8. Topology of finite-temperature and non equilibrium steady states of fermions

So far we have discussed isolating many-body ground states of fermion lattice hamiltonians.

- What survives of topological properties at $T \neq 0$?
- Can we extend the concept of topology to steady states of open systems?

8.1 Gaussian mixed states

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

$$H = \sum_{\vec{k}} \underline{\tilde{c}}^{+}(\vec{k})^{T} \, \underline{\underline{h}}(\vec{k}) \, \underline{\tilde{c}}(\vec{k})$$

Now we want to consider mixed states, i.e. density matrices in so-called Gaussian states which are the equivalent of non-interacting fermions.

Gaussian states are fully determined by single-particle correlations. We assume for simplicity that anomal correlations vanish, i.e.

$$\langle \tilde{c}_i \tilde{c}_j \rangle = \langle \tilde{c}_i^+ \tilde{c}_j^+ \rangle = 0$$

Then

$$\boxed{\rho = \frac{1}{Z} \exp\left\{ - \sum_{ij} \tilde{c}_i^+ G_{ij} \tilde{c}_j \right\}}$$

and

$$\boxed{\langle c_i^+ c_j \rangle = \frac{1}{2} \left[1 - \tanh\left(\frac{G}{2}\right) \right]_{ij}}$$

- Thermal states of non-interacting Hamiltonians

$$\rho = \frac{1}{Z} \exp\left(-\beta (H - \mu N)\right)$$

are obviously Gaussian. $\beta = 1/k_B T$

- They also arise as (unique) steady states of Lindbladians with quadratic Hamiltonians and linear Lindblad operators, if such a state exists.

$$0 = \frac{d}{dt} \rho = -\frac{i}{\hbar} [H, \rho] + \frac{1}{2} \sum_\mu \left(2 L_\mu \rho L_\mu^+ - \{ L_\mu^+ L_\mu, \rho \}_- \right)$$

with $$L_\mu = \sum_j \alpha_{\mu j} \hat{c}_j^+ + \beta_{\mu j} \hat{c}_j$$

properties of Gaussian states

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

- ρ is fully determined by matrix G_{ij}

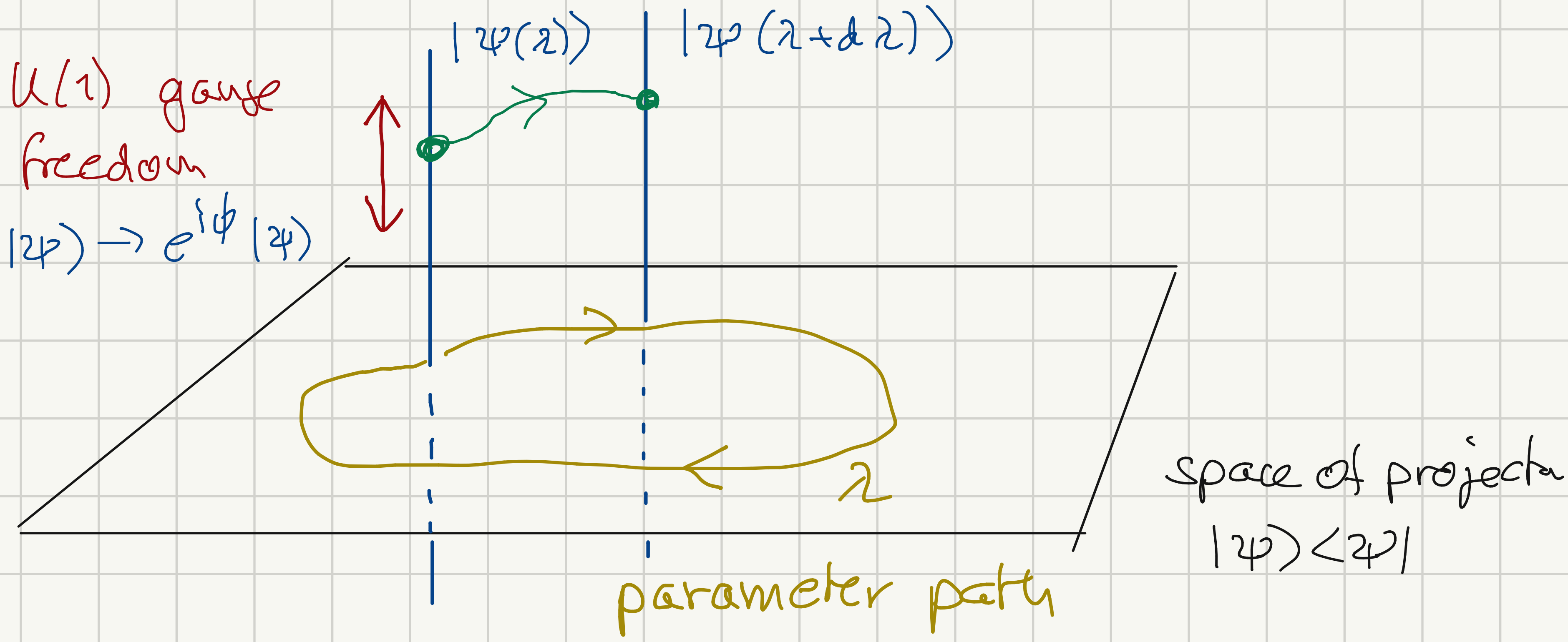
8.2 Topological invariants for mixed states I: The problem with geometric phases

In order to define topological invariants for pure states we made use of geometric phases. How can we generalize this to density matrices?

(A) Berry phase and Berry parallel transport

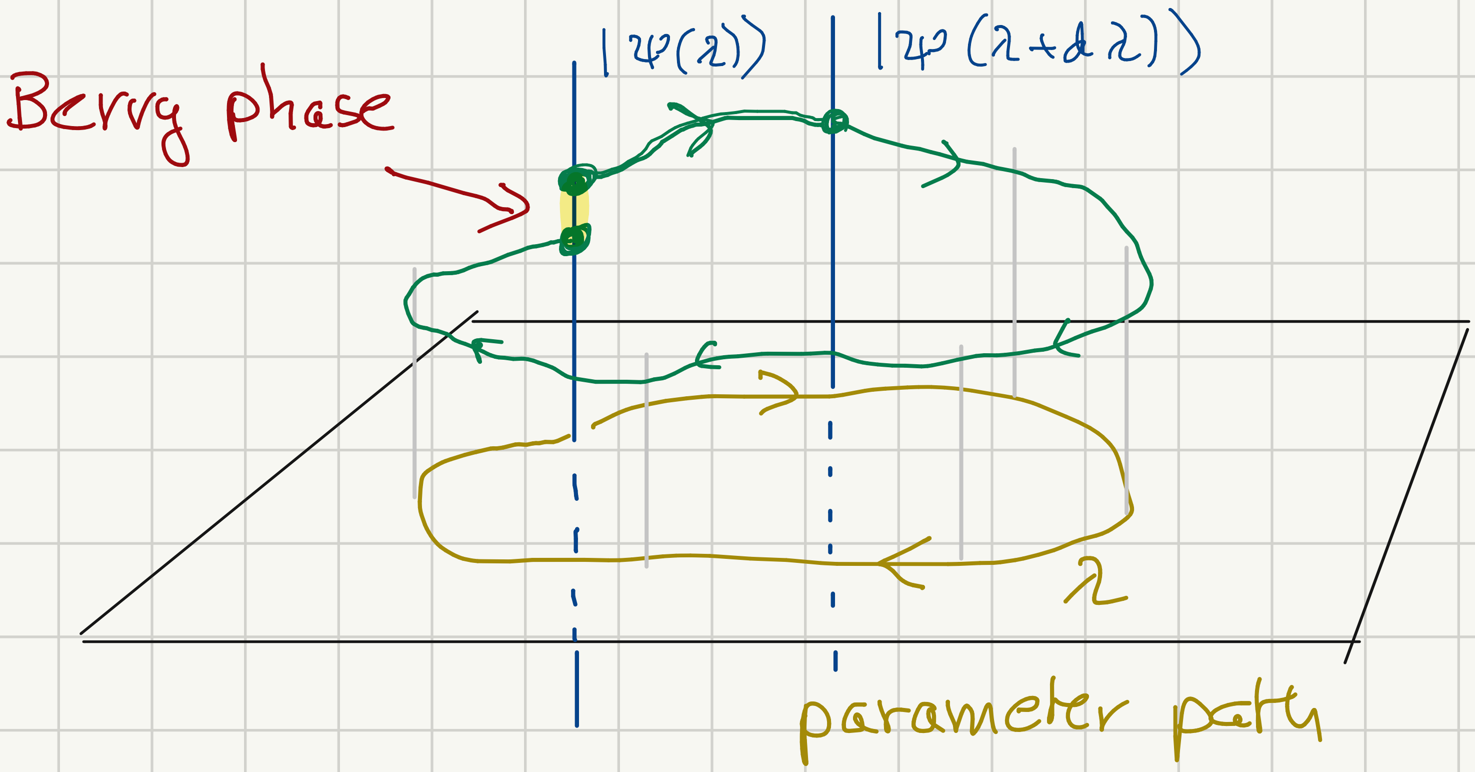
Consider pure states $\rho = |\psi\rangle\langle\psi|$ depending on a parameter λ in a periodic way

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



parallel transport of state $|\psi(\lambda)\rangle \rightarrow |\psi(\lambda+d\lambda)\rangle$

