

# Topological Invariants of Interacting Gapped Quantum Materials and Transport Phenomena

Thesis by  
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The logo for the California Institute of Technology (Caltech), featuring the word "Caltech" in a bold, orange, sans-serif font.

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## ABSTRACT

In this thesis we study transport properties of interacting lattice system focusing, on those which become topologically protected at low temperatures for gapped Hamiltonians. We prove the vanishing of the net energy currents in equilibrium states of lattice systems as well as systems of nonrelativistic particles with finite-range potential interactions. We derive Kubo-like formulas for the thermal and thermoelectric Hall conductances of arbitrary 2d lattice systems which are free from ambiguities associated with the definition of magnetizations. We use these formulas to define a relative topological invariant of gapped 2d lattice systems at zero temperature.

We define and study analogs of the Thouless charge pump and Berry Curvature for many-body gapped systems in spatial dimension  $D$ . We show how to attach a topological invariant to a  $D$ -dimensional family of such systems. For a large class of families we argue that this topological invariant is an integer.

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*Chapter 1*

## INTRODUCTION

**1.1 Topological phases and transport phenomena**

One of the most successful paradigms for describing phases of matter is the Landau-Ginzburg theory of second-order phase transitions. It classifies phases according to their global symmetries and predicts the behavior of the system near criticality based only on the symmetry breaking pattern. A classic example is the order-disorder transition of the Ising model associated to  $\mathbb{Z}_2$  symmetry. The mere knowledge of the symmetry breaking pattern is enough to predict the scaling dimensions at the critical point.

However, since the discovery of topological order, it is known that this theory cannot describe all phases of matter. Different plateaus of quantum Hall effect have the same symmetry even though they are separated by zero-temperature phase transitions. This raises a question of classification of zero-temperature phases. While it is enormously hard to address this question in full generality, it simplifies in the case of insulators and other gapped systems. At low temperatures, their transport properties become quantized and robust against small perturbations. In this thesis, we define some of these transport coefficients for a large class of interacting systems and study their properties.

Our chosen setting in this thesis is lattice system with finite-range interactions. Some of our results also apply to continuum systems of particles with rapidly decaying potential interactions. We introduce the main definitions and key observables in Chapter 3. In Chapters 5 and 6 we define thermal and thermoelectric Hall conductances, show that they become invariants of the phase at low temperatures and are related to anomalies of the boundary conformal field theory (CFT) whenever the boundary is described by one. One novelty is that we do not assume the existence of a field-theoretic or hydrodynamic description at long distances. Another outcome of our analysis is microscopic formulas for all transport coefficients which are free from ambiguities in the definition of currents and magnetizations. We show that ambiguities in magnetizations drop out of all measurable quantities if one takes into account that some transport phenomena involve both the bulk and the edges, and that their contributions cannot be unambiguously separated. The corresponding trans-

port coefficients are a property of a pair of materials rather than a single material. Ambiguities in the definition of currents, on the other hand, are cured by correcting "textbook" Kubo formulas with additional local terms.

The low-temperature thermal Hall effect is especially important for systems without any symmetries since it is the only transport quantity which characterizes topological phases. In the case of systems with a  $U(1)$ -symmetry, thermal Hall conductance can distinguish different phases having the same electric Hall conductance. One might expect that transverse thermoelectric coefficients can be used to make an even finer classification of phases. However, as we argue in Chapter 7, all such invariants are zero due to the Third Law of Thermodynamics.

Many of our arguments require an extension of F. Bloch's theorem on absence of net electric currents in equilibrium systems to the case of the energy currents. This result has an interest of its own and we prove energy Bloch's theorem in Chapter 4. Somewhat surprisingly, the arguments used to prove the usual Bloch's theorem [10] do not generalize to the case of the energy current which requires an entirely new approach.

## 1.2 Generalizations of the Berry curvature and the Thouless pump

Along with topological invariants of quantum many-body systems, one sometimes considers topological invariants of families of many-body systems. One example of such an invariant is the Thouless charge pump which is an integer assigned to a loop in the space of  $U(1)$ -invariant gapped systems in one dimension at zero temperature. It measures the net charge flowing through a section of a system as the parameters of the Hamiltonian are varied adiabatically. Thouless charge pump is a topological invariant in the sense that it does not change under continuous deformations of the loop, provided the loop stays away from the locus where the energy gap closes. An even simpler example arises from the Berry phase of single-body quantum systems. In that case, an integer is assigned to a family of quantum systems with a unique gapped ground state parameterized by a closed oriented two-dimensional surface (for example, a sphere). This integer is the integral of the curvature of the Berry connection divided by  $2\pi$ .

It was proposed by Alexei Kitaev that both the Berry curvature and the Thouless charge pump have higher dimensional "descendants" which assign topological invariants to families of gapped systems in  $D$  spatial dimensions. In the second part of this thesis we define and study these descendants for quantum lattice systems. In

Chapter 8 we deal with higher-dimensional generalizations of the Berry curvature and in Chapter 9 with higher-dimensional generalizations of the Thouless charge pump. These new invariants can detect zero-temperature phase transitions, similarly to how the integral of the Berry curvature on a sphere can detect degenerate points inside it. Further, whenever a family has a non-trivial descendant invariant, the edge must be gapless for at least one member of the family.

Family invariants of gapped many-body systems are particularly interesting when all systems in the family are in a trivial phase (or more generally, in an "invertible" phase). A. Kitaev have argued that infinite-dimensional spaces of all such systems have a nontrivial but highly constrained topology (from the homotopy theory viewpoint, when these spaces in all dimensions are considered simultaneously, they form a "loop spectrum"). This means that there is one-to-one correspondence between homotopy classes of families of  $(D + 1)$ -dimensional invertible states parametrized by a periodic parameter and  $D$ -dimensional invertible phases. Physically, a map from higher dimensions to lower dimensions corresponds to forming a soliton, while the inverse map corresponds to constructing a  $(D + 1)$ -dimensional pump which transmits a  $D$ -dimensional system during an adiabatic change of the parameter.

It is expected that at low energies and large length scales, a lattice system can be approximated by a continuum quantum field theory that captures the universal features of the system. Accordingly, invertible topological systems are expected to be approximated by invertible topological quantum field theories (TQFTs). As was shown in [20], invertible TQFTs indeed form a loop spectrum whose structure can be determined. Verifying that invertible lattice systems give rise to an equivalent loop spectrum remains an outstanding problem. Our construction of higher-dimensional analogs of the Berry curvature and the Thouless charge pump allows us to test some elements of this picture. In particular, in agreement with the conjectures sketched above, we argue that descendant topological invariants of families of invertible systems parameterized by spheres are integral in all dimensions.

## Chapter 2

### HYDRODYNAMICS OF THERMOELECTRIC COEFFICIENTS

#### 2.1 Generalities

In this section we recall the definition of transport coefficients and some of their properties. The discussion applies both in 2D and 3D; in later sections we specialize to 2D materials.

In the hydrodynamic limit, one can expand the electric current density and the energy current density to first order in the electric field and the temperature gradient.<sup>1</sup> For simplicity we will assume that the chemical potential is constant. For the electric current, this expansion has the form

$$\mathbf{j}_k^N = \sigma_{km} \mathbf{E}_m - \nu_{km} \partial_m T, \quad (2.1)$$

where  $\mathbf{E}_k = -\partial_k \varphi - \partial_t \mathbf{A}_k$  and  $\varphi$  is the electric potential. The conductivity tensor  $\sigma_{km}$  and the thermoelectric tensor  $\nu_{km}$  are functions of temperature only. Strictly speaking, this expansion applies in a non-equilibrium steady state (NESS). Thus we may assume  $\nabla \times \mathbf{E} = \frac{\partial \mathbf{B}}{\partial t} = 0$ . For the energy current the expansion is

$$\mathbf{j}_k^E = \varphi \mathbf{j}_k^N + \eta_{km} \mathbf{E}_m - \kappa_{km} \partial_m T. \quad (2.2)$$

Note that the first term on the r.h.s. is not invariant under a constant gauge transformation  $\varphi(x) \mapsto \varphi(x) + c$ . This is because the energy density operator also transforms under such gauge transformations,  $\hat{h}(\mathbf{r}) \mapsto \hat{h}(\mathbf{r}) + c \hat{\rho}(\mathbf{r})$ , where  $\hat{\rho}$  is the electric charge density. Since the current operators  $\mathbf{J}^{N,E}(\mathbf{r})$  are defined by the equations

$$i[H, h(\mathbf{r})] = -\nabla \cdot \mathbf{J}^E(\mathbf{r}), \quad i[H, \rho(\mathbf{r})] = -\nabla \cdot \mathbf{J}^N(\mathbf{r}), \quad (2.3)$$

this requires the energy current operator to transform as well,  $\mathbf{J}^E \mapsto \mathbf{J}^E + c \mathbf{J}^N$ . The tensor  $\nu_{km}$  describes the Seebeck and Nernst effects, while the tensor  $\eta_{km}$  describes the Peltier and Ettingshausen effects.

Transport coefficients are constrained by Onsager's reciprocity relations [36]:

$$\begin{aligned} \sigma_{km}(T, \mathbf{B}) &= \sigma_{mk}(T, -\mathbf{B}), \\ \kappa_{km}(T, \mathbf{B}) &= \kappa_{mk}(T, -\mathbf{B}), \\ \eta_{km}(T, \mathbf{B}) &= T \nu_{mk}(T, -\mathbf{B}), \end{aligned} \quad (2.4)$$

---

<sup>1</sup>More precisely, these are “transport” currents. There are also “magnetization” currents which are present even in equilibrium.

where we assumed for definiteness that time-reversal invariance is broken only by an external magnetic field  $\mathbf{B}$ . In general, Onsager reciprocity relates transport coefficients of a system and its time-reversal partner. Note that in a time-reversal-invariant situation the tensors  $\sigma$  and  $\kappa$  are required to be symmetric, but  $\nu$  and  $\eta$  can have both a symmetric and an anti-symmetric part. We will distinguish the symmetric and anti-symmetric components with superscripts  $S$  and  $A$ . Thus  $\sigma^S$  is the ordinary conductivity tensor, while  $\sigma^A$  is the Hall conductivity tensor, etc.

One can compute the bulk entropy production rate per unit volume following [36]. The rate of change of entropy density is

$$\frac{\partial s}{\partial t} = \frac{1}{T} \left( \frac{\partial h}{\partial t} - \varphi \frac{\partial \rho}{\partial t} \right) = \frac{1}{T} \left( -\nabla \cdot \mathbf{j}^E + \varphi \nabla \cdot \mathbf{j}^N \right). \quad (2.5)$$

Computing the divergences of currents and taking into account  $\nabla \times \mathbf{E} = 0$  we get

$$\frac{\partial s}{\partial t} = \frac{1}{T} \sigma_{km} \mathbf{E}_k \mathbf{E}_m + \frac{1}{T^2} \kappa_{km} \partial_k T \partial_m T - \frac{1}{T^2} (T \nu_{km} + \eta_{mk}) \mathbf{E}_k \partial_m T - \nabla \cdot \mathbf{j}_k^S, \quad (2.6)$$

where the entropy current density is

$$\mathbf{j}_k^S = \frac{1}{T} \eta_{km} \mathbf{E}_m - \frac{1}{T} \kappa_{km} \partial_m T. \quad (2.7)$$

Note that only the symmetric parts of the conductivity tensors  $\sigma_{km}$  and  $\kappa_{km}$  enter the expression for the entropy production rate. The anti-symmetric parts (the Hall conductance  $\sigma^A$  and the thermal Hall conductance  $\kappa^A$ ) drop out. The entropy current seems to depend on the whole tensor  $\kappa$ , but in fact one can replace  $\kappa$  with  $\kappa^S$ , since this changes the current only by a divergence-free vector field. One can say that  $\sigma^A$  and  $\kappa^A$  describe non-dissipative phenomena. On the other hand, both symmetric and anti-symmetric parts of  $\nu_{km}$  and  $\eta_{km}$  contribute to dissipation. Note also that Onsager reciprocity relations ensure that the entropy production rate does not change if one switches the direction of the external magnetic field (or replaces the system with its time-reversal partner).

## 2.2 Relative and absolute transport coefficients

The total current densities are usually divided into two parts:

$$\begin{aligned} \mathbf{j}_{\text{tot}}^N &= \mathbf{j}^N + \mathbf{j}_{\text{mag}}^N, \\ \mathbf{j}_{\text{tot}}^E &= \mathbf{j}^E + \mathbf{j}_{\text{mag}}^E, \end{aligned} \quad (2.8)$$

where magnetization currents are by definition divergence-free vector fields which do not contribute to net currents across any section of the system. Therefore they

must have the form

$$\mathbf{j}_{\text{mag}}^N = \nabla \times \mathbf{M}^N, \quad (2.9)$$

$$\mathbf{j}_{\text{mag}}^E = \nabla \times \mathbf{M}^E, \quad (2.10)$$

where  $\mathbf{M}^{N,E}$  are defined by these equations and are usually called magnetization density and energy magnetization density, respectively. In the following we will use the same term magnetization for both magnetization and magnetization density which should not lead to a confusion.

The magnetization currents can be present even in an equilibrium state. The transport currents  $\mathbf{j}^{N,E}$ , on the other hand, can be present only in a non-equilibrium steady state created by slowly varying gradients of external electric potential and temperature. This follows from the Bloch theorem [60, 10] and its energy analogue of Chapter 4. This constrains the form of transport currents.

A crucial point for this thesis is that the separation of the current densities in (2.8) is ambiguous. One can always remove a curl of a vector field from  $\mathbf{j}^{N,E}$  and add it to  $\mathbf{j}_{\text{mag}}^{N,E}$  without affecting the conservation equation and the form of the transport equations (2.1,2.2). While this should have no effect on physically observable quantities it can affect the transport coefficients. Let us specialize to the 2d case and decompose all two-index tensors into symmetric and anti-symmetric parts:  $\sigma_{km} = \sigma_{km}^S + \epsilon_{km}\sigma^A$  and similarly for the tensors  $\nu$ ,  $\eta$ , and  $\kappa$ . Taking into account the requirement of gauge-invariance, the allowed redefinitions of the transport currents have the form

$$j_k^N \mapsto j_k^N + \epsilon_{km}\partial_m (\sigma_0\phi + f(T)), \quad (2.11)$$

$$j_k^E \mapsto j_k^E + \epsilon_{km}\partial_m \left( \frac{1}{2}\sigma_0\varphi^2 + f(T)\phi + g(T) \right). \quad (2.12)$$

Here  $\sigma_0$  is a constant and  $f(T)$ ,  $g(T)$  are arbitrary functions of  $T$ . Simultaneously magnetizations are redefined as follows:

$$M^N \mapsto M^N - \sigma_0\phi - f(T), \quad (2.13)$$

$$M^E \mapsto M^E - \frac{1}{2}\sigma_0\varphi^2 - f(T)\phi - g(T). \quad (2.14)$$

After the redefinition transport coefficients change:

$$\begin{aligned}
 \sigma^A &\mapsto \sigma^A - \sigma_0, \\
 \nu^A &\mapsto \nu^A - \frac{df(T)}{dT}, \\
 \eta^A &\mapsto \eta^A - f(T), \\
 \kappa^A &\mapsto \kappa^A - \frac{dg(T)}{dT}.
 \end{aligned} \tag{2.15}$$

Using such a redefinition we can always set  $\sigma^A(T)$  to vanish at  $T = 0$  and make  $\kappa^A$  and  $\eta^A$  vanish identically for any homogeneous material. Instead of setting  $\eta^A(T) = 0$ , one can choose to set  $\nu^A(T) = 0$  and use the remaining freedom to set  $\eta^A(0) = 0$ . Note also that  $\frac{d\sigma^A}{dT}$  and  $\nu^A - \frac{d\eta^A}{dT}$  are invariant under such redefinitions.

So far we have ignored the vector potential, or equivalently gauge transformations which depend on the spatial coordinates. Allowing such gauge transformations changes the analysis as follows. Transport electric current  $\mathbf{j}^E$  and transport heat current  $\mathbf{j}^E - \varphi \mathbf{j}^N$  are now required to depend on  $\varphi$  only through the electric field  $E_k = -\partial_k \varphi - \frac{\partial A_k}{\partial t}$ . The only difference this makes is that only transformations (2.11) with  $\sigma_0 = 0$  are allowed. As a result, the Hall conductivity  $\sigma^A$  is now free from ambiguities.

There is a natural way to fix ambiguities in  $M^N$  and  $M^E$  and therefore also in  $\nu^A, \eta^A$  and  $\kappa^A$  [14]. If we consider a material with a boundary, the magnetizations as well as all transport coefficients can be set to zero outside. This removes all ambiguities from transport coefficients, but obscures the fact that some transport coefficients are defined relative to vacuum, while others do not depend on any choices and can be measured in the bulk. We will call them relative and absolute transport coefficients, respectively. According to the above analysis, all symmetric transport coefficients as well as  $\sigma^A$  are absolute, while  $\nu^A, \eta^A$ , and  $\kappa^A$  are relative. The combination  $\nu^A - \frac{d\eta^A}{dT}$  is also absolute.

This distinction has consequences for the microscopic formulas that can be derived for transport coefficients (Kubo formulas). As we just explained, determination of relative transport coefficients require solution of a boundary value type problem. On the other hand, as we show in the thesis, derivatives of relative transport coefficients with respect to temperature or the parameters of the Hamiltonian involves only correlation functions of a system without boundary. The values of relative transport coefficients for any particular material can be found by integrating this differential

over the parameters and/or temperature. The ambiguity in the choice of the base point of the integral is analogous to the ambiguity of the magnetization currents and can be fixed by choosing the base point of the integral to be a trivial insulator. The Kubo formula for relative transport coefficient so defined is manifestly independent of the choice of boundary conditions at the cost of depending on the correlation functions of whole family of systems which interpolates between the system of interest and a trivial insulator. On the other hand, Kubo formulas for absolute transport coefficients depend only on the correlation function of the system at fixed temperature and values of all parameters.

As a consistency check, let us verify that physical bulk quantities depend only on absolute transport coefficients. For the time derivatives of charge and energy densities we get

$$\frac{\partial \rho^N}{\partial t} = -\nabla \cdot \mathbf{j}^N = -\sigma_{km}^S \partial_k \mathbf{E}_m - \frac{d\sigma_{km}}{dT} \mathbf{E}_m \partial_k T - v_{km}^S \partial_k \partial_m T - \frac{dv_{km}^S}{dT} \partial_k T \partial_m T, \quad (2.16)$$

$$\begin{aligned} \frac{\partial \rho^E}{\partial t} = -\nabla \cdot \mathbf{j}^E = & -\varphi \nabla \cdot \mathbf{j}^N + \sigma_{km}^S \mathbf{E}_k \mathbf{E}_m - \left( v_{km} + \frac{d\eta_{mk}}{dT} \right) \mathbf{E}_k \partial_m T \\ & - \eta_{km}^S \partial_k \mathbf{E}_m + \kappa_{km}^S \partial_k \partial_m T + \frac{d\kappa_{km}^S}{dT} \partial_k T \partial_m T, \end{aligned} \quad (2.17)$$

where the external fields are assumed to be time-independent and thus  $\nabla \times \mathbf{E} = 0$ . As expected, these time derivatives are unaffected by transformations (2.15).

Since only absolute transport coefficients enter the expressions for the divergences of currents, measuring net currents through closed curves (or surfaces, if we are discussing a 3d material) does not allow to determine relative transport coefficients. This applies even to infinite curves with a boundary at infinity, provided  $\varphi$  and  $T$  tend to fixed values at infinity. The latter condition must be imposed to eliminate the contribution of magnetization currents. For example, if we compute the electric current  $I_x^N$  through a vertical line  $x = 0$ , then the contribution of  $v^A$  drops out because

$$\int_{-\infty}^{\infty} dy v^A \partial_y T dy = 0. \quad (2.18)$$

The above considerations apply to a homogeneous material whose transport coefficients are constants. If one considers a heterogeneous material, such as an interface between two homogeneous ones, then the expressions for net currents will involve



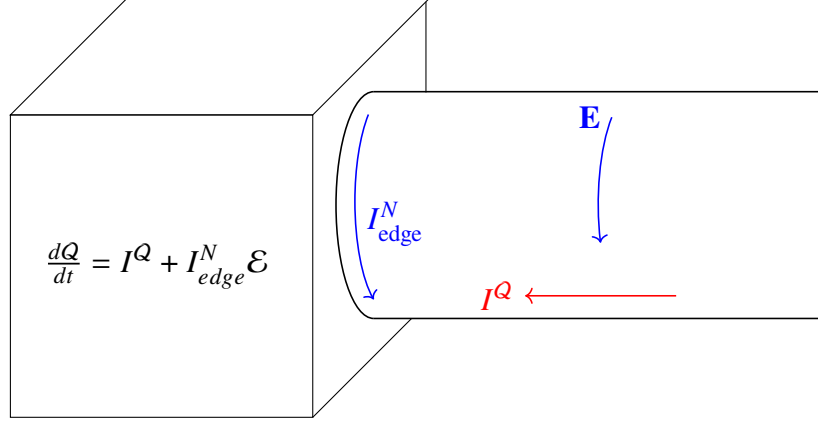


Figure 2.1: Insertion of a flux  $\Phi$  into a cylinder creates electric field around it. If  $\eta_{xy} \neq 0$ , this electric field  $\mathbf{E}$  drives a heat current  $I^Q$  along the axis of the cylinder. The jump of the magnetization gives rise to an edge current  $I^N_{\text{edge}}$ . Work done on the edge current by the electric field contributes to the net heat  $Q$  transferred to the heat bath.

differences between relative transport coefficients. For example, consider a sample such that  $v^A$  interpolates between  $v_1^A$  for  $y \ll 0$  and  $v_2^A$  for  $y \gg 0$ . Suppose that the temperature is a function of  $y$  only which is equal to  $T_b$  throughout the interface region and approaches  $T_\infty$  at  $y \rightarrow \pm\infty$ . Then the  $v^A$ -dependent contribution to the net electric current in the  $x$  direction is

$$- \int_{-\infty}^{\infty} dy v^A \partial_y T = (T_b - T_\infty)(v_2^A - v_1^A). \quad (2.19)$$

Similarly, the contribution of  $\kappa^A$  to the net heat current is  $= (T_b - T_\infty)(\kappa_2^A - \kappa_1^A)$ . By creating an electric potential  $\varphi$  which is equal to  $\varphi_b$  in the interface region and approaches  $\varphi_\infty$  at  $y \rightarrow \pm\infty$ , one can also measure  $\sigma_2^A - \sigma_1^A$  and  $\eta_2^A - \eta_1^A$ .

In the case of the electric Hall conductivity one can do better by utilizing a time-dependent vector potential rather than a scalar potential and working in a cylinder geometry or a torus geometry. Then in principle one can determine  $\sigma^A$  for a single material by measuring the net flow of electric charge across a section of a cylinder or a torus as one inserts a unit of magnetic flux through this section. This does not work for  $\eta^A$  because the physical quantity that needs to be measured is the net amount of heat transferred to the heat bath as one inserts a unit of magnetic flux (see Fig. 2.1). In this case heat transport will receive additional contribution from the work of the electromotive force  $\mathcal{E}$  on the net electric edge currents  $I^N_{\text{edge}}$ . The edge currents are proportional to the jump in the magnetization along the boundary and they make  $\eta$  relative even in cylinder geometry.

## Chapter 3

### LATTICE SYSTEMS

#### 3.1 Introduction

In this thesis we will work mostly with lattice system with finite range interaction. The precise definitions and constructions will be the main topic of this short chapter. While most of it is straightforward, some of the operators such as current and magnetization become functions of several lattice sites. A natural mathematical language to deal with it is explained in the Appendix A. However, we will avoid using it whenever possible in order to make the presentation more accessible.

#### 3.2 Electric currents on a lattice

A lattice system in  $d$ -dimensions has a Hilbert space  $V = \otimes_{p \in \Lambda} V_p$ , where  $\Lambda$  (“the lattice”) is a uniformly discrete subset of  $\mathbb{R}^d$  (that is, there is a minimal distance  $D > 0$  between all points), and all  $V_p$  are finite-dimensional. An observable is localized at a point  $p \in \Lambda$  if it has the form  $A \otimes 1_{\Lambda \setminus p}$  for some  $A : V_p \rightarrow V_p$ . An observable is localized on a subset  $\Lambda' \subset \Lambda$  if it commutes with all observables localized at any  $p \notin \Lambda'$ . A local observable  $A$  is an observable localized on a finite set  $\Lambda' \subset \Lambda$ , which will be called the support of  $A$ .

Hamiltonian of a lattice system has the form

$$H = \sum_{p \in \Lambda} H_p, \quad (3.1)$$

where the operators  $H_p : V_p \rightarrow V_p$  are Hermitian and local. We will assume that the Hamiltonian has a finite range  $R$ , which means that each  $H_p$  is a local observable supported in a ball of radius  $R$  centered at  $p$ . This implies that  $[H_p, H_q] = 0$  whenever  $|p - q| > 2R$ . We will also assume that the operators  $H_p$  are uniformly bounded, i.e. there exists  $C > 0$  such that  $\|H_p\| < C$  for all  $p \in \Lambda$ .

To define electric currents, we assume that the system has an on-site  $U(1)$  symmetry. Thus we are given a  $U(1)$  action on each  $V_p$ , with the generator  $Q_p$  (a Hermitian operator on  $V_p$  with integral eigenvalues). The total  $U(1)$  charge is  $Q_{tot} = \sum_{p \in \Lambda} Q_p$ . Further, we assume that  $[Q_{tot}, H_p] = 0$  for any  $p \in \Lambda$ . Since the time derivative of

$Q_q$  is

$$\frac{dQ_q}{dt} = i \sum_{p \in \Lambda} [H_p, Q_q], \quad (3.2)$$

it appears natural to define the  $U(1)$  current from  $q$  to  $p$  by  $J_{pq}^N = -i[H_p, Q_q]$ . However, this does not satisfy a physically desirable property  $J_{qp}^N = -J_{pq}^N$ . Instead we define

$$J_{pq}^N = i[H_q, Q_p] - i[H_p, Q_q]. \quad (3.3)$$

The lattice current thus defined satisfies  $J_{qp}^N = -J_{pq}^N$  as well as

$$\frac{dQ_q}{dt} = - \sum_{p \in \Lambda} J_{pq}^N. \quad (3.4)$$

Each of the operators  $J_{pq}^N$  is local in the above sense (it commutes with operators whose supports are sufficiently far from both  $p$  and  $q$ ). But the collection of all  $J_{pq}^N$  is also local in a different sense:  $J_{pq}^N$  vanishes when  $|p - q|$  is sufficiently large (specifically, greater than  $R$ ). Objects depending on two or more points of  $\Lambda$  which vanish when the any of the two points are sufficiently far will be called finite-range. So one can also say that the current  $J_{pq}^N$  is finite-range. The property of being finite-range makes sense not just for operators, but also for c-number quantities depending on several points of  $\Lambda$ .

While the above definition of the electric current seems natural, it is not completely unique. Let  $U_{pqr}$  be any function of three points which takes values in local operators, is skew-symmetric in all three variables, and is finite-range. If we define

$$J'_{pq}{}^N = J_{pq}^N + \sum_r U_{pqr}, \quad (3.5)$$

then it is easy to see that  $J'_{pq}{}^N$  satisfies the same requirements as  $J_{pq}^N$  and therefore is also a physically acceptable current. This is a lattice counterpart of the continuum statement that only  $\nabla \cdot \mathbf{J}^N$  has a physical significance, and thus one can replace  $\mathbf{J}^N \mapsto \mathbf{J}^N + \nabla \times \mathbf{u}$ , where  $\mathbf{u}$  is arbitrary, without affecting any physical predictions. In the lattice case, it is not obvious that the only ambiguity in the definition of the current is (3.5). This is shown in Appendix A under some natural assumptions on  $\Lambda$ .

Suppose  $\Lambda$  is decomposed into a disjoint union of two sets,  $\Lambda = A \cup B$ ,  $A \cap B = \emptyset$ . The current from  $B$  to  $A$  is defined as

$$J^N(A, B) = \sum_{p \in A} \sum_{q \in B} J_{pq}^N. \quad (3.6)$$

It is not difficult to check that  $J^N(A, B)$  does not change if one replaces  $J_{pq}^N$  with  $J'_{pq}$  defined in (3.5). This is because  $J^N(A, B)$  is physical: it is equal to minus the rate of change of the electric charge in region  $B$ . This is expressed by the equation

$$\frac{dQ(B)}{dt} = -J^N(A, B). \quad (3.7)$$

Here  $Q(B) = \sum_{p \in B} Q_p$ .

More generally, given a skew-symmetric function  $\eta(p, q) : \Lambda \times \Lambda \rightarrow \mathbb{R}$ , one can define

$$J^N(\eta) = \frac{1}{2} \sum_{p, q} \eta(p, q) J_{pq}^N. \quad (3.8)$$

In general, this expression is not physical: it changes under the redefinition (3.5). However, if  $\eta(p, q)$  satisfies

$$\eta(p, q) + \eta(q, r) + \eta(r, p) = 0, \quad \forall p, q, r \in \Lambda, \quad (3.9)$$

then one can check that  $J^N(\eta)$  is invariant under substitutions (3.5) and thus is physical. Such checks become much easier if one uses the mathematical machinery explained in Appendix A. In the case  $\eta(p, q) = \chi_B(q) - \chi_B(p)$ , where  $\chi_B(p) = 1$  for  $p \in B$  and  $\chi_B(p) = 0$  otherwise,  $J^N(\eta)$  reduces to  $J^N(A, B)$ .

### 3.3 Energy currents and energy magnetization on a lattice

For a quantum system on a lattice  $\Lambda \subset \mathbb{R}^d$ , the energy current from site  $q$  to site  $p$  is an operator  $J_{pq}^E$  which satisfies

$$\frac{dH_q}{dt} = - \sum_{p \in \Lambda} J_{pq}^E. \quad (3.10)$$

An obvious solution is [40, 1]

$$J_{pq}^E = -i[H_p, H_q]. \quad (3.11)$$

Since  $[H_p, H_q] = 0$  whenever  $|p - q| > 2R$ ,  $J_{pq}^E$  is nonzero only when  $p, q$  are nearby. The energy current from  $B$  to  $A = \Lambda \setminus B$  is defined to be

$$J^E(A, B) = \sum_{p \in A} \sum_{q \in B} J_{pq}^E, \quad (3.12)$$

where  $\chi_B$  is the same as before.

As in the case of the electric current, the expression for  $J_{pq}^E$  is not unique. One can always make a replacement

$$J_{pq}^E \mapsto J_{pq}^E + \sum_r U_{pqr}^E, \quad (3.13)$$

where the operator  $U_{pqr}^E$  is skew-symmetric under the exchange of the points  $p, q, r$  and vanishes if any two of them are farther than some fixed distance. The modified energy current is physically equivalent to  $J_{pq}^E$ . Physical quantities, such as  $J^E(A, B)$ , are not affected by such modifications.

### 3.4 Magnetization

The equilibrium expectation value of the currents satisfy

$$\sum_{p \in \Lambda} \langle J_{pq}^{N,E} \rangle = 0. \quad (3.14)$$

This equation is a lattice analog of the continuum equation

$$\nabla \cdot \langle \mathbf{J}^{N,E}(\mathbf{r}) \rangle = 0. \quad (3.15)$$

In the continuum the general solution to this equation

$$\langle J_k^{N,E}(\mathbf{r}) \rangle = -\epsilon_{kj} \partial_j M^{N,E}(\mathbf{r}) \quad (3.16)$$

defines the magnetization  $M^N$  and energy magnetization  $M^E$ . Analogously, on a lattice the solution of equation (3.14) is

$$\langle J_{qr}^{N,E} \rangle = \sum_{p \in \Lambda} M_{pqr}^{N,E}, \quad (3.17)$$

where  $M_{pqr}^{N,E}$  are skew-symmetric functions of the lattice points  $p, q, r \in \Lambda$ . These are lattice analogs of the magnetization and the energy magnetisation. Physically, in continuum case  $M^{N,E}(r)$  represent the circulating currents of the system in equilibrium. Similarly,  $M_{pqr}^{N,E}$  physically can be thought as quantity which measures the circulating current around a triangle formed by  $p, q, r$ .

Unfortunately,  $M_{pqr}^{N,E}$  is not unique: one can always redefine

$$M_{pqr}^{N,E} \mapsto M_{pqr}^{N,E} + \sum_{s \in \Lambda} N_{pqrs}, \quad (3.18)$$

where  $N_{pqrs}$  is skewsymmetric function of its subscripts which decays whenever any two of them are far apart. This corresponds to ambiguity in splitting of the circulating currents to contributions of magnetization from the different triangles and it is absent in continuum case.

There is an additional ambiguity corresponding to existence of solutions to the equation  $\sum_{r \in \Lambda} M_{pqr}^{N,E} = 0$  which are not of the form  $\sum_{s \in \Lambda} N_{pqrs}$ . It corresponds to

an ambiguity of addition of a constant to the magnetization in continuum case. A standard method to deal with the later is to consider a system with a boundary and fix the magnetization to be zero outside of the system. In this thesis, we want to think about all transport coefficients as manifestly bulk quantities and avoid dealing with boundaries. While magnetization itself suffers from ambiguities and depends non-locally on the boundary conditions, the variation of magnetization with respect to parameters of the Hamiltonian is local. Indeed, consider the variation of the equation (3.17) with respect to a parameter  $\lambda^\ell$  of the Hamiltonian

$$\frac{\partial}{\partial \lambda^\ell} \langle J_{pq}^{N,E} \rangle = \sum_{r \in \Lambda} \mu_{pqr,\ell}^{N,E}, \quad (3.19)$$

where  $\mu_{pqr,\ell}^{N,E} = \frac{\partial M_{pqr}^{N,E}}{\partial \lambda^\ell}$  and is given by [1]

$$\mu_{pqr,\ell}^{N,E} = -\beta \langle \langle \frac{\partial H_p}{\partial \lambda^\ell}; J_{qr}^{N,E} \rangle \rangle - \beta \langle \langle \frac{\partial H_r}{\partial \lambda^\ell}; J_{pq}^{N,E} \rangle \rangle - \beta \langle \langle \frac{\partial H_q}{\partial \lambda^\ell}; J_{rp}^{N,E} \rangle \rangle, \quad (3.20)$$

where  $\langle \langle A; B \rangle \rangle$  denotes the Kubo canonical pairing [57]. Using the properties of the Kubo pairing (see Appendix A), one can easily verify the identity (3.19). In the following we will combine derivatives of magnetizations with respect to different parameters into 1-forms on the parameter space  $\mu_{pqr}^{N,E} = \sum_\ell \mu_{pqr,\ell}^{N,E} d\lambda^\ell$ .

### 3.5 Equilibrium conditions and driving forces

In the following we will need to study response of the system to gradients of temperature. Follow Luttinger [39], we will find it by investigating the behavior of the system coupled to external potentials

$$H_p^{\psi,\phi} = (1 + \psi(p))(H_p + \phi(p)Q_p), \quad (3.21)$$

where  $\phi(p)$  is external electric potential and  $\psi(p)$  can be thought of as gravitational potential. The potentials are assumed to infinitesimally small slowly-varying functions of  $p$  which vanish at infinity. After coupling to external potentials the system will eventually relax into a state with the density matrix

$$\rho \sim \exp\left(-\frac{H^{\psi,\phi} - \mu_0 Q_{\text{tot}}}{T_0}\right), \quad (3.22)$$

where  $T_0$  and  $\mu_0$  are the temperature and local chemical potential of the system at infinity. On the other hand, on physical grounds we expect local observables supported in some small but macroscopic region around site  $p$  to be described by a

thermal density matrix

$$\rho(p) \sim \left( -\frac{H - \mu(p)Q_{\text{tot}}}{T(p)} \right), \quad (3.23)$$

where the local temperature  $T(p)$  and chemical potential  $\mu(p)$  are slowly varying functions of  $p$ . The equilibrium conditions can be found to be [39, 14, 47]

$$(1 + \psi(p))(\mu(p) + \phi(p)) = \mu_0, \quad (3.24)$$

$$(1 + \psi(p))T(p) = T_0. \quad (3.25)$$

These relations together with the absence of transport currents in equilibrium can be used to derive Einstein relations between transport coefficients [39]. The latter also leads to transport currents being proportional to the gradients of the left hand sides of eqs. (3.24) and (3.25). The fact that the driving forces depend only on specific combinations of  $\psi, \phi, T, \mu$  will be used to relate the response to variations of the thermodynamic parameter  $T$  to the response to variations of the external field  $\psi$ .

Note that, in section 2.2 for simplicity we assumed that chemical potential is constant. We will continue doing so in the rest of the thesis and we will assume  $\mu(p)$  to be constant. Generalization to a more general case of non-constant local chemical potential is straightforward, but clumsy due to ambiguities in the separation of electrochemical potential  $\mu + \phi$  into two parts.

## ENERGY BLOCH THEOREM

**4.1 Introduction**

An old argument of F. Bloch explained in detail by D. Bohm [10] shows that in an equilibrium state of a quasi-1d system of non-relativistic particles the net particle number current is zero. By an equilibrium state we mean either a ground state or a Gibbs state. A quasi-1d system is a system which is infinitely-extended in only one direction, but can have an arbitrary number of finite directions. Recently H. Watanabe extended Bloch's argument to lattice systems [59]. This result appears very general and likely to apply to currents of other conserved quantities. For example, a non-vanishing energy current in an equilibrium state would conflict with Fourier's law. However, the Bloch-Bohm argument does not immediately apply to the energy current, since it relies in an essential way on the quantization of the particle number which does not have an analog in the case of energy.

There are also examples of systems where equilibrium currents do not vanish. In a 1+1d Conformal Field Theory with unequal central charges  $c_L$  and  $c_R$  for left-movers and right-movers the energy current at temperature  $T$  is nonzero and equal to [9, 2]

$$\langle j_E \rangle = \frac{\pi T^2}{12} (c_R - c_L). \quad (4.1)$$

In a 1+1d CFT with a  $U(1)$  current algebra at levels  $k_L$  and  $k_R$  the net  $U(1)$  current at a chemical potential  $\mu$  and arbitrary temperature is [7]

$$\langle j_Q \rangle = \frac{\mu}{2\pi} (k_R - k_L). \quad (4.2)$$

This raises the question about the precise conditions under which equilibrium-state currents vanish. Note that in both examples symmetry anomalies (i.e. obstructions to gauging a symmetry) are present:  $k_R - k_L$  measures the anomaly of the  $U(1)$  symmetry, while  $c_R - c_L$  measures the anomaly of the diffeomorphism symmetry. In the case of the  $U(1)$  symmetry, this implies that a lattice system with an on-site  $U(1)$  symmetry or a system of non-relativistic particles cannot flow to a CFT with a non-zero  $k_R - k_L$ . Indeed, if a system can be consistently coupled to a  $U(1)$  gauge field, the same must hold for its long-wavelength limit, ruling out a low-energy theory with a nontrivial  $U(1)$  anomaly. This argument does not work for energy currents since



most microscopic Hamiltonians in condensed matter physics cannot be coupled to a gravity in any natural way. To linear order, a natural coupling to gravity requires a conserved symmetric stress-energy tensor. In relativistic field theory, such a tensor is present because the system is invariant under continuous translations in space and time and Lorentz transformations, but most microscopic models in condensed matter physics are invariant only under continuous time translations and discrete spatial translations. Nevertheless, it is widely believed that a system of particles with short-range interactions or a lattice system with short-range interactions cannot flow to a CFT with a non-zero  $c_R - c_L$ .

In this chapter, we prove the absence of equilibrium-state energy currents for quasi-1d lattice systems with finite-range interactions as well as for systems of non-relativistic particles with finite-range potential interactions. We make only very modest assumptions, which roughly amount to the absence of phase transitions in quasi-1d systems at positive temperatures.<sup>1</sup> Our arguments apply equally to bosons and fermions. An immediate corollary is that lattice systems or systems of particles with finite-range interactions cannot flow to a 1+1d CFT with a non-zero  $c_R - c_L$ . We also give an alternative derivation of the vanishing of the  $U(1)$  current in certain continuous systems and explain how 1+1d chiral CFTs perturbed by a chemical potential manage to evade this conclusion.

## 4.2 Assumptions

We are interested in Gibbs states at temperature  $T = 1/\beta$ . We assume that the state is clustering, i.e. correlators of local operators  $\langle AB \rangle - \langle A \rangle \langle B \rangle$  approach zero as  $L_{AB} = \text{dist}(\text{supp}(A), \text{supp}(B)) \rightarrow \infty$ . We also assume that the Kubo pairing (see Appendix B.1) of any two local operators  $A$  and  $B$  decays at least as  $L_{AB}^{-(1+\epsilon)}$  for some  $\epsilon > 0$ . The Kubo pairing arises when studying the response to an infinitesimal perturbation  $H \rightarrow H + \lambda B$  [57]. Then the change in the equilibrium expectation value of  $A$  is

$$\Delta \langle A \rangle = \langle \Delta A \rangle - \lambda \beta \langle \langle A; B \rangle \rangle. \quad (4.3)$$

Here the first term accounts for the possible dependence of the observable  $A$  on  $\lambda$ , while the second term is due to the change of the equilibrium state. Thus, up to a factor  $\beta$ , the Kubo pairing of local operators is the same as a generalized susceptibility for local perturbations. The assumption that the Kubo pairing decays faster than  $1/L_{AB}$  ensures that perturbations of the form  $\sum_x B_x$  where  $B_x$  is finite-range,

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<sup>1</sup>Many-body localization transitions are not accompanied by divergent susceptibilities and are not regarded as phase transitions for our purposes.

and  $\|B_x\|$  is uniformly bounded, lead to a well-defined change in the expectation values of all local observables.

These decay assumptions are likely true for any positive temperature. Correlators of local observables decay exponentially away from phase transitions. One also expects the generalized susceptibilities for uniform perturbations to be finite away from phase transitions, although we are not aware of a proof. Since we are considering 1d systems, we do not expect any phase transitions at positive temperatures. Zero-temperature states can then be treated as  $T \rightarrow 0$  limits of Gibbs states.

### 4.3 Energy currents in lattice systems

In this section we will consider 1d lattice system. Any  $a \in \mathbb{R} \setminus \Lambda$  divides  $\Lambda$  into two parts:  $\Lambda = \Lambda_+(a) \cup \Lambda_-(a)$ , where  $\Lambda_+(a)$  (resp.  $\Lambda_-(a)$ ) is defined by the condition  $p > a$  (resp.  $p < a$ ). The net current from  $\Lambda_-(a)$  to  $\Lambda_+(a)$  is

$$J^E(a) = \sum_{p>a, q<a} J_{pq}^E. \quad (4.4)$$

For any  $a, b \notin \Lambda$  and  $b > a$  we have

$$J^E(b) - J^E(a) = - \sum_{a<p<b} i[H, H_p]. \quad (4.5)$$

Since  $\langle [H, A] \rangle = 0$  for any local observable  $A$ , we get that  $\langle J^E(a) \rangle$  is independent of  $a$ .

Consider an infinitesimal variation of the Hamiltonian  $\Delta H$  such that  $\Delta H_p = 0$  for sufficiently large positive  $p$ . Then

$$\Delta \langle J^E(a) \rangle = \langle \Delta J^E(a) \rangle - \beta \langle \langle J^E(a); \Delta H \rangle \rangle. \quad (4.6)$$

Pick an  $R > 0$  such that  $a + R \notin \Lambda$ . Using the equation (4.5) and the property of the Kubo pairing

$$\langle \langle [H, A]; B \rangle \rangle = \frac{1}{\beta} \langle [B, A] \rangle, \quad (4.7)$$

the second term in (4.6) can be written as

$$-\beta \langle \langle J^E(a); \Delta H \rangle \rangle = -\beta \langle \langle J^E(a+R); \Delta H \rangle \rangle - \sum_{a<p<a+R} \langle i[\Delta H, H_p] \rangle. \quad (4.8)$$

On the other hand, varying eq. (4.5) we can re-write the first term in eq. (4.6) as

$$\langle \Delta J^E(a) \rangle = \langle \Delta J^E(a+R) \rangle + \sum_{a<p<a+R} \langle i[\Delta H, H_p] \rangle. \quad (4.9)$$

Hence

$$\Delta\langle J^E(a) \rangle = \langle \Delta J^E(a+R) \rangle - \beta \langle \langle J^E(a+R); \Delta H \rangle \rangle. \quad (4.10)$$

Now let us take the limit  $R \rightarrow +\infty$ . The first term is zero for sufficiently large  $R$  since  $\Delta H_p = 0$  for sufficiently large positive  $p$ , and both  $H_p$  and  $\Delta H_p$  are assumed to have finite support, for all  $p \in \Lambda$ . Using the assumed decay of the Kubo pairing, the second term can be estimated to be no larger than  $C/R^\epsilon$  for some  $C > 0$  and thus goes to zero for  $R \rightarrow +\infty$ . Hence  $\Delta\langle J^E(a) \rangle = 0$ .

A similar argument shows that  $\Delta\langle J^E(a) \rangle = 0$  for variations of  $H$  which vanish for sufficiently large negative  $p$ . Now, any deformation of the Hamiltonian can be decomposed into a sum of two deformations: one vanishing for  $p \gg 0$  and one vanishing for  $p \ll 0$ . Linearity of response to infinitesimal deformation implies that variation of the current expectation value is the sum of variations corresponding to the two deformations. Since each of them vanishes, we conclude that  $\Delta\langle J^E(a) \rangle = 0$  for arbitrary variations of  $H$  within the allowed class.

Now we consider the temperature dependence of the net energy current. Re-scaling simultaneously the temperature  $T \mapsto \lambda T$  and the Hamiltonian  $H \mapsto \lambda H$  leaves the state unchanged, thus for any observable  $A$  which does not depend explicitly on  $T$  or  $H$  we have

$$\left( T \frac{d}{dT} + \lambda \frac{d}{d\lambda} \right) \langle A \rangle_\lambda = 0, \quad (4.11)$$

where  $\langle A \rangle_\lambda$  denotes the average over a Gibbs state with a Hamiltonian  $\lambda H$  and temperature  $T$ . More generally, if  $A$  is multiplied by  $\lambda^p$  under  $H \mapsto \lambda H$ , then

$$\left( T \frac{d}{dT} + \lambda \frac{d}{d\lambda} \right) \left\langle \frac{A}{T^p} \right\rangle_\lambda = 0. \quad (4.12)$$

The energy current  $J^E$  has  $p = 2$ . On the other hand, since re-scaling the Hamiltonian by a constant factor is an allowed deformation, we have

$$\frac{d}{d\lambda} \langle J^E(a) \rangle_\lambda = 0. \quad (4.13)$$

Therefore

$$\langle J^E(a) \rangle = CT^2, \quad (4.14)$$

where  $C$  is some constant which is unchanged under all allowed variations of the Hamiltonian.

Finally, let us assume that our state can be continuously connected to the maximally mixed state  $T = \infty$ . Then the above temperature dependence is incompatible with the fact that the operators  $J^E(a)$  are bounded, unless  $C = 0$ . Thus the net energy current vanishes.

#### 4.4 Energy currents in particle systems

There is a well-known difficulty with defining a local energy current in systems of particles with a potential interaction. It is related to the non-locality of the potential interaction. One way of dealing with this difficulty involves a formal expansion of the potential  $V(\mathbf{x} - \mathbf{y})$  into an infinite sum of zero-range potentials (the Dirac delta-function  $\delta(\mathbf{x} - \mathbf{y})$  and its derivatives) [29]. If desired, one can smear the delta-function into a Gaussian, but the infinite sum remains [25]. Such an energy current is local only up to exponentially small “tails.” For 1d or quasi-1d systems with a finite-range potential there is an alternative approach which avoids both infinite series and “tails”: one can define the energy density and the energy current which are local only in one dimension. This is sufficient for our purposes. To simplify notation, we will only discuss the strictly 1d case, but the modifications to the quasi-1d case are minor.

The second-quantized Hamiltonian has the form

$$H = \int dx k(x) + \int dx \rho(x)W(x) + \frac{1}{2} \int dx dy \rho(x)\rho(y)V(x, y), \quad (4.15)$$

where  $k(x)$  is the usual kinetic energy density operator,

$$k(x) = \frac{1}{2m} \partial_x \psi^\dagger(x) \partial_x \psi(x), \quad (4.16)$$

$\rho(x) = \psi^\dagger(x)\psi(x)$  is the particle density operator,  $W(x)$  is the external potential, and  $V(x, y) = V(y, x)$  is the pairwise interaction potential. We define the potential energy density as

$$\pi(x) = W(x)\rho(x) + \frac{1}{2}\rho(x) \int V(x, y)\rho(y)dy, \quad (4.17)$$

and the total energy density as  $h(x) = k(x) + \pi(x)$ . To find the energy current  $j^E(x)$ , we need to solve the conservation equation

$$i[H, h(x)] = -\partial_x j^E(x). \quad (4.18)$$

When computing the commutator on the left, the following identities are useful:

$$[\rho(x), \rho(y)] = 0, \quad (4.19)$$

$$[\rho(x), j^N(y)] = \frac{i}{m} \rho(y) \partial_y \delta(x - y), \quad (4.20)$$

$$[k(x), \rho(y)] = -ij^N(x) \partial_x \delta(x - y), \quad (4.21)$$

where  $j^N = \frac{-i}{2m}(\psi^\dagger \partial_x \psi - (\partial_x \psi^\dagger) \psi)$  is the particle-number current. A solution has the form  $j^E(x) = j_k^E(x) + j_\pi^E(x)$ , where

$$j_k^E(x) = \frac{-i}{4m^2} \left( \partial_x \psi^\dagger(x) \partial_x^2 \psi(x) - \partial_x^2 \psi^\dagger(x) \partial_x \psi(x) \right), \quad (4.22)$$

and

$$\begin{aligned} j_\pi^E(x) = & j^N(x)W(x) + j^N(x) \int V(x, y)\rho(y)dy + \frac{i}{2m}\rho(x) (\partial_x V(x, y))|_{y=x+} \\ & + \frac{1}{2} \int_{z < x < y} \left( \partial_y j^N(y)\rho(z) - \partial_z j^N(z)\rho(y) \right) V(y, z)dydz. \end{aligned} \quad (4.23)$$

One can check that the energy current is Hermitian. Note that if the potential  $V(x, y)$  has range  $R$ , i.e. vanishes whenever  $|x - y| \geq R$ , all terms in  $j_\pi^E(x)$  are quasi-local: they commute with all local observables whose support is farther from  $x$  than  $R$ . It is important for what follows that a quasi-local energy current can be constructed for an arbitrary symmetric finite-range potential  $V(x, y)$ .

For any bounded function  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  we can consider a modified potential  $V_\phi(x, y) = \phi(x)\phi(y)V(x, y)$ , which is also symmetric and finite-range. If  $\phi(x)$  is small in some region of space, particle interactions are suppressed there. We claim that the energy current  $\langle j^E(a) \rangle$  does not change as one varies  $\phi$ , provided the Kubo pairings of local operators decay at least as  $1/L^{1+\epsilon}$ . Indeed, consider an arbitrary infinitesimal variation of  $\phi(x)$ . It can be decomposed into a sum of two contributions: one vanishing for  $x \ll 0$  and another one vanishing for  $x \gg 0$ . It is sufficient to show that the energy current is unchanged under the two separately. Let us consider a variation of  $\phi$  which vanishes for  $x \gg 0$ . As in the previous section, using the conservation equation and its variation we find:

$$\Delta \langle j^E(a) \rangle = \langle \Delta j^E(a + R) \rangle - \beta \langle \langle j^E(a + R); \Delta H \rangle \rangle, \quad (4.24)$$

where  $R$  is arbitrary. Taking the limit  $R \rightarrow +\infty$ , we conclude that  $\langle j^E(a) \rangle$  is unchanged under arbitrary infinitesimal variations of  $\phi$  which vanish for  $x \gg 0$ . An identical argument shows that  $\langle j^E(a) \rangle$  is unchanged under arbitrary infinitesimal variations of  $\phi$  which vanish for  $x \ll 0$ . Linearity of response then implies that  $\langle j^E(a) \rangle$  is unchanged under arbitrary bounded variations of  $\phi$ .

Now let us take a constant  $\phi = 1$  and decrease it to 0 (while keeping the temperature fixed). Unless one passes through a phase transition with divergent susceptibilities,  $\langle j^E(a) \rangle$  is unchanged. Since it vanishes when  $V(x, y) = 0$ , it must also be zero for the initial potential  $V(x, y)$ . It is widely believed that finite-temperature phase transitions

cannot occur in systems of 1d particles with finite-range potential interactions. Assuming this, we proved that the equilibrium energy current vanishes for all  $T > 0$  and therefore also for  $T = 0$ .

#### 4.5 $U(1)$ currents in continuous systems

In this section we discuss why Bloch's result does not apply to some continuous systems, like chiral 1+1d CFTs, but applies to others, like non-relativistic particles.

Consider a continuous system in  $n$  spatial dimensions with a Hamiltonian  $H = \int h(\mathbf{x})d^n x$ . We assume time-translation symmetry but not necessarily spatial translation symmetry. The space is assumed to have the form  $\mathbb{R} \times W$ , where  $W$  is compact. The energy density  $h(\mathbf{x})$  is assumed to be quasi-local, in the sense that there exists a  $R > 0$  such that for any strictly local  $A(\mathbf{x})$  (i.e. a function of fields and their derivatives at a point  $\mathbf{x}$ ) we have  $[h(\mathbf{y}), A(\mathbf{x})] = 0$  whenever  $|\mathbf{x} - \mathbf{y}| > R$ . Both local field theories (whether Lorentz-invariant or not) and non-relativistic particles with finite-range interactions obey this.

We assume that the  $U(1)$  generator  $Q$  is  $Q = \int \rho(\mathbf{x})d^n x$  where  $\rho$  is a local operator, and that there exists a quasi-local  $U(1)$  current  $\mathbf{j}^N(\mathbf{x})$  satisfying

$$i[H, \rho(\mathbf{x})] = -\nabla \cdot \mathbf{j}^N(\mathbf{x}). \quad (4.25)$$

This condition is satisfied for local field theories as well as for systems of non-relativistic particles.

Suppose we can promote  $U(1)$  symmetry to a local  $U(1)$  symmetry with generators

$$Q_f = \int \rho(\mathbf{x})f(\mathbf{x})d^n x, \quad (4.26)$$

where  $f(\mathbf{x})$  is an arbitrary function. Requiring  $[Q_f, Q_g] = 0$  for all  $f, g$  we get

$$[\rho(\mathbf{x}), \rho(\mathbf{y})] = 0. \quad (4.27)$$

Using (4.27) we can deduce that the net  $U(1)$  current, if present, cannot depend on the chemical potential  $\mu$ . Indeed, consider an infinitesimal deformation of the Hamiltonian of the form

$$\Delta H = \int f(\mathbf{x})\rho(\mathbf{x})d^n x. \quad (4.28)$$

The condition (4.27) implies that the current is undeformed,  $\Delta \mathbf{j}^N = 0$ , regardless of  $f(\mathbf{x})$ . Following the same procedure as above, we find the change in the expectation value of  $J^N(a) = \int_W j_1^N(a, w)d^{n-1}w$ :

$$\Delta \langle J^N(a) \rangle = -\beta \langle \langle J^N(a+R); \int f(\mathbf{y})\rho(\mathbf{y})d^n y \rangle \rangle, \quad (4.29)$$

where  $R$  is arbitrary. Writing a general bounded  $f(\mathbf{x})$  as a sum of two functions vanishing for  $x \gg 0$  and  $x \ll 0$  we argue as before that  $\langle J^N(a) \rangle = 0$ . Then, taking  $f$  to be constant, we deduce that  $\langle J^N(a) \rangle$  is independent of the chemical potential, provided we stay away from phase transitions. For non-relativistic particles, we can deform  $\mu$  to  $-\infty$  and get Bloch's result.

In 1+1d CFTs with a non-zero  $k_R - k_L$  instead of (4.27) one has  $[\rho(x), \rho(y)] = -ic\delta'(x - y)$  where  $c = (k_R - k_L)/2\pi$ . Such  $c$ -number terms in the commutators are known as Schwinger terms. Since the deformation (4.28) no longer commutes with  $\rho(x)$ , the current now depends on  $f$ . One finds  $j^N(x, f) = j^N(x) + cf(x) \cdot 1$ . Going through the same argument as above, one finds that  $\langle j^N(x, f) \rangle$  is independent of  $f$ . Setting  $f(x) = -\mu$ , we seem to find that the equilibrium current vanishes at arbitrary  $\mu$ , in contradiction with (4.2). However, the current which appears in (4.2) is not  $j^N(x, f)$  for  $f(x) = -\mu$ , but the undeformed current  $j^N(x)$ . For a constant  $f(x)$ , the conservation equation can be satisfied without changing the current thanks to  $[Q, \rho(x)] = 0$ , and this is the standard choice in CFT. Taking into account the relation between  $j^N(x, f)$  and  $j^N(x)$ , we indeed find (4.2).

The discrepancy between  $j^N(x, f)$  and  $j^N(x)$  is a manifestation of  $U(1)$  anomaly. One can think of the deformation (4.28) as coupling the theory to an external electric potential  $\varphi = f(x)$ . The current  $j^N(x, f)$  depends on  $f(x)$  locally, but it is not invariant under the transformation  $f(x) \mapsto f(x) + f_0$ , which is a particular gauge transformation. To patch this up one can define a current  $\tilde{j}^N(x, f) = j^N(x, f) - cf(a) \cdot 1$ , where  $a$  is an arbitrary point. This current is gauge invariant and reduces to  $j^N(x)$  when  $f(x) = -\mu$ . However,  $\tilde{j}^N(x, f)$  is non-local. The conflict between gauge-invariance and locality is a manifestation of  $U(1)$  anomaly.

## 4.6 Applications

We showed that the equilibrium energy current vanishes both for infinitely-extended 1d lattice systems with finite-range interactions and quasi-1d systems of non-relativistic particles with finite-range potential interactions. The only assumption was the absence of phase transitions at positive temperatures, which is expected to hold for such systems. In view of eq. (4.1), our result implies that such systems cannot flow to a 1+1d CFT with a nonzero  $c_R - c_L$ .

One subtlety in this argument is that the CFT energy current  $T^{10}$  might not be the same as the infrared limit  $j^E$  of the microscopic energy current. As any locally conserved quantity, stress-energy tensor  $T^{\mu\nu}$  is not completely unique, and the

freedom to redefine it might be important in order to ensure that it is symmetric and traceless. However, since both  $T^{00}$  and the microscopic energy density  $h(x)$  must integrate to the same low-energy Hamiltonian, they can differ at most by a total derivative:  $T^{00} = h + \partial_x O$ , where  $O$  is a local operator. Then the CFT energy current  $T^{10}$  is related to  $j^E$  by  $T^{10} = j^E - \partial_t O$ . Hence the equilibrium expectation values of  $T^{10}$  and  $j^E$  are the same, and the vanishing of  $\langle j^E \rangle$  implies  $\langle T^{10} \rangle = 0$  and  $c_R - c_L = 0$ .

It is well-known that a nonzero  $c_R - c_L$  may appear in 1+1d CFTs describing the gapless edge of a gapped 2d system. The above result shows that  $c_R - c_L$  is determined by the bulk properties of the 2d material and does not depend on the edge. Indeed, we may consider a strip of the 2d phase bounded by two different edges (with opposite orientations) as a 1d material, and then the above result shows that  $c_R - c_L$  must be equal for the two edges. This is not surprising since  $c_R - c_L$  is related to the bulk thermal Hall conductance. The same comments apply, *mutatis mutandis*, to  $k_R - k_L$  and the Hall conductance.

The vanishing of the net  $U(1)$  current is implicitly assumed in the definition of magnetization. Usually, one says that since  $\nabla \cdot \langle \mathbf{J}^N(\mathbf{x}) \rangle = 0$  in an equilibrium state, one can define the magnetization by the equation  $\nabla \times \mathbf{M}^N(\mathbf{x}) = \langle \mathbf{J}^N(\mathbf{x}) \rangle$ . If the net current in some direction were nonzero, the magnetization so defined would be either multi-valued (if the direction is periodically identified) or would grow linearly with distance. In either case, it could not be regarded as a local property of the material. Bloch's theorem shows that the magnetization is well-defined. An analogous quantity for energy currents ("energy magnetization") is of importance in the theory of the thermal Hall effect of Chapter 5. Our results on the vanishing of the net energy current justify the existence of energy magnetization in a wide variety of situations.

One final remark is that the vanishing of  $U(1)$  and energy currents strictly applies to infinite systems in equilibrium. In a large but finite quasi-1d system, like a macroscopic ring, there can be a non-vanishing  $U(1)$  or energy current in equilibrium. However, it must go to zero when the size of the system goes to infinity.



## Chapter 5

### THERMAL HALL EFFECT

#### 5.1 Introduction

There has been much theoretical as well as experimental interest in the thermal Hall effect. Just to give a couple of recent examples: (1) thermal Hall effect has been used to probe the non-Abelian nature of the  $\nu = 5/2$  FQHE state [6]; (2) an unusual behavior of thermal Hall conductivity at low temperatures was observed in cuprate superconductors in the pseudogap region [24].

Despite many theoretical works on the thermal Hall effect (see e.g. [14, 47, 50, 11, 21]), there are still unresolved issues with the very definition of thermal Hall conductivity. In fact, all known approaches to defining thermal Hall conductivity as a bulk property are plagued with ambiguities. To see what the issue is in the simplest possible setting, consider a macroscopic system where the only conserved quantity carried by the low-energy excitations is energy (for example, an insulator at temperatures well below the band gap). One could expect that thermal Hall conductivity appears as a transport coefficient in the hydrodynamic description, but this is not the case: there is no physical time-reversal-odd transport coefficient at leading order in the derivative expansion as it was explained in chapter 2.

In the 2d case the tensor  $\kappa_{m\ell}^A$  reduces to a single quantity <sup>1</sup>, the thermal Hall conductivity  $\kappa^A = \frac{1}{2}\epsilon_{m\ell}\kappa_{m\ell}^A$ , and there is an alternative line of reasoning which suggests that in certain circumstances  $\kappa^A$  can be defined in bulk terms. Consider a material with a bulk energy gap. There might still be gapless excitations at the edges, and we will assume that they are described by a 1+1d Conformal Field Theory. Then it seems natural to relate  $\kappa^A(T)$  to the chiral central charge of the edge CFT:

$$\kappa^A(T) \simeq \frac{\pi T}{6}(c_R - c_L). \quad (5.1)$$

To see why this is natural, recall that a chiral 1+1d CFT at temperature  $T$  carries an equilibrium energy current  $I^E = \frac{\pi T^2}{12}(c_R - c_L)$  [9, 2]. Thus in a strip of a 2d material whose boundaries are kept at temperatures  $T$  and  $T + \Delta T$ , where  $T$  is much smaller

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<sup>1</sup>We use the notation  $\kappa^A$  instead of the more standard  $\kappa_{xy}$  to avoid confusion with the off-diagonal component of  $\kappa^S$  which may be nonzero if rotational invariance is broken.

than the bulk energy gap and  $\Delta T \ll T$ , there is a net energy current

$$I^E \simeq \frac{\pi T}{6}(c_R - c_L)\Delta T. \quad (5.2)$$

If we define  $\kappa^A = I^E/\Delta T$ , we get (5.1).

On the other hand, it has been shown in chapter 4 that the chiral central charge of the edge modes (and more generally, the equilibrium energy current carried by the edge modes) is independent of the particular edge. Hence the low-temperature thermal Hall conductivity of a gapped 2d material defined via (5.1) is a well-defined bulk property.<sup>2</sup>

The results of Chapter 4 also imply that the chiral central charge of the edge modes does not vary as one changes the parameters of the Hamiltonian. Therefore the low- $T$  thermal Hall conductivity is a topological invariant of the gapped 2d material. Finally, the above arguments make no assumption about the way the temperature varies within the strip. Thus the low-temperature thermal Hall *conductance* of a strip of a gapped 2d material coincides with its thermal Hall conductivity and is a well-defined bulk property as well. One does not expect this to hold at arbitrary temperatures, or for gapless materials at low  $T$ .

This leads us to ask the following questions.

Q1. Is the thermal Hall conductivity measured in experiments (at general temperatures) a well-defined bulk quantity? If yes, then how is this compatible with the above arguments that thermal Hall conductivity is not a well-defined bulk transport coefficient?

Q2. Is there a microscopic Kubo-type formula for the thermal Hall conductance and conductivity measured in experiments (at general temperatures) which makes no reference to the choice of the edge?

Q3. Is it true that the low-temperature thermal Hall conductance of a gapped 2d material is independent of the detailed shape of the temperature profile and thus coincides with the thermal Hall conductivity even if the edge is not described by Conformal Field Theory?

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<sup>2</sup>For gapped 2d systems at low temperatures, one can also try to define thermal Hall conductivity as the coefficient of the gravitational Chern-Simons term in the low-energy effective action [49, 58, 44]. As explained in [50], the energy current corresponding to the gravitational Chern-Simons term is of higher order in derivatives, in agreement with the above discussion. However, there is no natural way to couple a typical condensed matter system to gravity, and therefore this prescription is ambiguous.

Q4. Is it true that the low-temperature thermal Hall conductance of a gapped 2d material is linear in  $T$  at low  $T$  even if the edge is not described by Conformal Field Theory?

Q5. Is it true that the low-temperature thermal Hall conductance of a gapped 2d material is a topological invariant of the phase, in the sense that it does not change when the parameters of the Hamiltonian vary without crossing a bulk zero-temperature phase transition?

The goal of this chapter is to provide answers to the above questions in the case of lattice 2d systems. We show (with varying degree of rigor) that the answers to all these questions is "yes". In addition, we show that for systems described by Commuting Projector Hamiltonians thermal Hall conductance vanishes identically for all temperatures. We also show that for 2d gapped free fermionic systems of class A (that is, for non-interacting possibly disordered 2d insulators) thermal Hall conductance at low temperatures and electric Hall conductance are related via the Wiedemann-Franz law.

Our main observation is that, as was explained in Section 2.2, while it is problematic to give a definition of thermal Hall conductance which is not "contaminated" with edge effects, there is no such difficulty for derivatives of the thermal Hall conductance with respect to parameters of the Hamiltonian. We derive microscopic Kubo-type formulas for all such derivatives in a straightforward manner. A limitation of such formulas is that they hold only away from phase transitions. This is a common limitation of the usual linear response theory which assumes that correlations are short-range in order to be able to make a derivative expansion.

Kubo-like formulas for the derivatives of the thermal Hall conductance can be used to compute the difference of thermal Hall conductances  $\kappa_{MM'}^A = \kappa_M^A - \kappa_{M'}^A$  of two 2d materials  $M$  and  $M'$ . One chooses a path in the parameter space connecting the two Hamiltonians and avoiding bulk phase transitions and integrates the derivative along this path. Specializing to a linear temperature profile, we also get a formula for the difference of thermal Hall *conductivities*.

Our Kubo-like formula satisfies an important consistency check: the integral defining the "relative thermal Hall conductance"  $\kappa_{MM'}^A$  is independent of the choice of the path. We give both an intuitive argument based on the absence of macroscopic energy currents in equilibrium (which has been proved in Chapter 4) and a more formal mathematical argument for lattice systems. This allows us to standardize

the choice of paths used to compute  $\kappa_{\mathcal{M}\mathcal{M}'}^A$ . For example, for lattice systems with a finite-dimensional on-site space of states (such as fermion systems and spin systems) one can use paths which pass through the infinite-temperature phase. Since the infinite-temperature phase is the same for all lattice Hamiltonians, this makes it more plausible that a suitable path can be found for all pairs of materials  $\mathcal{M}, \mathcal{M}'$ .

One can interpret the integral formula for the relative thermal Hall conductance in more physical terms if one considers a smooth edge between the materials  $\mathcal{M}$  and  $\mathcal{M}'$  which interpolates between the two Hamiltonians in the physical space. If one applies linear response theory to this system and assumes that the temperature gradient is negligible in the edge region, one gets precisely our integral formula. Path-independence of the integral formula is then equivalent to the independence of the choice of the edge between  $\mathcal{M}$  and  $\mathcal{M}'$ . The latter property can be traced again to the absence of macroscopic energy currents in equilibrium.

This physical interpretation clarifies why it is not possible to write a well-defined microscopic formula for  $\kappa_{\mathcal{M}}^A$  even though it is possible to write down such a formula for the electric Hall conductance  $\sigma_{\mathcal{M}}^A$  of a single material  $\mathcal{M}$ . In the electric case, torus geometry provides a theoretical set-up where  $\sigma_{\mathcal{M}}^A$  can be measured without introducing edges. In this geometry, electric field is created using a time-dependent vector potential rather than a scalar potential. There is no thermal analogue of the torus set-up, and this is why only the relative thermal Hall conductance  $\kappa_{\mathcal{M}\mathcal{M}'}^A$  of two materials has a physical significance.

In most experiments, one of the materials is the vacuum and the difference between the thermal Hall conductances of the material and the vacuum is measured. If one normalizes the thermal Hall conductance of the vacuum to be zero, then the thermal Hall conductance of a material  $\mathcal{M}$  relative to the vacuum can be declared to be the “absolute” thermal Hall conductance of  $\mathcal{M}$ . Nevertheless, it is important to keep in mind that this is just a normalization condition, not something forced on us by physics.<sup>3</sup> One consequence of this is that there is no microscopic formula for the thermal Hall conductance which is local in the parameter space (that is, depends only on correlators for a particular Hamiltonian).

The results described above answer questions Q1 and Q2. Specifically, although thermal Hall conductivity is not a well-defined bulk transport coefficient and can

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<sup>3</sup>This was first noticed by H. Casimir in his landmark paper on Onsager reciprocity [12]. Casimir showed that invariance under time-reversal, strictly speaking, does not require the anti-symmetric part of the thermal conductivity tensor to vanish. Vanishing is only obtained if one normalizes the thermal Hall conductivity of the vacuum to be zero.

be measured only in the presence of an edge or another inhomogeneity, thermal Hall energy flux can be shown to be independent of the properties of the edge, provided the variation of the temperature on the length scale determined by the edge is negligible.

To answer Q3, Q4 and Q5 we study the low-temperature behavior of our formula for  $\kappa_{MM'}^A$ . Using the same method as in the work of Niu and Thouless on the electric Hall conductance [43], we show that the low- $T$  behavior of  $\kappa_{MM'}^A$  is independent of the precise temperature profile, up to terms exponentially suppressed in the temperature. This answers Q3. We also argue that derivatives of the thermal Hall conductance of a gapped 2d system with respect to parameters of the Hamiltonian are exponentially small for low  $T$  if there is a bulk energy gap. This answers Q5. Then we explain how to include the temperature  $T$  among the parameters and argue that the  $T$ -derivative of the dimensionless quantity  $\kappa_{MM'}^A/T$  is also exponentially small at low  $T$  if there is an energy gap. This implies that  $\kappa_{MM'}^A$  is linear in  $T$  up to exponentially small corrections. This answers Q4. Together with Q5, this shows that the coefficient of the  $T$ -linear term in  $\kappa_{MM'}^A$  is a topological invariant of the phase.

In this chapter we focus on lattice 2d systems. This allows to give a completely general formula for derivatives of the thermal Hall conductance with respect to arbitrary parameters of the Hamiltonian. Since the definition of thermal Hall conductance is rather subtle, we begin with a discussion of the electric Hall conductance. Some of the subtleties arise already in this context. Then we move on to the thermal case and derive a Kubo-like formula for derivatives of the thermal Hall conductance with respect to parameters. We argue that the integral defining the difference of thermal Hall conductances of two materials is independent of the path used to compute it. Then we discuss the low-temperature behavior of the thermal Hall conductance and show that for gapped systems it is linear in  $T$  up to exponentially small corrections and that its slope is a topological invariant of the phase. We also show that for systems described by Local Commuting Projector Hamiltonians thermal Hall conductance vanishes identically. Therefore such systems cannot have edge modes described by a CFT with a nonzero chiral central charge. This is an energy counterpart of the recently proved result that in such systems the zero-temperature electric Hall conductance vanishes [30]. To make the thesis more accessible, we relegate most mathematical details to appendices. In one of the appendices, we show by a direct computation that for gapped free fermionic systems of class A the relative

thermal Hall conductance of the  $T = 0$  and  $T = \infty$  states is related to the zero-temperature electric Hall conductance through a version of the Wiedemann-Franz law. The derivation does not assume translational invariance. Other appendices set up the mathematical machinery mentioned above and supply some details of the derivation.

## 5.2 Electric Hall conductance

### Kubo formula for the electric Hall conductance

Usually, Kubo formula is written down for conductivity rather than conductance. That is, it is assumed that the electric field is uniform across all relevant scales. For our purposes, it will be important to have a formula for the electric Hall current which does not assume that the electric field is uniform.

Consider a time-dependent perturbation of the Hamiltonian of the form

$$\Delta H(t) = \epsilon e^{st} \sum_{p \in \Lambda} \widehat{g}(p) Q_p, \quad (5.3)$$

where the real parameter  $\epsilon$  is small and  $\widehat{g} : \Lambda \rightarrow \mathbb{R}$  is arbitrary for now. This perturbation corresponds to adiabatically switching on an electric potential  $\epsilon \widehat{g}$ . Assuming that at  $t = -\infty$  the system is in an equilibrium state at temperature  $T$ , at  $t = 0$  the system will be in a non-equilibrium steady state. The change in the expectation value of an observable  $A$  at  $t = 0$  relative to the expectation value at  $t = -\infty$  is given by the general Kubo formula for dynamic response derived in Appendix B.2

$$\Delta \langle A \rangle = \epsilon \lim_{s \rightarrow 0^+} \beta \int_0^\infty e^{-st} \left\langle \left\langle A(t); \sum_p \frac{1}{i} [H, \widehat{g}(p) Q_p] \right\rangle \right\rangle dt. \quad (5.4)$$

Here Heisenberg-picture operators are defined as usual,  $A(t) = e^{iHt} A e^{-iHt}$ , and double brackets  $\langle \langle \dots \rangle \rangle$  denote Kubo's canonical pairing, see Appendix B. We also assumed that  $A$  doesn't have an explicit dependence on  $\epsilon$ .

For an infinite system, the existence of the limit  $s \rightarrow 0^+$  in eq. (5.4) is far from obvious. When both the perturbation  $\Delta H$  and the observable  $A$  are supported on a compact set  $K \subset \Lambda$ , the existence of the limit has been proved in [41]. When  $\widehat{g}$  is nonzero only on a compact set  $K \subset \Lambda$ , but  $A$  is supported on a non-compact set, we still expect the limit to exist, at least away from phase transitions. Indeed, if the correlation length is finite, the state of the system far from  $K$  is unaffected by the perturbation, and we can effectively truncate the support  $A$  to be compact, thereby

reducing to the case when both  $\widehat{g}$  and  $A$  are compactly supported. More generally, when the intersection of the supports of  $\widehat{g}$  and  $A$  is compact, the same argument suggests that  $\Delta\langle A \rangle$  is well-defined.

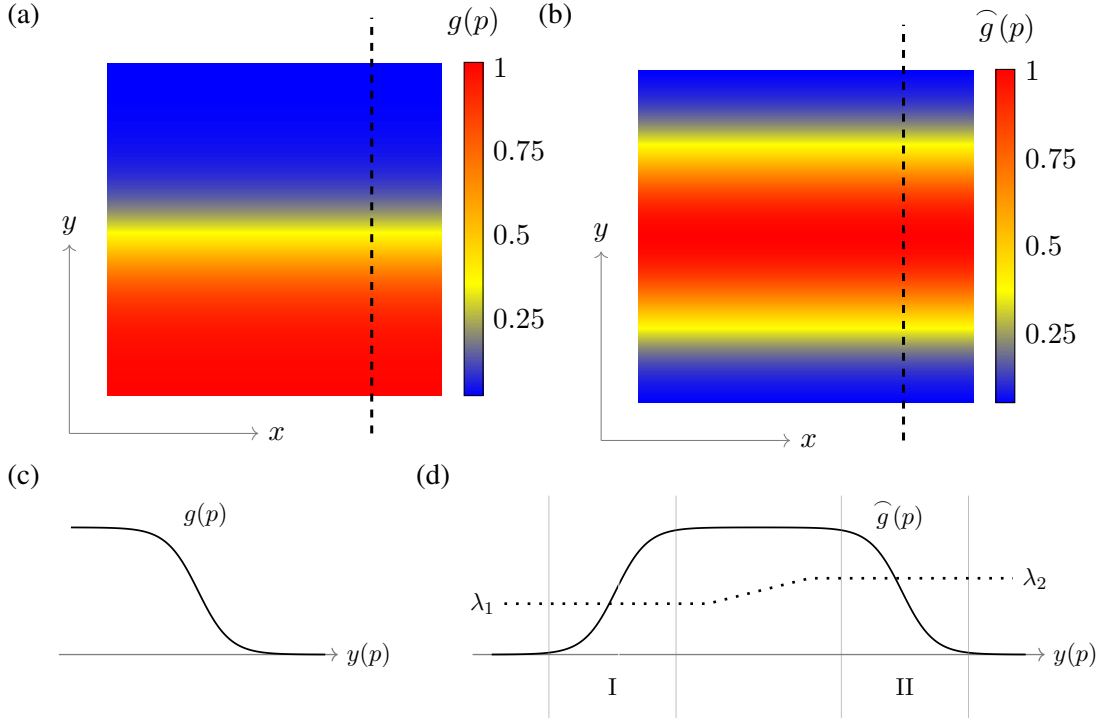


Figure 5.1: (a) Heat map of the function  $g(p)$  corresponding to a temperature gradient in a horizontal strip. (b) Heat map of the function  $\widehat{g}(p)$  corresponding to two horizontal strips with the opposite signs of the temperature gradient. (c) The function  $g(p)$  restricted to the dashed line in (a). (d) The function  $\widehat{g}(p)$  restricted to the dashed line in (b). Dotted line in (d) represents the dependence of some parameter  $\lambda$  of the Hamiltonian on  $y(p)$ .

From now on we specialize to the 2d case, unless explicitly stated otherwise. To compute the quantum Hall conductance of an infinite 2d system, we would like  $A$  to be the electric current across a vertical line  $x = a$ , and  $\widehat{g}$  to be a function which depends only on  $y$ , vanishes at  $y = +\infty$  and approaches 1 at  $y = -\infty$ , see Fig. 5.1a. Such a function  $\widehat{g}$  corresponds to the net electric potential change  $-\epsilon$  from  $y = -\infty$  to  $y = +\infty$ . However, such  $A$  and  $\widehat{g}$  do not satisfy the condition on supports explained above. Another way to explain a potential problem is to note that while the electric field corresponding to such a function  $\widehat{g}$  is vanishingly small for  $y \ll 0$  and all  $t$ , the state of the system at  $t = 0$  and  $y \ll 0$  is different from that at  $t = -\infty$  and  $y \ll 0$  because the electrochemical potential changes by  $-\epsilon$ . Since the expectation value of the current density is nonzero even in equilibrium and may

depend on the electrochemical potential, the change in the current density between  $t = 0$  and  $t = -\infty$  need not vanish at large negative  $y$ , and then the change in the net current across the line  $x = a$  will be ill-defined.

One way to avoid this difficulty is to make the  $y$  direction periodic and to perturb the system by a constant vector potential rather than a scalar potential. However, this approach does not have an analog in the case of thermal transport, which is our primary interest. Alternatively, one can take  $\widehat{g}$  to vanish both for  $y \ll 0$  and  $y \gg 0$ . For example, one can take  $\widehat{g}$  to look as in Fig. 5.1a. Then the electric field is smooth in the regions *I* and *II* and has opposite magnitudes there. Elsewhere it is zero. If the system is homogeneous, the net electric Hall current in the  $x$  direction will be zero. However, if the system is inhomogeneous, then the electric Hall conductance of the two regions may be different, and the net electric Hall current will be given by

$$\Delta\langle A \rangle = -\epsilon \int_{-\infty}^{+\infty} \sigma_{xy} \partial_y \widehat{g} dy = \epsilon \int_{-\infty}^{+\infty} \widehat{g} \partial_y \sigma_{xy} dx = \epsilon \int_{\lambda_1}^{\lambda_2} \frac{\partial \sigma_{xy}}{\partial \lambda} d\lambda. \quad (5.5)$$

Here we assumed that the system is homogeneous in regions *I* and *II* in Fig. 5.1d, while in the intermediate region some parameter of the Hamiltonian  $\lambda$  varies from  $\lambda_1$  to  $\lambda_2$  as  $y$  is increased. This approach allows one to compute the derivatives of the Hall conductance with respect to parameters. Integrating these derivatives along a path in the space of parameters, one can compute the relative electric Hall conductance of two systems, provided the path avoids phase transitions. This is good enough, since in practice one usually measures the relative electric Hall conductance of a particular material and vacuum.

As discussed in Chapter 3, the net current through a vertical line  $x = a$  is defined as

$$J_a^N = \frac{1}{2} \sum_{p,q} J_{pq}^N (f(q) - f(p)), \quad (5.6)$$

where  $f(p) = \theta(a - x(p))$  is a step-function. More generally, one can consider the expression (3.8) where one sets  $\eta(p, q) = f(q) - f(p)$  for some function  $f : \Lambda \rightarrow \mathbb{R}$  which is equal to 1 if  $x(p) \ll 0$  and equal to 0 if  $x(p) \gg 0$ . That is,  $f$  is a smeared step-function in the  $x$ -direction.

In what follows, we will use the following notation. Given any function  $f : \Lambda \rightarrow \mathbb{R}$ , we define a function  $\delta f : \Lambda \times \Lambda \rightarrow \mathbb{R}$  by  $(\delta f)(p, q) = f(q) - f(p)$ . One can view the operation  $\delta$  as a lattice analogue of the gradient operator  $\nabla$ . For more details on this notation see Appendix A. Thus the smeared current (3.8) with  $\eta(p, q) = f(q) - f(p)$



will be denoted  $J^N(\delta f)$ . While  $J_a^N$  is the rate of change of the charge in the region  $x > a$ ,  $J^N(\delta f)$  is the minus the rate of change of the operator

$$Q(f) = \sum_p f(p)Q_p. \quad (5.7)$$

That is,

$$i[H, Q(f)] = -J^N(\delta f). \quad (5.8)$$

It is very important for what follows that when  $f$  is a smeared step-function,  $J^N(\delta f)$  is a local operator supported in a vertical strip on  $\mathbb{R}^2$ , roughly where  $f$  is neither 0 nor 1. Indeed, on the one hand,  $J_{pq}^N$  is nonzero only if  $|p - q| < R$ . On the other hand,  $f(q) - f(p)$  is zero if both  $x(p)$  and  $x(q)$  are sufficiently large and positive, as well as when both  $x(p)$  and  $x(q)$  are sufficiently large and negative. The combined effect of this is that  $J^N(\delta f)$  is a sum of local operators supported in a vertical strip which is infinite in the  $y$ -direction but has a finite width in the  $x$ -direction.

Applying the general Kubo formula (5.4) to  $A = J^N(\delta f)$ , we get

$$\Delta\langle J^N(\delta f) \rangle = \epsilon\beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle\langle J^N(\delta f, t); J^N(\delta \widehat{g}) \rangle\rangle dt. \quad (5.9)$$

Here we identified  $\sum_p \frac{1}{i} [H, \widehat{g}(p)Q_p]$  with  $J^N(\delta g)$  and denoted by  $J^N(\delta f, t)$  the time-translation of  $J^N(\delta f)$  by  $t$ . Note that  $J^N(\delta g)$  is supported in a horizontal strip on  $\mathbb{R}^2$ . More precisely, if  $g$  is as in Fig. 5.1a, then  $J^N(\delta g)$  is supported in a horizontal strip. If  $\widehat{g}$  depends on  $y$  as in Fig. 5.1b, then  $J^N(\delta \widehat{g})$  is supported in two horizontal strips corresponding to regions I and II in Fig. 5.1d.

Recall now that we consider a Hamiltonian depending on a parameter  $\lambda$  which varies with  $y$  such that in region I  $\lambda = \lambda_1$ , in region II  $\lambda = \lambda_2$ , and in the intermediate region  $\lambda$  interpolates between these two values without crossing a phase transition. We assume that  $\lambda_2 - \lambda_1$  is small. We also choose  $g$  as in Fig. 5.1b. Then  $J^N(\delta \widehat{g})$  is a sum of operators supported in regions I and II. We can make this explicit by writing  $\delta \widehat{g} = \delta g_{II} - \delta g_I$ , where  $g_{I,II}$  interpolate between 0 and 1 as one moves from  $y = +\infty$  to the intermediate region. If the electric field in region I is minus the translate of the electric field in region II, then  $J^N(\delta g_I)$  is the translate of  $J^N(\delta g_{II})$ , and to linear order in  $\Delta\lambda$  we get

$$\Delta\langle J^N(\delta f) \rangle = \epsilon(\lambda_2 - \lambda_1) \frac{\partial}{\partial \lambda} \left[ \beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle\langle J^N(\delta f, t); J^N(\delta g_{II}) \rangle\rangle dt \right] + O((\lambda_2 - \lambda_1)^2), \quad (5.10)$$

where  $g$  is as in Fig. 5.1a which is translate of  $g_{I,II}$ . Here we implicitly assumed that the correlator

$$\lim_{s \rightarrow 0^+} \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle, \quad (5.11)$$

depends only on the Hamiltonian in some neighborhood of the intersection of supports of  $J^N(\delta f)$  and  $J^N(\delta g)$ , and thus when evaluating it one may assume that either  $\lambda = \lambda_1$  or  $\lambda = \lambda_2$ .

Comparing eq. (5.10) with eq. (5.5), we get

$$\frac{\partial \sigma_{xy}}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left[ \beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle dt \right], \quad (5.12)$$

where  $g$  is now a function depending only on  $y$  which interpolates between 1 and 0 as  $y$  varies from  $-\infty$  to  $+\infty$ , and  $f(p) = \theta(a - x(p))$ . This formula determines the electric Hall conductance up to an arbitrary constant. If we define the electric Hall conductance of vacuum to be zero, then we get a Kubo formula for the electric Hall conductance itself:

$$\sigma_{xy} = \beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle dt. \quad (5.13)$$

Note that it still depends on the exact profile of the electric potential  $g$  as well as on the choice of  $f$ . To get the electric Hall conductivity one needs to take the limit where  $g$  is linear over a very large region in  $y$ . One also has to set  $f(p) = \theta(x(p) - a)$  and average over  $a$ . We will see in the next section that at  $T = 0$  the precise choice of  $f$  and  $g$  becomes immaterial.

### Zero-temperature electric Hall conductance as a topological invariant

In this section we argue that for a gapped system at  $T = 0$  the electric Hall conductance  $\sigma_{xy}$  is independent of the precise choice of functions  $f$  and  $g$  and unchanged under variations of the Hamiltonian which do not close the gap. This is an adaptation of the arguments of Niu and Thouless [43]. We will also make use of the recent rigorous results on the decay of certain correlation functions in gapped systems obtained by H. Watanabe [60]. Ref. [60] assumes that the system is finite, so strictly speaking we need a generalization of these results to infinite systems. This generalization is straightforward, since Watanabe's estimates are uniform in the system's size.

After specializing to  $T = 0$ , we follow Ref. [43] and rewrite  $\sigma_{xy}$  in terms of the many-body Green's function  $G = (z - H)^{-1}$ :

$$\sigma_{xy} = -i \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J^N(\delta f) G^2 J^N(\delta g) \right). \quad (5.14)$$

Here  $E_0$  is the energy of the ground state, the contour of integration encloses the point  $z = E_0$  counter-clockwise and trace is taken over the Hilbert space of the whole system. We also denote by  $a$  the  $x$ -coordinate of the mid-line of the vertical strip where  $J^N(\delta f)$  is supported, and denote by  $b$  the  $y$ -coordinate of the mid-line of the horizontal strip where  $J^N(\delta g)$  is supported.

First we will argue that shifting  $f \mapsto f + f_0$ , where  $f_0(p)$  depends only on  $x(p)$  and is compactly supported in the  $x$ -direction, does not affect  $\sigma_{xy}$ . Under such a shift  $\sigma_{xy}$  changes by

$$-i \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J^N(\delta f_0) G^2 J^N(\delta g) \right) = - \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G [H, Q(f_0)] G^2 J^N(\delta g) \right). \quad (5.15)$$

Using the identity  $[H, A] = -[G^{-1}, A]$ , this expression can be written as

$$\oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( Q(f_0) G^2 J^N(\delta g) \right) - \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G Q(f_0) G J^N(\delta g) \right). \quad (5.16)$$

The first term can be written as

$$\oint_{z=E_0} \frac{dz}{2\pi i} \frac{\partial}{\partial z} \text{Tr} \left( Q(f_0) G J^N(\delta g) \right) \quad (5.17)$$

and thus vanishes. The second term is well-defined because according to [60] correlators of the form

$$\oint_{z=E_0} \text{Tr} (G A G B) \quad (5.18)$$

are exponentially small when the supports of  $A$  and  $B$  are separated by a large distance, and  $Q(f_0)$  and  $J^N(\delta g)$  are sums of local operators supported in a vertical and a horizontal strip, respectively.

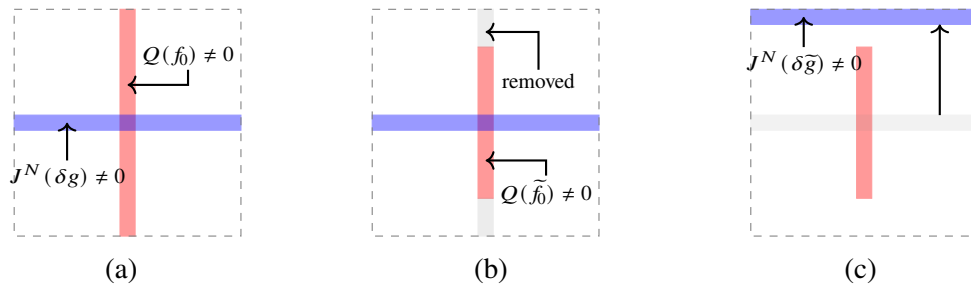


Figure 5.2: (a) The red vertical line represents the support of  $Q(f_0)$ , the blue horizontal line represents the support of  $J^N(\delta g)$ . (b) Grey parts are far away from the blue line, give a negligible contribution and can be dropped. (c) One can use the conservation law to move the blue line so that the blue and red lines are separated by a large distance.

As a matter of fact, the second term in (5.16) is also zero. To see this, let us replace the function  $f_0$  with a function  $\tilde{f}_0$  which is equal to  $f_0$  for  $|y - b| < L/2$  but vanishes for  $|y - b| \geq L/2$ . If  $L$  is large, the exponential decay of the correlator (5.18) implies that the second term in (5.16) changes by an amount of order  $L^{-\infty}$ . Let  $\tilde{g}$  denote the translate of  $g$  in the  $y$  direction by  $L$ , see Fig 5.2. Clearly,  $g_0 = g - \tilde{g}$  is a function which depends only on  $y(p)$  and is compactly supported in the  $y$  direction. Therefore

$$\begin{aligned} & \oint \frac{dz}{2\pi i} \text{Tr} \left( GQ(f_0)GJ^N(\delta g) \right) = \\ & = \oint \frac{dz}{2\pi i} \text{Tr} \left( GQ(\tilde{f}_0)GJ^N(\delta \tilde{g}) \right) - i \oint \frac{dz}{2\pi i} \text{Tr} \left( GQ(\tilde{f}_0)G[H, Q(g_0)] \right) + O(L^{-\infty}). \end{aligned} \quad (5.19)$$

The first term here is of order  $L^{-\infty}$  since the supports of  $Q(\tilde{f}_0)$  and  $J^N(\delta \tilde{g})$  are separated by a distance of order  $L$ . The second term is zero, since

$$\begin{aligned} \oint \frac{dz}{2\pi i} \text{Tr} \left( GQ(\tilde{f}_0)G[H, Q(g_0)] \right) & = - \oint \frac{dz}{2\pi i} \text{Tr} \left( GQ(\tilde{f}_0)G[G^{-1}, Q(g_0)] \right) = \\ & = - \oint \frac{dz}{2\pi i} \text{Tr} \left( G[Q(\tilde{f}_0), Q(g_0)] \right) = 0, \end{aligned} \quad (5.20)$$

due to ultra-locality of the charge. Taking the limit  $L \rightarrow \infty$ , we conclude that the second term in (5.16) is zero. This concludes the proof that  $\sigma_{xy}$  is independent of the precise choice of  $f$ . Independence of  $g$  is proved similarly.

Note that the status of  $f$  and  $g$  was somewhat different until now. The function  $g$  describes the profile of the electric potential and thus is a smeared step-function of nonzero width. The physically preferred value for  $f$  was an unsmeared step-function of the  $x$  coordinate. However, the difference between a smeared and unsmeared step-function is a function  $f_0$  supported on an interval. The above argument shows that for  $T = 0$  shifting  $f \mapsto f + f_0$  does not affect  $\sigma_{xy}$ . Thus at  $T = 0$  we can take both  $f$  and  $g$  to be unsmeared step-functions centered at  $x = a$  and  $y = b$ , respectively. Exchanging  $x$  and  $y$  is then the same as exchanging  $a$  and  $b$ . It is easy to see that  $\sigma_{xy}$  is anti-symmetric under such an exchange, hence at  $T = 0$  it coincides with  $\sigma^A$ . This is to be expected, since at  $T = 0$  the dissipative part of the conductance tensor vanishes.

Next we show that deformations of the Hamiltonian which do not close the energy gap do not affect  $\sigma_{xy}$ . It is sufficient to show this for families of Hamiltonians of the form  $H(\lambda) = H + \lambda V$ , where  $V$  is a local operator supported on a region of a fixed

diameter  $D$ . The general case is an immediate consequence, since we can write an arbitrary deformation as a sum of such deformations.

As explained above, we can choose  $f$  and  $g$  to be step-functions centered at  $x = a$  and  $y = b$ , respectively. We will denote the corresponding current operators  $J_a^N$  and  $J_b^N$  and write

$$\sigma^A = -i \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J_a^N G^2 J_b^N \right). \quad (5.21)$$

Since changing  $a$  and  $b$  does not affect  $\sigma^A$ , we can choose them so that the distance between the support of the perturbation  $V$  and the lines  $x = a$  and  $y = b$  is of order  $L$  where  $L$  is arbitrarily large. The variation of (5.21) under the deformation of the Hamiltonian is proportional to

$$\begin{aligned} \frac{\partial}{\partial \lambda} \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J_a^N G^2 J_b^N \right) &= \oint_{z=E_0} \frac{dz}{2\pi i} \left\{ \text{Tr} \left( G V G J_a^N G G J_b^N \right) \right. \\ &\quad \left. + \text{Tr} \left( G J_a^N G V G G J_b^N \right) + \text{Tr} \left( G J_a^N G G V G J_b^N \right) \right\}, \end{aligned} \quad (5.22)$$

where we have used the fact that variations of  $J_a^N, J_b^N$  are zero since the supports of  $J_a^N$  and  $J_b^N$  are more than a distance  $2R$  away from the support of  $V$ . We also used

$$\frac{\partial G}{\partial \lambda} = G \frac{\partial H}{\partial \lambda} G = G V G. \quad (5.23)$$

Subtracting a total derivative

$$\begin{aligned} 0 &= \oint \frac{dz}{2\pi i} \text{Tr} \frac{\partial}{\partial z} \left( G J_a^N G V G J_b^N \right) = \oint \frac{dz}{2\pi i} \left\{ \text{Tr} \left( G G J_a^N G V G J_b^N \right) \right. \\ &\quad \left. + \text{Tr} \left( G J_a^N G G V G J_b^N \right) + \text{Tr} \left( G J_a^N G V G G J_b^N \right) \right\}, \end{aligned} \quad (5.24)$$

from the above expression, we get

$$\frac{\partial}{\partial \lambda} \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J_a^N G^2 J_b^N \right) = - \oint \frac{dz}{2\pi i} \text{Tr} \left( [V, G J_a^N G] G J_b^N G \right). \quad (5.25)$$

In Appendix B.3 we show that correlators of the form

$$\oint \frac{dz}{2\pi i} \text{Tr} \left( [A, G B G] G C G \right), \quad (5.26)$$

where  $A, B, C$  are local operators and the support of  $A$  is away from the support of  $B$ , are exponentially suppressed for gapped systems. Therefore we have

$$\frac{\partial \sigma^A}{\partial \lambda} = -i \frac{\partial}{\partial \lambda} \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} \left( G J_a^N(x_0) G^2 J_b^N(y_0) \right) = O(L^{-\infty}). \quad (5.27)$$

Since  $L$  can be made arbitrarily large, this concludes the proof.

### 5.3 Thermal Hall Conductance

#### Kubo formula for the derivatives of the thermal Hall conductance

To derive a Kubo formula for derivatives of the thermal Hall conductance we follow the same strategy as in the case of electric Hall conductance. Following Luttinger [39], we perturb the Hamiltonian by a term

$$\Delta H(t) = \epsilon e^{st} \sum_{p \in \Lambda} \widehat{g}(p) H_p, \quad t \in (-\infty, 0]. \quad (5.28)$$

It is shown in 3.5 that this is equivalent to a time-dependent and space-dependent infinitesimal temperature deformation

$$\delta T(t, \mathbf{r}) = \epsilon T e^{st} \widehat{g}(\mathbf{r}).$$

As in the electric case, we cannot take  $\widehat{g}$  to be a smeared step-function of  $y$ , since then the change in the expectation value of the net energy current across a line  $x = a$  will be ill-defined. Instead we take  $\widehat{g}$  to be a function as in Fig. 5.1b, and consider an inhomogeneous system whose Hamiltonian depends on a parameter  $\lambda$  which varies with  $y$  as in Fig. 5.1d. This allows one to compute the derivative of the thermal Hall conductance with respect to  $\lambda$ .

One difference compared to the electric case is that the energy current operator  $A = J^E(\delta f)$  now has an explicit dependence on  $\epsilon$  (the magnitude of the perturbation). This happens because  $[H_p, H_q] \neq 0$ , in general. The change in  $A$  due to this explicit dependence is

$$\Delta A = -\frac{\epsilon}{2} \sum_{p,q} i[H_p, H_q] (f(q) - f(p)) (\widehat{g}(p) + \widehat{g}(q)). \quad (5.29)$$

The corresponding change in the expectation value of  $A$  is

$$\frac{\epsilon}{2} \sum_{p,q} \langle J_{pq}^E \rangle (f(q) - f(p)) (\widehat{g}(p) + \widehat{g}(q)) = \frac{\epsilon}{3} \sum_{p,q,r} M_{pqr}^E (f(q) - f(p)) (\widehat{g}(q) - \widehat{g}(r)). \quad (5.30)$$

Here we used skew-symmetry of  $M_{pqr}^E$  with respect to arbitrary permutations of  $p, q, r$ .

Since  $M_{pqr}^E$  decays rapidly when  $q$  and  $r$  are far apart, and since  $\widehat{g}(q) - \widehat{g}(r)$  vanishes when  $q$  and  $r$  are both in a region where  $\widehat{g}$  is constant, eq. (5.30) receives contributions only from the regions *I* and *II* where the temperature gradient is nonzero. We make this explicit by writing  $\delta \widehat{g} = \delta g_{II} - \delta g_I$ , where  $g_{I,II}(p)$  depends only on  $y(p)$  and interpolates between 0 and 1 as one moves from  $y = +\infty$  to the

intermediate region. If the temperature gradients in regions  $I$  and  $II$  are equal and opposite,  $\delta g_{I,II}$  are the translate of  $g$  as in Fig. 5.1a. In these two regions the parameter  $\lambda$  takes constant values  $\lambda_1$  and  $\lambda_2$ , respectively. Therefore the expression (5.30) can be written as

$$2\epsilon(\lambda_2 - \lambda_1) \mu_\lambda^E(\delta g \cup \delta f) + O\left((\lambda_2 - \lambda_1)^2\right), \quad (5.31)$$

where  $\mu_{pqr,\lambda}^E = \partial M_{pqr}^E / \partial \lambda$ , and we introduced a shorthand

$$\mu_\lambda^E(\delta f_1 \cup \delta f_2) = \frac{1}{6} \sum_{p,q,r} \mu_{pqr,\lambda}^E (f_1(q) - f_1(p))(f_2(r) - f_2(q)) \quad (5.32)$$

for any two functions  $f_1, f_2 : \Lambda \rightarrow \mathbb{R}$ . For generic functions  $f_1, f_2$  the triple sum over  $p, q, r$  has a large-volume divergence which arises from the region where  $p, q, r$  are all close together. However, for  $f_1 = g$  and  $f_2 = f$  it is easy to check that the summation is absolutely convergent, so the expression is well-defined.

Combining (5.31) with the change in  $\langle A \rangle$  arising from the change in the state of the system, we get

$$\begin{aligned} \Delta \langle A \rangle \approx \epsilon(\lambda_2 - \lambda_1) \frac{\partial}{\partial \lambda} \left[ \beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle \langle J^E(\delta f, t); J^E(\delta g) \rangle \rangle dt \right] \\ + 2\epsilon(\lambda_2 - \lambda_1) \mu_\lambda^E(\delta g \cup \delta f). \end{aligned} \quad (5.33)$$

On the other hand, the expected net energy current across the line  $x = a$  is

$$-\epsilon T \int_{-\infty}^{+\infty} \kappa_{xy} \partial_y g \, dy = \epsilon T \int_{\lambda_1}^{\lambda_2} \frac{\partial \kappa_{xy}}{\partial \lambda} d\lambda.$$

Comparing these two expressions we get a formula for the  $\lambda$ -derivative of the thermal Hall conductance:

$$d\kappa_{xy} = d \left[ \beta^2 \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle \langle J^E(\delta f, t); J^E(\delta g) \rangle \rangle dt \right] - 2\beta \mu^E(\delta f \cup \delta g), \quad (5.34)$$

where we combined  $\lambda$ -derivatives into 1-form  $\mu = \mu_\lambda d\lambda$ . Unlike in the electric case, there is no canonical formula for  $\kappa_{xy}$ . We can still define the difference of thermal Hall conductances of two materials  $\mathcal{M}$  and  $\mathcal{M}'$  by integrating the 1-form  $d\kappa_{xy}$  along a path in the parameter space connecting  $\mathcal{M}$  and  $\mathcal{M}'$ . This path must avoid phase transitions, otherwise objects like  $\mu^E(\delta f \cup \delta g)$  might diverge.

### Path-independence of the thermal Hall conductance

We have defined a 1-form  $d\kappa_{xy}$  on the space of parameters of a lattice system whose integral along a curve  $\Gamma$  can be identified with the difference of thermal Hall conductances of the initial and final points of  $\Gamma$ . The definition of the 1-form depended on the rapid spatial decay of the Kubo pairings of local operators. Thus when choosing a curve connecting two points  $\mathcal{M}$  and  $\mathcal{M}'$  in the parameter space, one needs to avoid loci where phase transitions occur. Since we are allowed to enlarge the parameter space by adding arbitrary local terms to the Hamiltonian, it is very plausible that such a curve exists for any two points  $\mathcal{M}$  and  $\mathcal{M}'$ . Indeed, phase transitions at nonzero temperatures are usually associated with spontaneous symmetry breaking and typically can be turned into cross-overs by adding suitable symmetry-breaking perturbations. Quantum phase transitions at zero-temperature defy the symmetry-breaking paradigm, but as explained in the next section temperature can be considered as one of the parameters of the Hamiltonian, and at non-zero temperature quantum phase transitions become cross-overs.

An important consistency requirement is that the difference of the thermal Hall conductances thus computed does not depend on the choice of  $\Gamma$ . To show this, consider an arbitrary closed loop  $\Gamma$  in the parameter space. By assumption, the ‘‘Kubo’’ part of the thermal Hall conductance

$$\kappa_{xy}^{\text{Kubo}} = \beta^2 \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle\langle J^E(\delta f, t); J^E(\delta g) \rangle\rangle dt \quad (5.35)$$

is well-defined for each point of  $\Gamma$ . Therefore  $d\kappa_{xy}^{\text{Kubo}}$  is an exact 1-form and its integral over any closed curve vanishes.

We are going to argue that the energy magnetization contribution  $\mu^E(\delta f \cup \delta g)$  is also exact. This is a 1-form on the parameter space which depends on  $f$  and  $g$ . Its physical meaning is the differential of the energy magnetization in the region where both  $f$  and  $g$  vary substantially. We would like to show that the integral of this 1-form along any loop  $\Gamma$  avoiding phase transitions is zero. Heuristically, this must be true in order to avoid contradiction with the theorem about the absence of net energy currents in equilibrium quasi-1d systems proved in Chapter 4. Imagine slowly varying the parameters of the system as a function of  $y \in [0, L]$  while following a loop  $\Gamma$ . Then we can compactify the  $y$  direction with period  $L$ , and regard this as a quasi-1d system. If  $L$  is large compared to the correlation length, this should not affect local properties, including the differential of the energy magnetization  $\mu^E$ . The energy current in the  $x$  direction can be computed using the continuum equation



(3.16). Since the net energy current should vanish, we get

$$0 = \int \langle J_x^E \rangle dy = \int_0^L \partial_y M^E dy \simeq \int \partial_\lambda M^E d\lambda = \int_\Gamma \mu^E. \quad (5.36)$$

The error in this computation should become arbitrarily small for  $L \rightarrow \infty$ , so we get the desired result. A more precise argument is given in Appendix B.4.

### A relative invariant of gapped 2d lattice systems

In this section we use the 1-form  $d\kappa_{xy}$  to define a relative topological invariant of gapped 2d lattice systems at zero temperature. We anticipate that in the case when both lattice systems admit a conformally-invariant edge, the invariant will be equal to  $\pi/6$  times the difference of the chiral central charges for the two systems. We cannot necessarily connect two such systems by a curve  $\Gamma$  in the space of Hamiltonians without encountering a bulk phase transition. If we could, this would mean that they are in the same zero-temperature phase, and then by the result of Chapter 4 they would have to have the same chiral central charge for the edge modes, and therefore the relative invariant would vanish. Rather, the idea is to treat the temperature  $T$  as yet another parameter, and connect the two systems in the enlarged parameter space  $(T, \lambda)$ . At positive temperatures quantum phase transitions are smoothed out into cross-overs, and the two systems can now be deformed into each other while maintaining a finite correlation length.

Formally, the temperature can be regarded as a parameter because re-scaling the temperature by a positive factor is equivalent to re-scaling the Hamiltonian by the inverse factor. Therefore one can extend the form  $\kappa_{xy}$  to the open subset of the enlarged parameter space given by  $T > 0$ . In detail, this is done as follows. Given a Hamiltonian  $H$ , we define a one-parameter family of Hamiltonians by  $H(\lambda^0) = \lambda^0 H$  (the Hamiltonian  $H$  still depends on other parameters  $\lambda^\ell$  which we collectively call  $\lambda$  opposed to specific overall scaling parameter  $\lambda^0$ ). Then the above mentioned scaling symmetry implies

$$T \frac{d}{dT} \frac{\kappa_{xy}^{\text{Kubo}}}{T} = - \lambda^0 \frac{d}{d\lambda^0} \Big|_{\lambda^0=1} \frac{\kappa_{xy}^{\text{Kubo}}(\lambda^0)}{T}, \quad (5.37)$$

where  $\kappa_{xy}^{\text{Kubo}}(\lambda^0)$  denotes the Kubo part of  $\kappa_{xy}$  computed with the Hamiltonian  $H(\lambda^0)$ . We have to divide  $\kappa_{xy}$  by  $T$  in order to get an observable which is invariant under the rescaling  $H \mapsto \lambda^0 H, T \mapsto \lambda^0 T$ . Similarly, we have

$$2T \frac{d}{dT} \left( \beta^2 M_{pqr}^E \right) = -2 \lambda^0 \frac{d}{d\lambda^0} \Big|_{\lambda^0=1} \left( \beta^2 M_{pqr}^E \right) = \frac{2}{T^2} \tau_{pqr}^E, \quad (5.38)$$

where  $\tau_{pqr}^E$  is  $-\mu_{pqr}^E$  with  $dH_p$  replaced with  $H_p$ :

$$\tau_{pqr}^E = \beta \langle \langle H_p; J_{qr}^E \rangle \rangle + \beta \langle \langle H_r; J_{pq}^E \rangle \rangle + \beta \langle \langle H_q; J_{rp}^E \rangle \rangle. \quad (5.39)$$

We can now define a 1-form on the subset  $T > 0$  of the enlarged parameter space which represents the total derivative of  $\kappa_{xy}/T$ :

$$\Psi(f, g) = \frac{d\kappa_{xy}^{\text{Kubo}}}{T} - \frac{2}{T^2} \mu^E(\delta f \cup \delta g) + \frac{d}{dT} \left( \frac{\kappa_{xy}^{\text{Kubo}}}{T} \right) dT - 2\tau^E(\delta f \cup \delta g) \frac{dT}{T^3}. \quad (5.40)$$

Its integral around any closed curve in the  $(T, \lambda)$  space is zero by the same argument as before, therefore  $\Psi$  is exact.

Given any two gapped zero-temperature lattice systems  $\mathcal{M}$  and  $\mathcal{M}'$ , we would like to define a relative topological invariant by integrating  $\Psi$  along a curve in the enlarged parameter space which connects  $\mathcal{M}$  and  $\mathcal{M}'$ . See Fig. 3b. We need to check three things: that the integral converges, that it does not change as one deforms  $\mathcal{M}$  and  $\mathcal{M}'$  while keeping  $T = 0$  and finite correlation length, and that result of integration does not change as we modify the functions  $f, g$  while keeping their asymptotic behavior fixed. Neither of these is obvious. The  $T$ -component of the 1-form  $\Psi$  is

$$\begin{aligned} \Psi_n(f, g) &= \frac{d}{dT} \left( \frac{\kappa_{xy}^{\text{Kubo}}}{T} \right) - \frac{2}{T^3} \tau^E(\delta f \cup \delta g) \\ &= -\frac{1}{T^3} \left[ \frac{d}{d\lambda^0} \Big|_{\lambda^0=1} \int_0^\infty \beta \langle \langle J_{\lambda^0}^E(\delta f, t); J_{\lambda^0}^E(\delta g) \rangle \rangle_{\lambda^0} dt + 2\tau^E(\delta f \cup \delta g) \right]. \end{aligned} \quad (5.41)$$

Here  $\langle \langle \dots \rangle \rangle_{\lambda^0}$  denotes the Kubo pairing at temperature  $T$  with respect to the Hamiltonian  $H(\lambda^0) = \lambda^0 H$ , and  $J_{\lambda^0}^E$  is the energy current for the Hamiltonian  $H(\lambda^0)$ . We denoted the  $T$ -component  $\Psi_n$  to emphasize that it is the normal component to the boundary  $T = 0$  of the enlarged parameter space. The convergence of the integral of  $\Psi$  requires the expression in parentheses to vanish faster than  $T^2$  as  $T \rightarrow 0$ . Similarly, the independence of the integral of  $\Psi$  on the deformation of the endpoints requires the tangential component of  $\Psi$ ,

$$\Psi_t(f, g) = \frac{1}{T^2} \left( d \int_0^\infty \beta \langle \langle J^E(\delta f, t); J^E(\delta g) \rangle \rangle dt - 2\mu^E(\delta f \cup \delta g) \right), \quad (5.42)$$

to vanish at  $T = 0$ . Thus the expression in parentheses should vanish faster than  $T^2$  as  $T \rightarrow 0$ .

In Appendix B.5 we argue (not completely rigorously) that both expressions vanish exponentially fast as  $T \rightarrow 0$ . To see why this is plausible, consider eq. (5.42) for

definiteness and denote the expression in parentheses as  $\Omega(T)$ . It is a 1-form on the space of parameters of the Hamiltonian. The first term in  $\Omega(T)$  is the exterior derivative of the same kind of current correlator which defines the electric Hall conductance, except that the electric current  $J$  is replaced with the energy current  $J^E$ . The key point is that at  $T = 0$  this correlator is sensitive mainly to the state of the system in a compact region  $S \subset \mathbb{R}^2$  which is an intersection of the vertical strip corresponding to  $f$  and the horizontal strip corresponding to  $g$ . The same argument as in Section 5.2 shows that at  $T = 0$  the derivative of this correlator with respect to a deformation of the Hamiltonian localized at a distance  $L$  from  $S$  is of order  $L^{-\infty}$ . The same is true for the second term, because of the assumed decay of Kubo pairings. Since the sum of the two terms does not change as one varies  $f$  and  $g$ ,  $L$  can be made arbitrarily large, and we conclude that  $\Omega(0) = 0$  when evaluated on any deformation of the Hamiltonian supported on a quadrant in  $\mathbb{R}^2$ . Therefore  $\Omega(0) = 0$  identically. Further, in the presence of the energy gap one expects the low-temperature expansion to have a finite radius of convergence, therefore  $\Omega(T) - \Omega(0)$  is exponentially suppressed for low  $T$  (it is this part of the argument which is not rigorous). Combining these statements, we show that integral converges and independent of deformations of  $\mathcal{M}$  and  $\mathcal{M}'$  which do not cross phase transitions. In order to show that the value of integral is independent of the shift of cochains  $f, g$  we can use the fact that one form  $\Psi(f, g)$  is exact and integral is given by difference of antiderivatives of  $\Psi$  at endpoints. The latter can be shown to vanish if either  $f$  or  $g$  is hat-shaped as in Fig. 5.1b. For more details see Appendix B.5.

There is another limit where one can evaluate  $\Psi$ , namely  $T \rightarrow \infty$ . In this limit the expectation value  $\langle A \rangle$  of a local operator  $A$  becomes the normalized trace over the local Hilbert space, while the Kubo pairing becomes

$$\lim_{T \rightarrow \infty} \langle \langle A; B \rangle \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle. \quad (5.43)$$

Thus all components of  $\Psi$  are of order  $1/T^3$  for large  $T$ , and therefore the relative thermal Hall conductance of any two high-temperature states is of order  $1/T^2$ . Hence another natural choice of a reference state (apart from the trivial insulator at  $T = 0$ ) is the  $T = \infty$  state. That is, one can define an absolute topological invariant of a gapped zero-temperature system  $\mathcal{M}$  by integrating the 1-form  $\Psi$  along any path connecting  $\mathcal{M}$  to the  $T = \infty$  state.

The case of a Locally Commuting Projector Hamiltonian is particularly simple. In this case, since  $J_{pq}^E = -i[H_p, H_q] = 0$  for all  $p, q$ , the  $T$ -component of the 1-form

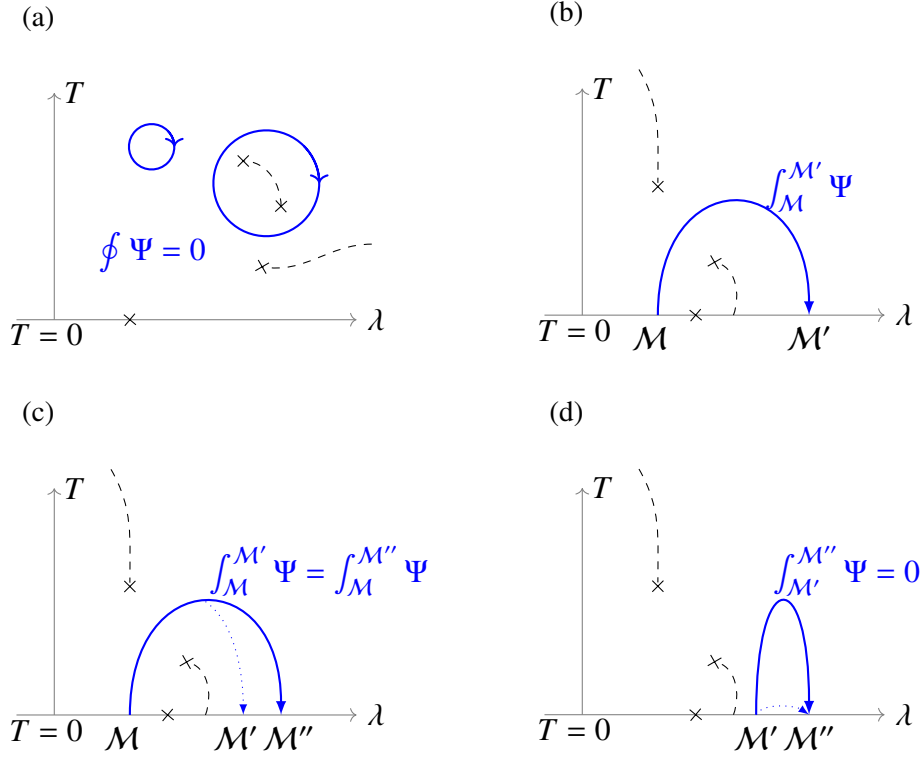


Figure 5.3: Phase diagrams. The horizontal axis represents a parameter of the Hamiltonian, the vertical axis is temperature. Dashed lines and crosses represent phase transitions. Blue lines are integration contours. (a) The integral of  $\Psi$  along a loop is zero regardless of whether there are phase transitions in the interior. (b) The invariant  $I(\mathcal{M}, \mathcal{M}')$  for zero-temperature phases  $\mathcal{M}$  and  $\mathcal{M}'$  can be computed by integrating  $\Psi$  along the blue line. (c) The points  $\mathcal{M}'$  and  $\mathcal{M}''$  are in the same phase, therefore one expects the integrals along the solid and dotted blue lines to be the same. (d) The difference of the two paths can be deformed to a near-zero-temperature path from  $\mathcal{M}''$  to  $\mathcal{M}'$ .  $\Psi$  is exponentially small on this path.

$\Psi$  vanishes identically. Integrating  $\Psi$  along a path  $\Gamma$  along which only  $T$  changes, we find that  $\kappa^A(T) - \kappa^A(\infty) = 0$ . Thus the thermal Hall conductance relative to the  $T = \infty$  state is zero for all temperatures.<sup>4</sup> This implies that the chiral central charge of the edge modes must vanish for such a Hamiltonian. One can also show that the zero-temperature electric Hall conductance vanishes for such systems, but the proof is very different [30].

The case of gapped systems of free fermions is also fairly simple, since there are

<sup>4</sup>Strictly speaking, to avoid potential phase transitions at  $T > 0$ , one needs to work with a finite-volume version of  $\Psi$  defined on torus. Its  $T$ -component still vanishes for a system described by a Local Commuting Projector Hamiltonian, so the integral from any  $T$  to  $T = \infty$  is still zero. Taking the infinite-volume limit we conclude that the relative thermal Hall conductance is identically zero.

no phase transitions at any  $T > 0$ , and one can again integrate  $\Psi$  along a path with only  $T$  varying. Then one only needs to know the  $T$ -component of  $\Psi$ , which can be evaluated in complete generality. This computation is performed in Appendix B.6 where it is shown that

$$\int_{T=0}^{T=\infty} \Psi = \left. \frac{\kappa^A}{T} \right|_{T=\infty} - \left. \frac{\kappa^A}{T} \right|_{T=0} = -\frac{\pi^2}{3} \sigma^A, \quad (5.44)$$

where  $\sigma^A$  is the electric Hall conductance at  $T = 0$ . If one defines  $\kappa^A/T$  to vanish at  $T = \infty$ , then this can be regarded as a form of the Wiedemann-Franz law. Note however that it cannot be interpreted too naively. For example, since  $\Psi$  is exponentially small for low  $T$ , most of the contribution to the integral (5.44) comes from  $T$  of order of the energy gap. Although one can define the absolute thermal Hall conductance at temperature  $T$  as

$$\kappa^A(T) = T \int_{\infty}^T \Psi, \quad (5.45)$$

and it will obey the Wiedemann-Franz law  $\kappa^A \simeq \frac{\pi^2}{3} T \sigma^A$  at low  $T$ ,  $\kappa^A(T)$  is not determined by correlators measured at temperature  $T$  and a fixed Hamiltonian.

#### 5.4 Concluding remarks

We have derived a formula for the derivatives of the thermal Hall conductance with respect to parameters of the Hamiltonian and temperature. The relative thermal Hall conductance is obtained by integrating the derivative along a path in parameter space connecting the two materials. We have argued that this is the best one can do, since only differences of thermal Hall conductances of materials are well-defined physical quantities. What is usually measured in experiments is the thermal Hall conductance of a particular material relative to the vacuum.

We also argued that for gapped 2d lattice systems the thermal Hall conductance at low  $T$  is linear in  $T$  up to exponentially small corrections. The slope of the thermal Hall conductance is a topological invariant, in the sense that it does not change under variations of the Hamiltonian which keep the correlation length finite. It can change only when the bulk undergoes a zero-temperature phase transition.

This result can be interpreted as a form of bulk-boundary correspondence. Consider a strip of a gapped 2d material  $\mathcal{M}$  at temperatures below the gap as well as below any temperatures at which bulk phase transitions occur. Suppose there is an effective field theory description of this system which reproduces all observations. Since there

are no bulk excitations, such an effective field theory describes only edge excitations. Let us assume that these edge excitations are described by a 1+1d CFT. There may also be terms in the effective action which describe the bulk response to the external fields, such as the Chern-Simons term (if the system has a  $U(1)$  symmetry and can be coupled to a background electromagnetic field) and the gravitational Chern-Simons term. However, such terms in the action do not contribute to the thermal Hall current at leading order in the temperature gradient [50]. Thus the net energy current for the edge modes should be equal to  $\kappa_{\mathcal{M}\mathcal{M}_0}^A(T)\Delta T$ , where  $\mathcal{M}_0$  is the vacuum and it is assumed that the temperature difference between the edges  $\Delta T$  is much smaller than  $T$ . On the other hand, as explained in Section 5.1, the net energy current computed from CFT is equal to  $\frac{\pi}{6}(c_R - c_L)T\Delta T$ . Therefore the slope of  $\kappa_{\mathcal{M}\mathcal{M}_0}^A(T)$  at low  $T$  is equal to  $\frac{\pi}{6}(c_R - c_L)$ .

## THERMOELECTRIC HALL EFFECTS

### 6.1 Introduction

Hydrodynamics in a general sense is a coarse-grained description of matter in local thermal equilibrium which incorporates all local conservation laws. It depends on the microscopic details only through transport coefficients. Dissipative transport coefficients such as viscosity, thermal conductivity and electric conductivity are particularly important for applications and their theory is better known. More recently a lot of attention has been devoted to non-dissipative time-reversal-odd transport coefficients such as electric Hall conductivity and Hall viscosity. This interest is explained in part by the contribution that gapless edge modes make to some of these coefficients at low temperatures.

Theoretical studies of transport phenomena often take Kubo formulas as their starting point. These are microscopic formulas for transport coefficients in terms of correlators of currents of conserved quantities. Although Kubo formulas go back to [57, 39] and can be found in many textbooks, there are a number of subtleties in their derivation. It is well appreciated by now that naive Kubo formulas for skew-symmetric parts of the transport tensors must be supplemented by additional terms involving magnetization and "energy magnetization" [14]. Such terms affect thermal Hall conductivity and the skew-symmetric parts of thermoelectric coefficients. Since magnetizations are intrinsically ambiguous, it is not obvious how to evaluate such terms, see [47] for a thorough discussion.

The theory of transport coefficients developed in [39, 14, 47] applies to continuum systems. It cannot be directly applied to lattice systems because it assumes certain scaling relations for electric and energy currents which do not hold on a lattice. (In fact, they do not hold for interacting continuum systems either, except after some spatial averaging [14]). Since tight-binding models and other lattice Hamiltonians are ubiquitous in theoretical condensed matter physics, it is important to develop an analogous formalism for them. In previous chapter we described such a formalism and used it to derive microscopic formulas for the Hall conductivity and thermal Hall conductivity of lattice systems. In this chapter we extend it to other transport coefficients.

## 6.2 Microscopic formulas for thermoelectric coefficients

### Nernst effect

Derivations here are analogous to the ones for electric and thermal effects.

In order to find the thermoelectric coefficient coefficient  $\nu_{xy}$  we deform the Hamiltonian density by

$$\Delta H_p = \epsilon e^{st} \widehat{g}(p) H_p, \quad (6.1)$$

where  $\widehat{g}(p)$  is a hat-shaped function as in Fig. 5.1b,  $\epsilon$  is an infinitesimal parameter, and  $s$  is a small positive number which controls how fast the perturbation is turned on. We will consider the so-called fast regime [39] in which the characteristic time  $1/s$  is large but not large enough in order for the two slopes of the hat  $\widehat{g}(p)$  to come into equilibrium.

The change in the electric current across a vertical line  $x = a$  is

$$\Delta \langle J^N(\delta f) \rangle = \langle \Delta J^N(\delta f) \rangle + \epsilon \beta \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^E(\delta \widehat{g}) \rangle \rangle, \quad (6.2)$$

where  $f(p) = \theta(a - x(p))$  is a step function. The explicit variation of the current is

$$\begin{aligned} \langle \Delta J^N(\delta f) \rangle &= \frac{i\epsilon}{2} \sum_{p,q \in \Lambda} \langle \widehat{g}(q) [H_q, Q_p] - \widehat{g}(p) [H_p, Q_q] \rangle (f(q) - f(p)) \\ &= \frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) \\ &\quad + \frac{i\epsilon}{4} \sum_{p,q \in \Lambda} \langle [H_q, Q_p] + [H_p, Q_q] \rangle (f(q) - f(p)) (\widehat{g}(q) - \widehat{g}(p)), \end{aligned} \quad (6.3)$$

where in the last line we separated the result into two contribution formally skew-symmetric and symmetric in  $f, \widehat{g}$ . The second term depends only on difference of values of  $\widehat{g}$  at different sites as expected for a transport current. On the other hand, the first term depends on the value of  $\widehat{g}$  and does not seem to be of the form expected for a transport current. As was explained in [14] this contribution is related to magnetization currents. Indeed we can rewrite

$$\begin{aligned} \frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) \\ = \sum_{p,q,r \in \Lambda} M_{pqr}^N (f(q) - f(p)) (\widehat{g}(q) - \widehat{g}(r)), \end{aligned} \quad (6.4)$$

where we used skew-symmetry of  $M_{pqr}^N$ .



Written in this form, the response is proportional to the differences of  $\widehat{g}$  at different points and therefore receives appreciable contributions only from regions  $I$  and  $II$  in Fig. 5.1d. However, transformation (6.4) contains an important subtlety. The right-hand side contains magnetization which is ambiguously defined while left-hand side is unambiguous. There is no contradiction because the ambiguity in the region  $I$  will compensate the one in the region  $II$ . Moreover, in a homogeneous system the response will be zero, because these two regions compensate each other exactly. One way to deal with it is to introduce a boundary somewhere in between the two regions and enforce magnetization  $M$  to be 0 outside of the sample. This approach is used in [14] in the continuum case. However, an explicit boundary introduces additional computational challenges and makes the bulk nature of the Nernst effect obscure.

Instead of introducing a sharp boundary, we will make one parameter of the Hamiltonian  $\lambda$  to have slightly different values in regions  $I$  and  $II$  (see Fig. 5.1d). We can write the hat-shaped function  $\widehat{g}$  as a difference of two functions  $g_I$  and  $g_{II}$ ,  $\widehat{g}(p) = g_{II}(p) - g_I(p)$ , each of which is a translate of the function  $g(p)$  which depends only on  $y(p)$  and is shown in Fig. 5.1c. The functions  $g_{I,II}$  are non-constant only in regions  $I$  and  $II$  respectively. Then the magnetization contribution can be rewritten as

$$\epsilon(\lambda_{II} - \lambda_I)\mu_\lambda^N(\delta g \cup \delta f) + O((\lambda_{II} - \lambda_I)^2), \quad (6.5)$$

where  $\mu_{pqr,\lambda}^N = \frac{\partial M_{pqr}^N}{\partial \lambda}$ , and we introduced a notation

$$\mu_\lambda^N(\delta f_1 \cup \delta f_2) = \frac{1}{6} \sum_{p,q,r \in \Lambda} \mu_{pqr,\lambda}^N (f_1(q) - f_2(p))(f_2(r) - f_2(q)). \quad (6.6)$$

Combining this with other contributions we find

$$\delta \langle J^N(\delta f) \rangle \approx \epsilon(\lambda_{II} - \lambda_I) \left\{ \frac{\partial}{\partial \lambda} \left[ \beta \int_0^\infty dt e^{-st} \langle \langle J^N(\delta f, t); J^E(\delta g) \rangle \rangle + U(\delta f, \delta g) \right] + \mu_\lambda^N(\delta g \cup \delta f) \right\}, \quad (6.7)$$

where

$$U(\delta f, \delta g) = \frac{i}{4} \sum_{p,q \in \Lambda} \langle [H_q, Q_p] + [H_p, Q_q] \rangle (f(q) - f(p))(g(q) - g(p)). \quad (6.8)$$

The function  $g$  as in Fig. 5.1c is not compactly supported and thus it takes an infinite time for the system to equilibrate. Therefore, one can take the limit  $s \rightarrow 0$  while

staying in the “fast” regime. From eqs. (3.24,3.25) one finds that electric current after perturbation by gravitational potential  $\epsilon g(p)$  is equal to the current generated by

$$T(p) = \epsilon g(p)T_0, \quad (6.9)$$

$$\phi(p) = \epsilon g(p)\mu_0. \quad (6.10)$$

From continuum phenomenological equation (2.1) one finds the current across  $x = a$  line to be

$$-\epsilon T_0 \int_{-\infty}^{\infty} v_{xy} \partial_y g dy - \epsilon \mu_0 \int_{-\infty}^{\infty} \sigma_{xy} \partial_y g dy = \epsilon T_0 \int_{\lambda_I}^{\lambda_{II}} \frac{\partial v_{xy}}{\partial \lambda} d\lambda + \epsilon \mu_0 \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \sigma_{xy}}{\partial \lambda} d\lambda. \quad (6.11)$$

Comparing it to (6.7) we find

$$dv_{xy} = d \left[ \beta^2 \lim_{s \rightarrow 0} \int_0^{\infty} dt e^{-st} \langle \langle J^N(\delta f, t); J^Q(\delta g) \rangle \rangle + \beta U(\delta f, \delta g) \right] - \beta \mu^N(\delta f \cup \delta g), \quad (6.12)$$

where we introduced the notation  $J^Q = J^E - \mu J^N$  for the heat current, inverse temperature  $\beta = \frac{1}{T}$ , we dropped the subscript 0 from  $T_0$  and  $\mu_0$  since this formula contains correlation functions of the unperturbed system in equilibrium. We combined differential with respect to parameter into the differential form  $\mu^N(\delta f \cup \delta g) = \mu^N(\delta f \cup \delta g) d\lambda$  and the derivation can be straightforwardly extended to involve several parameters. The exterior derivative  $d = \sum_{\ell} d\lambda_{\ell} \frac{\partial}{\partial \lambda_{\ell}}$  acts on the parameter space.

Since rescaling the temperature is equivalent to rescaling the Hamiltonian, we can extend this exact 1-form to the enlarged parameter space which includes  $T$ . Then we can define the difference of coefficients  $\eta_{xy}$  for any two 2d materials, regardless of the temperature. