6. Topology of finite temperature and non-equilibrium states in Chern-class systems

So far we have discussed topological properties of band structures that manifest themselves in topological properties of many-particle systems in insulating ground states, i.e. at $T=0$. Interesting questions are:

- What survives of these properties at $T \neq 0$?
- Can we define topological properties for open, driven systems?

These are questions which we currently address in our research. This chapter is thus an excurse to ongoing research in my group.

6.1 Gaussian systems

So far we have discussed non-interacting fermions with Bloch hamiltonians of the structure

$$H = \sum_{\vec{k}}' \underline{c}^{+}(\vec{k})^{T} \underline{\underline{h}}(\vec{k}) \underline{c}(\vec{k}) \tag{234}$$

When $\underline{\underline{h}}(\vec{k})$ has bands that are separated by non-vanishing gaps, and if these bands have non-vanishing Chern numbers insulating many-particle ground states showed interesting properties such as quantized bulk transport (Thouless pump, Hall conductivity) and protected edge states or edge currents.

Now we want to consider thermal states, described by a density matrix

(235) $$\rho = \frac{1}{Z} \exp(-\beta H) \qquad \beta = \frac{1}{k_B T}$$

Such density matrices with H of the form of (234) are so-called Gaussian states. They can be written as

(236) $$\rho \sim \exp\left\{ - \sum_{ij} \hat{c}_i^{(+)} G_{ij} \hat{c}_j \right\}$$

where G_{ij} is the single-particle correlation matrix or covariance matrix. If all anomal correlations vanish, i.e. $\langle \hat{c}_i \hat{c}_j \rangle = \langle \hat{c}_i^+ \hat{c}_j^+ \rangle = 0 \quad \forall\, i,j$ which is the case for (235) with H from (234) then

(237) $$\left[\tanh \frac{G}{2} \right]_{ij} = \langle c_i^+ c_j \rangle + \langle c_j c_i^+ \rangle$$

properties of Gaussian states

- Wick's theorem holds, i.e. all higher-order correlations can be reduced to single particle correlations $\langle c_i^+ c_j \rangle$ or $\langle c_i c_j \rangle$

- thus ρ is fully determined by the single-particle correlation matrix G_{ij}

- Any initial Gaussian state remains Gaussian under a unitary time evolution with a quadratic Hamiltonian

(238) $$H = \sum_{ij} h_{ij} \hat{c}_i^{(+)} \hat{c}_j$$

- The steady state of a Markov Lindblad-master equation ($\dot{\varrho}_{ss} = 0$)

(239) $$\frac{d}{dt}\varrho = -i\left[H, \varrho\right] + \frac{1}{2}\sum_\mu \left(2\hat{L}_\mu \varrho \hat{L}_\mu^+ - \{\hat{L}_\mu^+ \hat{L}_\mu, \varrho\}\right)$$

is Gaussian if H is of the structure (238) and if the Lindblad operators $\hat{L}_\mu$ are linear in particle operators

(240) $$\hat{L}_\mu = \sum_j \alpha_{\mu j} \hat{c}_j^{\,+} + \beta_{\mu j} \hat{c}_j$$

and if the steady state is unique. If multiple steady states exists, then they are Gaussian if also the initial state is Gaussian

We now want to discuss

- thermal states of free fermions

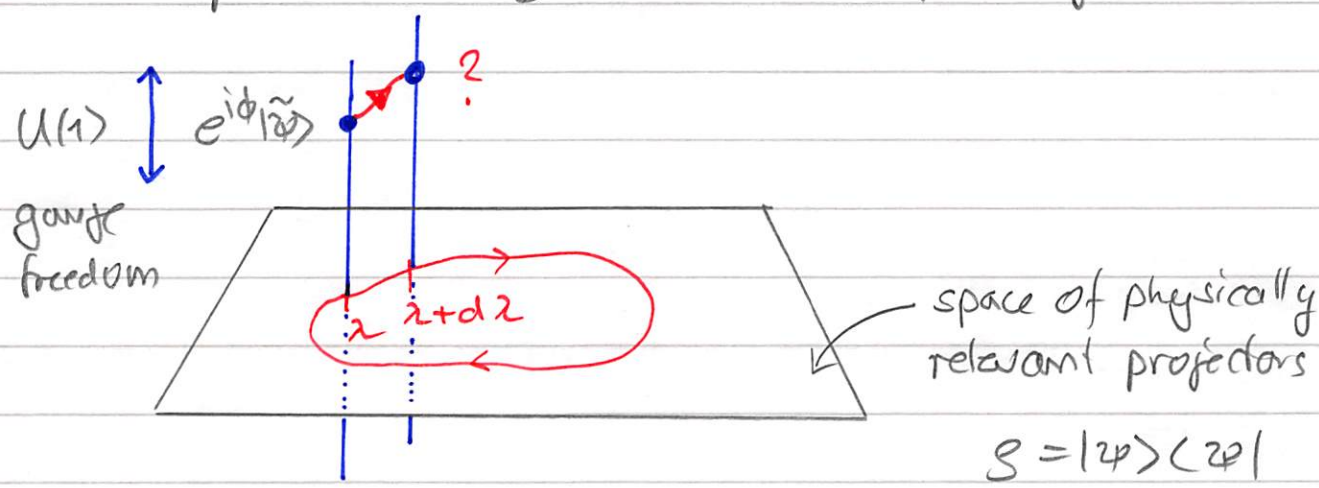
- Gaussian steady states of fermions (non-equilibrium steady state)

6.2 topological invariants I: the problem with geometric phases

To define a topolog. invariant we had made use of geometric phases of states in Hilbert space. How to generalize this to density matrices?

(A) Berry phase and parallel transport of states

consider pure states $\rho = |\psi\rangle\langle\psi|$ depending on λ



If we fix the U(1) gauge freedom at λ, how to choose the state at $\lambda+d\lambda$?

(241) $$\| \, |\psi(\lambda)\rangle - |\psi(\lambda+d\lambda)\rangle \, \| \overset{!}{=} \min$$ parallel transport

Makin a closed loop in λ one does not end up at the same state as one started from but picks up a phase, the Berry phase

(242) $$\phi_{\text{Berry}} = i \oint d\lambda \, \langle\psi(\lambda)| \partial_\lambda |\psi(\lambda)\rangle$$

(B) Uhlmann connection and Uhlmann phase

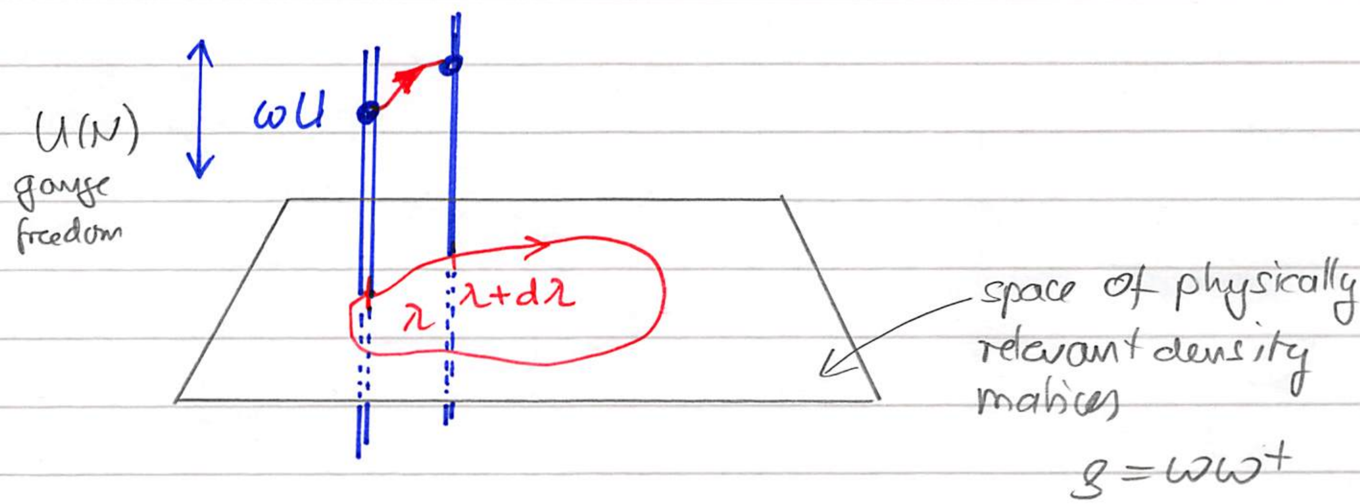
A generalization of Berry phases ($U(1)$) to density matrices was given by Uhlmann (Rep. Math. Phys. 24, 229 (1986))

(243) $\quad \rho$: $N \times N$ matrix $\qquad \rho = \omega \omega^+ \qquad \omega$: $N \times N$ matrix

gauge degree of freedom

(244) $\quad \omega \to \omega U \qquad \omega^+ \to U^+ \omega^+$

consider $\omega = \omega(\lambda)$



One can again define a parallel transport, requiring

(245) $\quad || \omega(\lambda) - \omega(\lambda + d\lambda) || \overset{!}{=} \min$

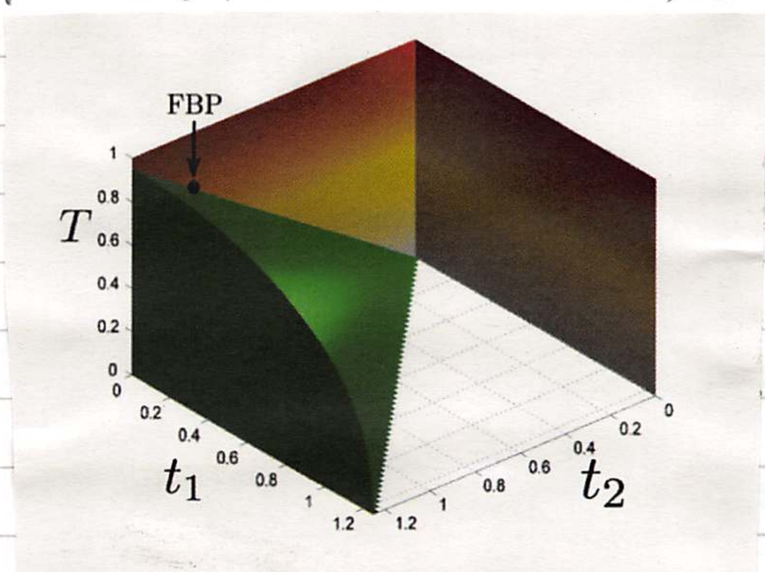
Making a closed loop leads to a $U(N)$ generalization of Berry phase. Note: N is the dimension of Hilbert space!

One can define a phase, the $U(1)$ Uhlmann phase

$$(243) \qquad \phi_u = \arg \oint d\lambda \, \mathrm{Tr}\{ w^\dagger(\lambda) \partial_\lambda w(\lambda) \}$$

The Uhlmann phase can be used in analogy to the Zak phase to define a topological invariant in 1D systems (Viyuela et al PRL 112, 130401 (2014))

For example for the SSH model (eq. (73), chapter 1.3) one finds a phase transition from the topologically non-trivial phase ($\phi_u = \phi_{ZAK} = \pi$ at $T=0$) to a trivial phase ($\phi_u = 0$ at $T \gtrsim T_c$)



The Uhlmann phase is however not suitable in 2D as shown by J.C. Budich and S. Diehl, PRB 91, 165140 (2015). They considered a finite-temperature state of the 2D Bloch hamiltonian with 2 bands

$$(244) \quad H = \sum_{\vec{k}} \begin{pmatrix} c_A^\dagger(k) \\ c_B^\dagger(k) \end{pmatrix}^T \underline{\underline{h}}(k) \begin{pmatrix} \hat{c}_A(k) \\ \hat{c}_B(k) \end{pmatrix} \qquad \underline{\underline{h}}(k) = \sum_{j=1}^{3} d_j(k) \underline{\underline{\sigma}}_j$$

where (note the difference to the QWZ model eq. (92))

$$(245) \quad d_1(k) = \sin(k_x) \qquad d_2(k) = 3\sin(k_y) \qquad d_3(k) = 1-\cos(k_x)-\cos(k_y)$$

One finds that for certain values of T

$$(246) \quad C_u \equiv \frac{1}{2\pi}\int_{BZ_x} \frac{\partial \phi_u(k_x)}{\partial k_x}\, dk_x \neq \tilde{C}_u \equiv \frac{1}{2\pi}\int_{BZ_y} \frac{\partial \phi_u(k_y)}{\partial k_y}\, dk_y$$

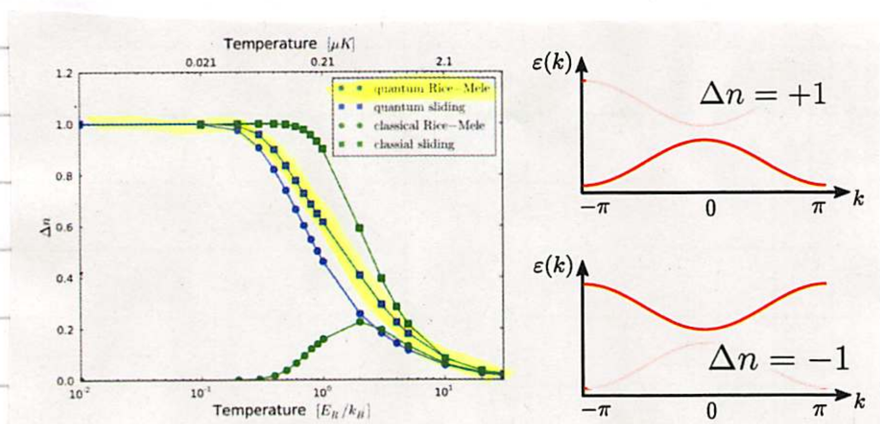
Thus $\boxed{\text{no proper Uhlmann-Berry connection exists !} \ ⚡}$

6.3 topological invariants II: Many-body polarization vs. bulk charge transport

In Chapter 1.2 we have seen that a non-trivial winding of the Zak phase in the Rice-Mele model has lead to quantized bulk transport, see eq. (73), (74)

$$(247) \qquad \Delta n = \frac{1}{2\pi}\oint d\lambda \, \frac{\partial \phi_{ZAK}}{\partial \lambda}$$

So, while ϕ_{ZAK} can no longer be used, perhaps Δn can?



Wang, Troyer, Dai
PRL 111 026802 (2013)

As soon as $T \sim \Delta\varepsilon_{gap}$ there is a sizable population of the upper band in which the transport is in the opposite direction

$$\Rightarrow \boxed{\text{break-down of quantized charge transport at finite } T}$$

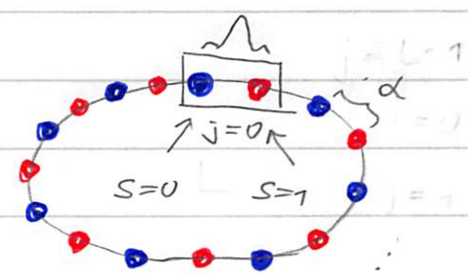
(A) Many-body polarization

In Chapter 1.2 we have used the center of mass of Wannier functions in a unit cell (eq. (60)) and found

(248) $$\langle W_n | \hat{x} | W_n \rangle = \int dx\, W_n^*(x)\, x\, W_n(x) = \frac{i}{2\pi} \int_{BZ} dk \langle u_{nk} | \partial_k u_{nk} \rangle$$

This quantity is referred to as polarization. As shown by Resta (PRL 80, 1800 (1998)), this polarization can be formulated for periodic systems as the phase of a many-body observable for unit filling of unit cell

(249) $$\boxed{P = \frac{1}{2\pi} \operatorname{Im} \ln \left\langle \exp\left(i \frac{2\pi}{L} \hat{x}\right) \right\rangle}$$



where

(250) $$\hat{x} = \sum_{j=0}^{L-1} \sum_{s} (j + s\alpha)\, \hat{n}_{js}$$

Shift of origin $j \to j+n$ leads to (unit filling of unit cell)

(251) $$\hat{x} \to \hat{x} + n \sum_{j=0}^{L-1} \sum_{s} \hat{n}_{js} = \hat{x} + nL$$

and thus

(252) $$P \to P' = \frac{1}{2\pi} \operatorname{Im} \ln \langle \exp(i \tfrac{2\pi}{L}(\hat{X} + nL)) \rangle = P$$

(B) Ensemble geometric phase

Eq. (249) can trivially be generalized to mixed states

$$\langle \psi | e^{i\frac{2\pi}{L}\hat{X}} | \psi \rangle \longrightarrow \operatorname{Tr}\{ \rho\, e^{i\frac{2\pi}{L}\hat{X}} \}$$

Thus we define an ensemble geometric phase

(253) $$\boxed{\phi_{EGP} \equiv \operatorname{Im} \ln \operatorname{Tr}\{ \rho\, e^{i\frac{2\pi}{L}\hat{X}} \}}$$

For $T=0$ $\phi_{EGP} = \phi_{ZAK}$. Being a phase of a complex number its winding upon a closed loop in a uniquely defined state ρ must be quantized!

In C. Bardyn, L. Wawer, A. Altland, M.F. and S. Diehl PRX 8, 011035 (2018) it was shown that for every Gaussian state ρ of fermions

(254) $$\boxed{P(\rho) = P(|\psi\rangle\langle\psi|) + \mathcal{O}(L^{-1})}$$

where $|\psi\rangle$ is a pure state

i.e. in the limit $L \to \infty$

(255) $$\boxed{\phi_{EGP}(\varrho) \underset{L\to\infty}{=} \phi_{ZAK}(|\psi\rangle)}$$

where $|\psi\rangle$ is the ground state of the so-called fictitious hamiltonian

(256) $$H_{fict} = \sum_{ij} \hat{c}_i^{\dagger} G_{ij} \hat{c}_j$$

with G_{ij} being the single-particle correlation matrix of the Gaussian state ϱ. From (254) follows

(257) $$\boxed{\oint d\lambda \frac{\partial}{\partial\lambda} P(\varrho) = \oint d\lambda \frac{\partial}{\partial\lambda} P(|\psi\rangle\langle\psi|)}$$

irrespective of system size L

example: finite-T Rice Mele model