienergies so that $\mu - \Omega < e_a(k) < \mu$ and set

$$\widehat{v}(t,k) \;=\; \widehat{u}(t,k) \sum_{a=1}^{N} \mathrm{e}^{\mathrm{i}te_a(k)}\, |\phi_a(k)\rangle\langle\phi_a(k)| \;=\; \widehat{v}(t+T,k)$$

W is defined as the homotopy invariant of the periodized evolution $\hat{v}$:

$$W \;=\; \frac{1}{24\pi^2} \int\limits_{\mathbb{R}/(T\mathbb{Z})\times\mathbb{T}^2} \mathrm{tr}\,(\widehat{v}^{-1}\mathrm{d}\widehat{v})^3 \;\in\; \mathbb{Z}$$

- For periodically driven crystals there is a special family of states ω (that deserve the name of **Gibbs-Floquet** states, unlike the so called **Floquet-Gibbs** states) corresponding to the occupation numbers

$$n_a(k) \;=\; \sum_{p\in\mathbb{Z}} \frac{1}{\mathrm{e}^{\beta(e_a(k)+p\Omega-\mu)}+1}\, \big|\phi_{ap}(k)\big|^2$$

where

$$\phi_{ap}(k) \;=\; \int_0^T \frac{dt}{T}\; \mathrm{e}^{\mathrm{i}t(e_a(k)+p\Omega)}\, \widehat{u}(t,k)\, \phi_a(k)$$

- Such **Gibbs-Floquet** states are obtained by weakly coupling the periodically driven system to the environment kept at inverse temperature β and chemical potential μ (**Alicki** *et al.* 2006)

- It would be interesting to obtain more explicit formulae for $\sigma^{\perp}$ in those states, in particular in the "ground state" obtained in the limit $\beta \to \infty$ with $\mathrm{e}^{-\mathrm{i}T\mu}$ in a gap of $u(T)$ for which

$$n_a(k) = \sum_{\substack{p \\ e_a(k)+p\Omega<\mu}} \big|\phi_{ap}(k)\big|^2$$

- The original aim of this research was to find a response interpretation for the invariant W. Unfortunately preliminary results failed to relate W to $\sigma^{\perp}$ in any of the states considered here

- This leaves the response interpretation of the **Kane-Mele** $\mathbb{Z}_2$-valued invariant for TRI $2d$ crystals and of its **Floquet** generalization (**Carpentier-Delplace-Fruchart-G.-Tauber** 2015) even more open