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



(B) Uhlmann connection and Uhlmann phase

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

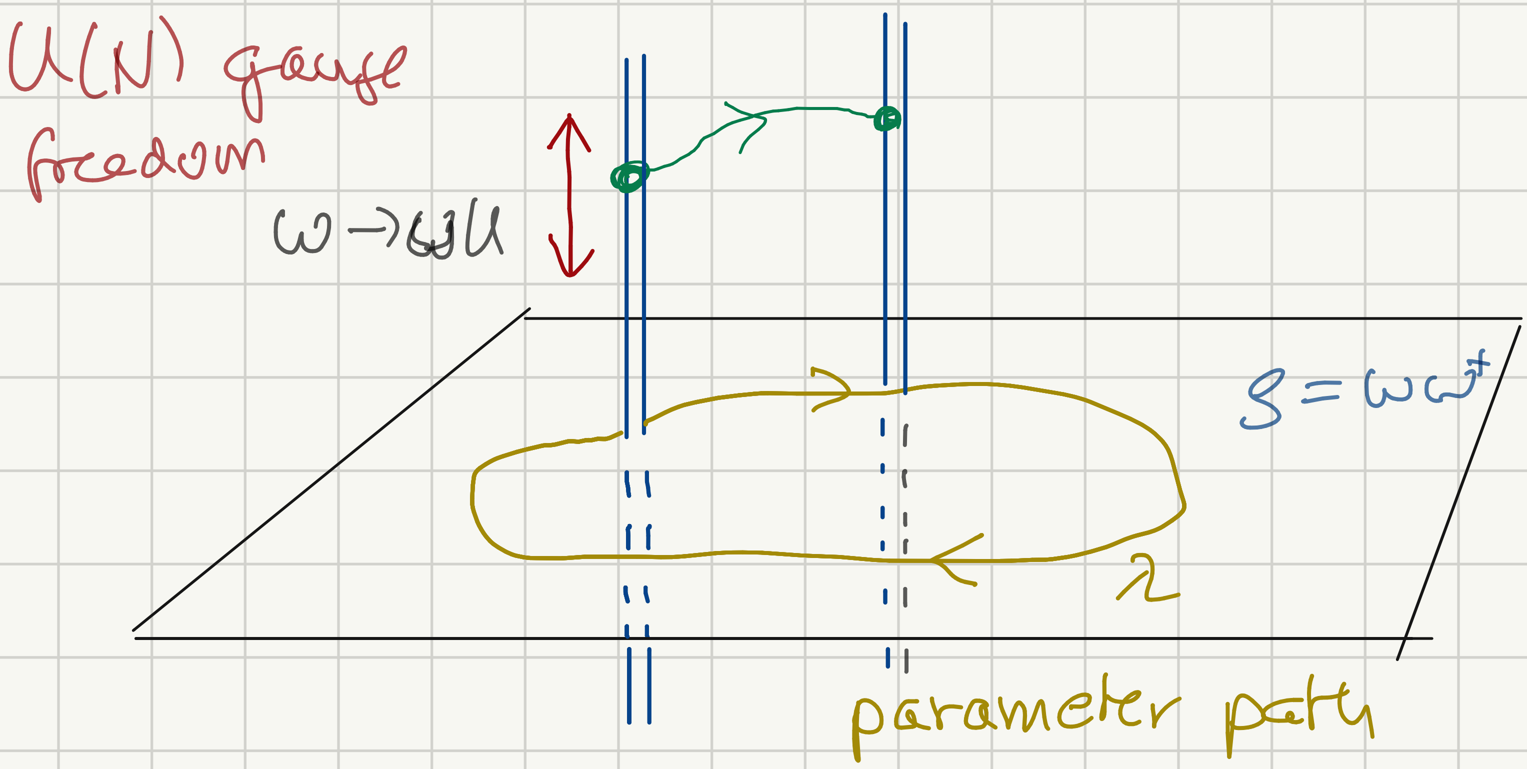
$\mathcal{g}$: $N \times N$ matrix

$$\mathcal{g} = \omega \omega^{+}$$ $\omega = N \times N$ matrix

gauge degree of freedom $U^{+} = U^{-1}$ unitary $N \times N$

$\omega \to \omega U$ $\omega^{+} \to U^{+} \omega$

Now consider $\mathcal{g} = \mathcal{g}(\lambda) = \omega(\lambda) \omega^{+}(\lambda)$



One can define a parallel transport of matrices $\omega(\lambda) \to \omega(\lambda + d\lambda)$ requiring

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

Making a closed loop in the parameter λ leads to a $U(N)$ generalization of the Berry phase.

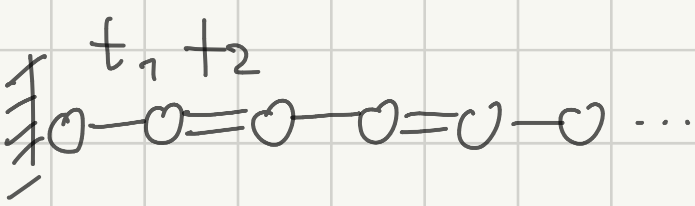
One can reduce this to a $U(1)$ phase

$$\boxed{\phi_u = \arg \oint dk\, \mathrm{Tr}\{w^\dagger(k)\,\partial_k w(k)\}}$$

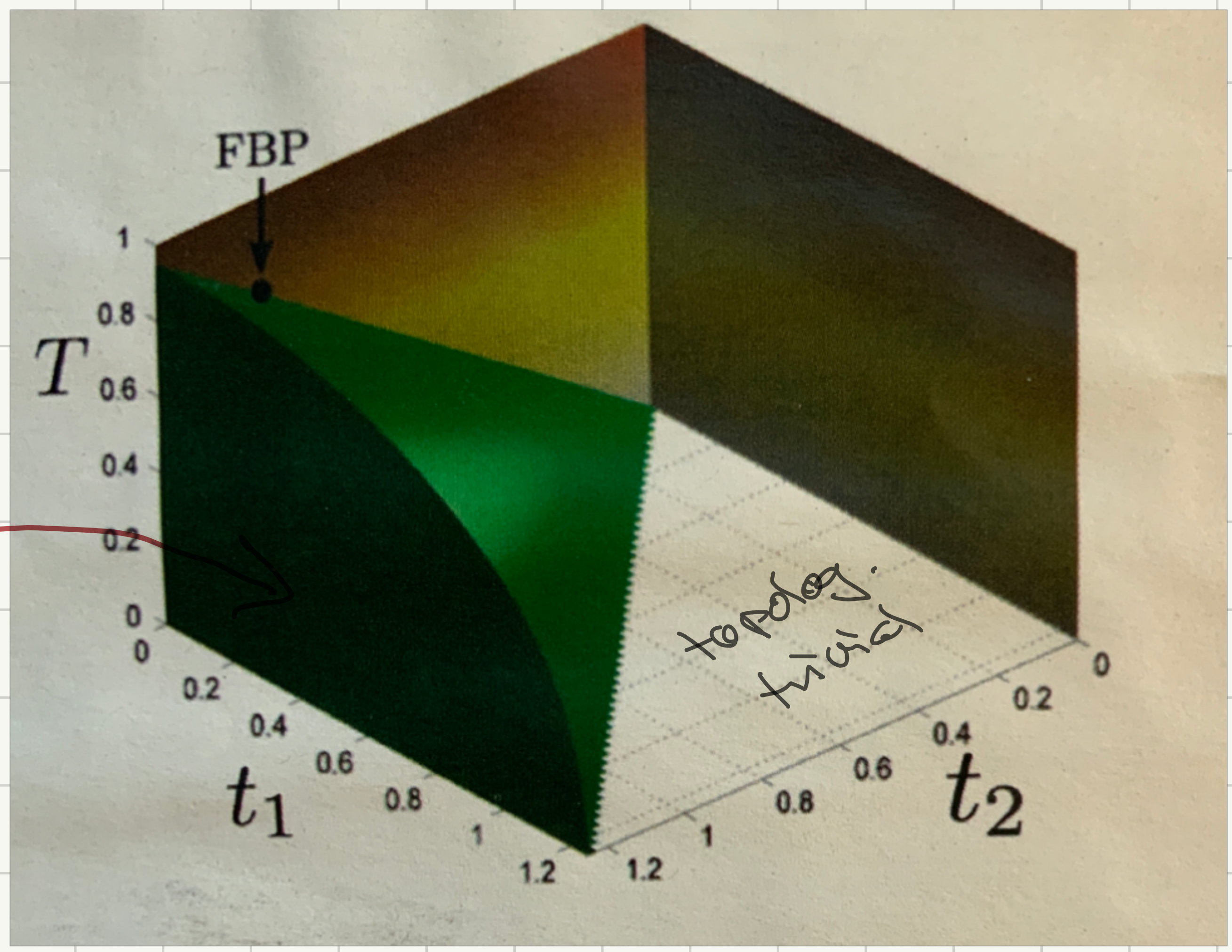
Uhlmann phase

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

Example: SSH model at finite T



$t_1 < t_2$



finite-T topological phase transition at $T = T_c$

The Uhlmann phase is however not suitable in 2D as shown by Budich and Diehl PRB 91, 165140 (2015)

They considered the <u>asymmetric</u> Qi-Wu-Zhang model in 2D

$$H = \sum_{\vec{k}} \begin{pmatrix} \tilde{c}_A^{\dagger}(\vec{k}) \\ \tilde{c}_B^{\dagger}(\vec{k}) \end{pmatrix}^T \underline{\underline{h}}(\vec{k}) \begin{pmatrix} \tilde{c}_A(\vec{k}) \\ \tilde{c}_B(\vec{k}) \end{pmatrix}$$

where

$$\underline{\underline{h}}(\vec{k}) = \sum_{j=1}^{3} d_j(\vec{k})\, \underline{\underline{\sigma}}_j$$

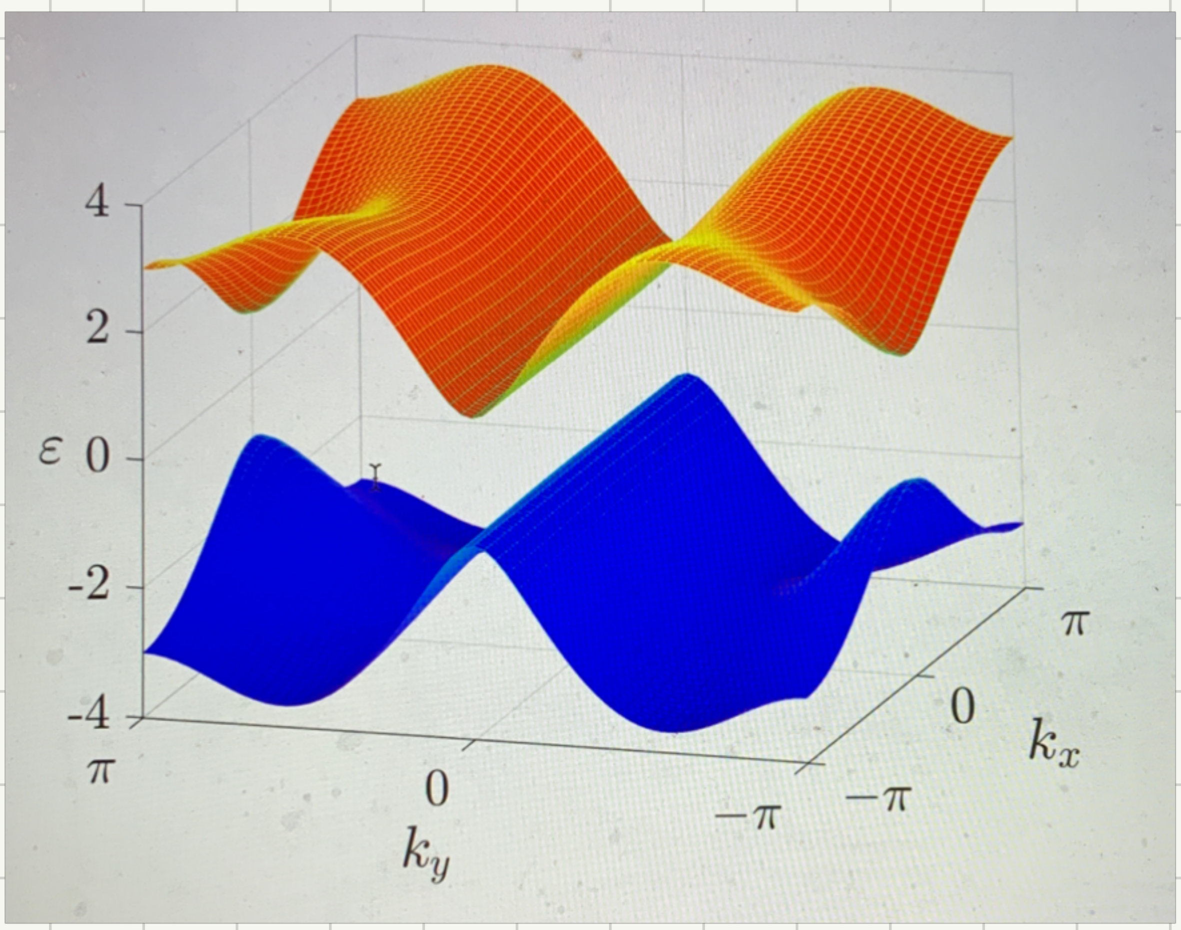
and

$$d_1(\vec{k}) = \sin(k_x) \qquad d_2(\vec{k}) = 3\sin(k_y)$$

$$d_2(\vec{k}) = 1-\cos(k_x)-\cos(k_y)$$

Note the factor of 3 as compared to eq. (92) which makes the band structure asymmetric in k_x and k_y

2 band model with $C \neq 0$



asymmetric Qi-Wu-Zhang

One finds for certain value of T

$$C_u^x \equiv \frac{1}{2\pi} \int_{BZ_x} dk_x \, \frac{\partial \phi_u(k_x)}{\partial k_x}$$

$$\neq C_u^y \equiv -\frac{1}{2\pi} \int_{BZ_y} dk_y \, \frac{\partial \phi_u(k_y)}{\partial k_y}$$

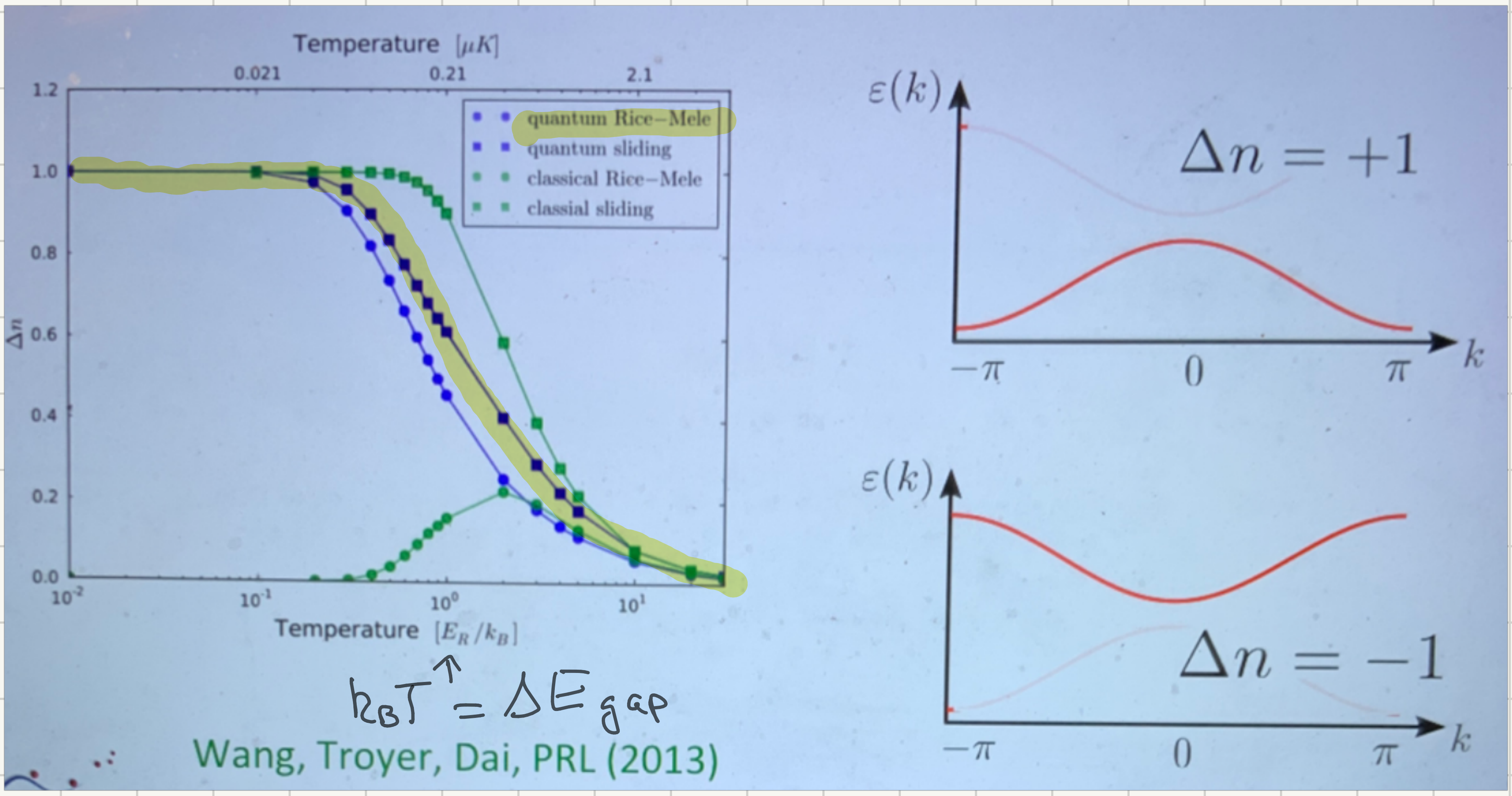
$\Rightarrow$ $\boxed{\nexists \text{ proper Uhlmann-Berry connection}}$

8.3 Topological invariant for mixed state II: Bulk transport and many-body polarization

In Chapter 1 we have seen that a non-trivial winding of the Zak phase in an insulating many-body state of a time periodic Hamiltonian leads to a quantized adiabatic particle transport in the bulk

$$\Delta n = \frac{1}{2\pi} \oint d\lambda \, \frac{\partial \phi_{ZAK}}{\partial \lambda} \in \mathbb{Z},$$

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



As soon as $k_B T \simeq \Delta E_{gap}$ there is a sizable fraction of particles in the upper band in which the transport is in the opposite direction

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

(A) Many-body polarization

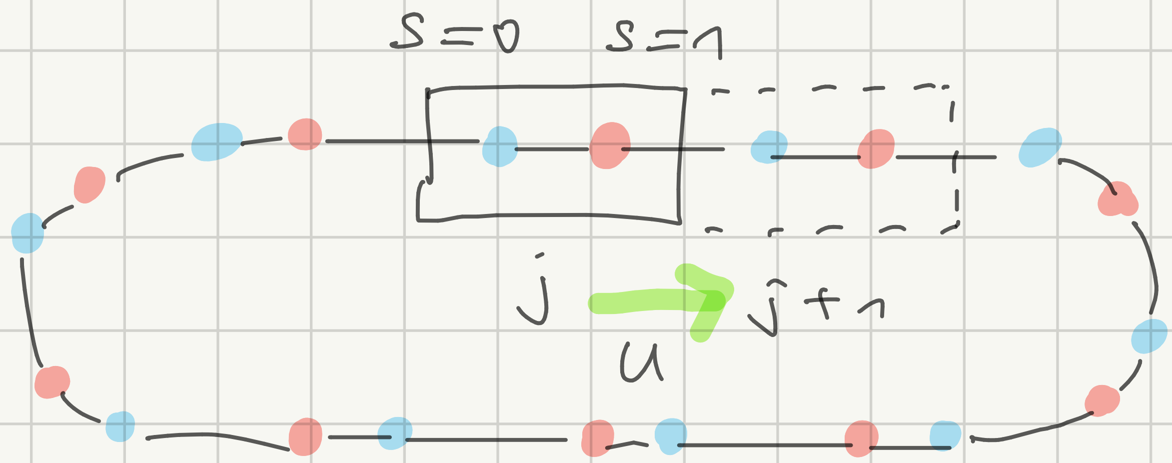
In Chapter 1 we have used the center of mass of Wannier functions in a unit cell, eq. (50), and found

$$\langle w_n | \hat{x} | w_n \rangle = \int dx\, w_n^*(x)\, x\, w_n(x) = \frac{i}{2\pi} \int_{BZ} dk\, \langle u_n(k) | \partial_k u_n(k) \rangle$$

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

$$P = \frac{1}{2\pi} \arg \langle \exp(i \tfrac{2\pi}{L} \hat{X}) \rangle$$
$$= \frac{1}{2\pi} \operatorname{Im} \log \langle \exp(i \tfrac{2\pi}{L} \hat{X}) \rangle$$

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



L : # of unit cells

Note that $\hat{T} \equiv e^{\frac{2\pi i}{L}\hat{X}}$ is the unitary momentum shift operator. Since the system is translational invariant

$$U e^{\frac{2\pi i}{L}X} U^{-1} = \exp\Big(\frac{2\pi i}{L} \sum_j \sum_s (j+1+s\alpha)\, \hat{n}_{js}\Big)$$
$$= \exp\Big(\frac{2\pi i}{L}\hat{X} + \frac{2\pi i}{L}\hat{N}\Big)$$

so
$$\langle \hat{T} \rangle = 0 \quad \text{unless } \frac{\langle \hat{N} \rangle}{L} \text{ is integer!}$$

$\Rightarrow$ $\boxed{\text{integer filling per unit cell needed}}$

(B) Ensemble geometric phase

The expression for P can trivially be extended to mixed states

$$\langle \Psi_0 | \hat{T} | \Psi_0 \rangle \longrightarrow \mathrm{Tr}\{ \rho \hat{T} \}$$

This defines the ensemble geometric phase

$$\boxed{\phi_{EGP} \equiv \mathrm{Im} \log \mathrm{Tr}\{ \rho \hat{T} \}}$$

For $T = 0$ $\quad \phi_{EGP} = \phi_{ZAK}$

In Bardyn et al. PRX $\underline{8}$, 011035 (2018) we have shown that for Gaussian mixed states with integer filling per unit cell

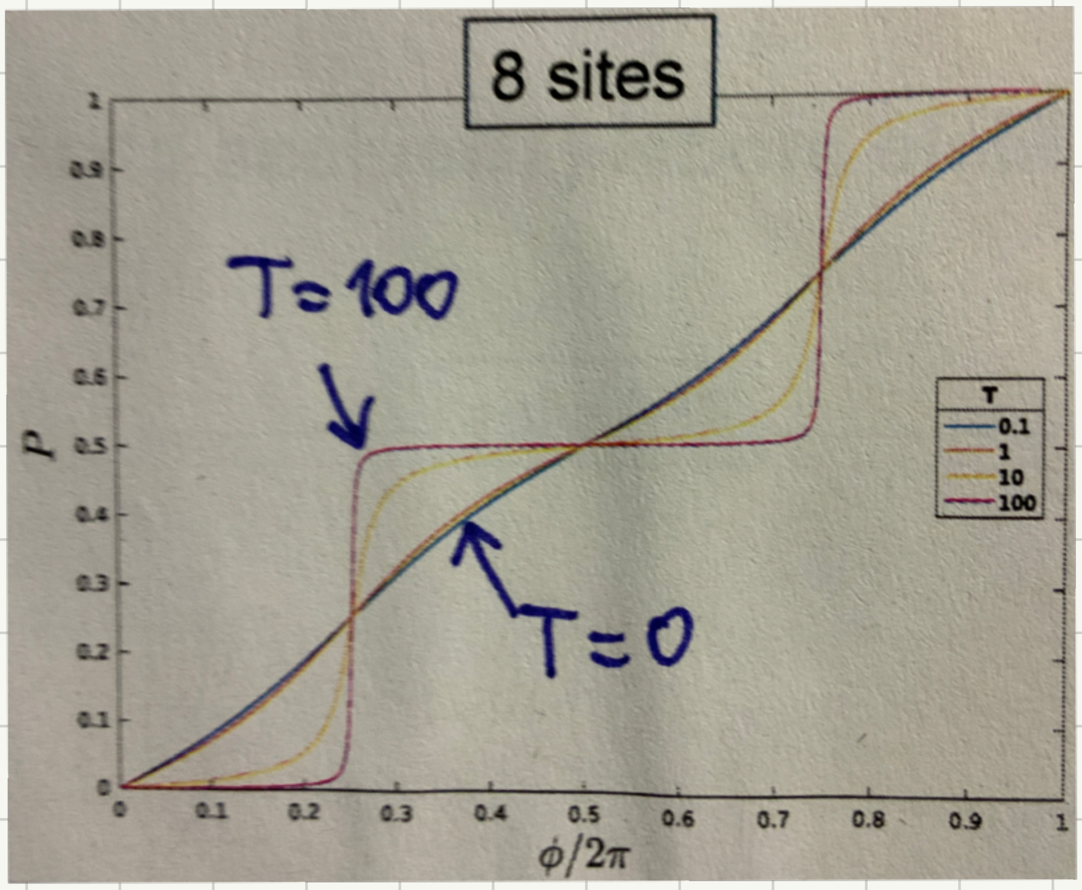
$$\boxed{P(\rho) = P(|\Psi\rangle\langle\Psi|) + \mathcal{O}(L^{-\alpha})}$$

where $|\Psi\rangle$ is the ground state of the fictitious Hamiltonian

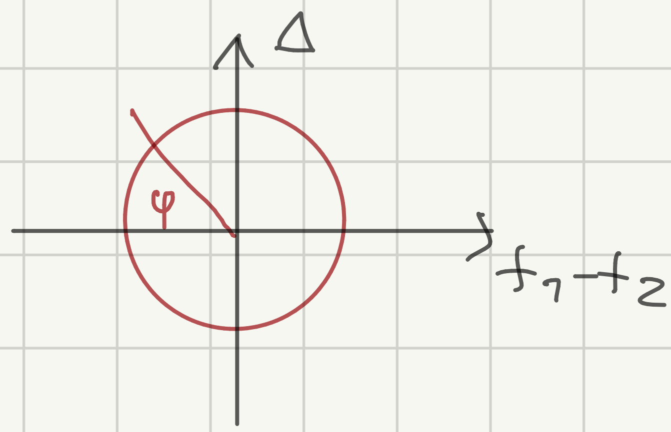
$$H_{fict} = \sum_{ij} \hat{c}_i^+ G_{ij} \hat{c}_j$$

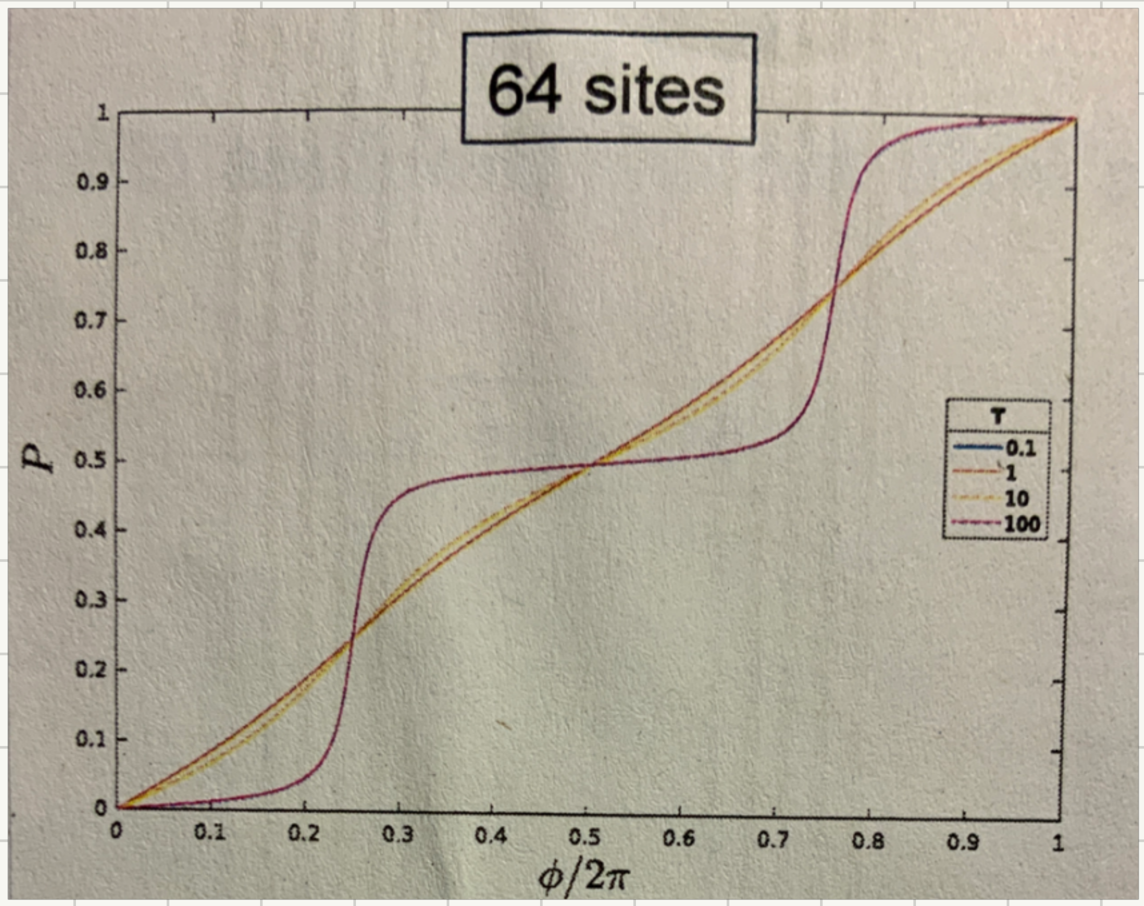
It follows for all values of L

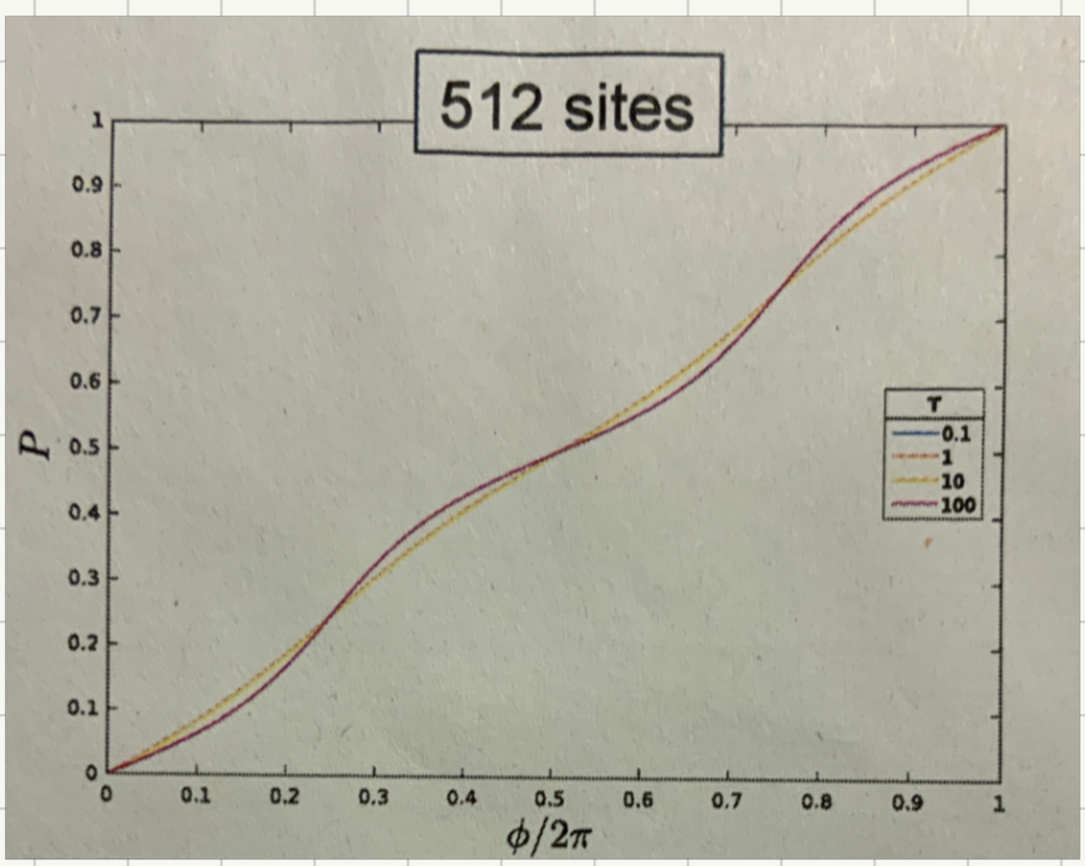
$$\boxed{\oint d\lambda \frac{\partial P(\rho)}{\partial \lambda} = \oint d\lambda \frac{\partial}{\partial \lambda} P(|\Psi\rangle\langle\Psi|) = \frac{1}{2\pi} \oint d\lambda \frac{\partial}{\partial \lambda} \phi^{ZAK}_{|\Psi\rangle}}$$



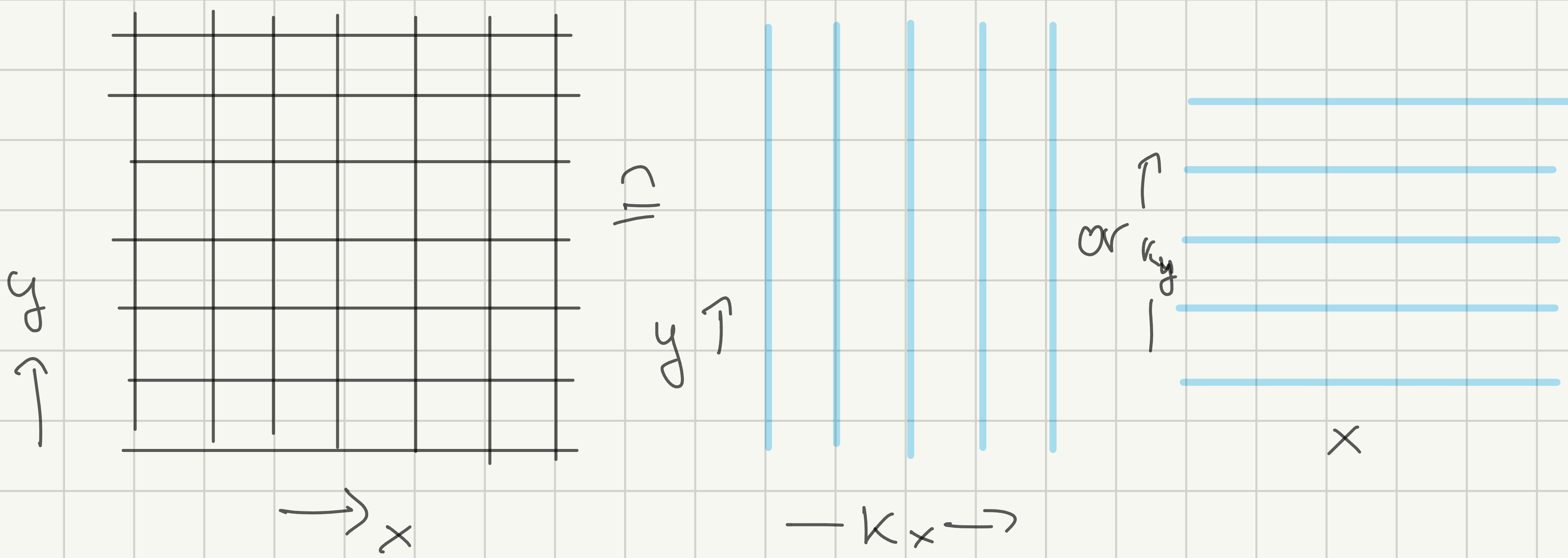
example Rice-Mele model at different T and L







Also the Polarization can be used to define a proper Chern number in 2D



decomposition $\qquad P_y(k_x) \qquad P_x(k_y)$

$$C^x_{EGP} = \oint dk_x \frac{\partial P_y}{\partial k_x} \qquad C^y_{EGP} = -\oint dk_y \frac{\partial P_x(k_y)}{\partial k_y}$$

for EGP

$$\boxed{C^x_{EGP} \overset{!}{=} C^y_{EGP} = C_{EGP}}$$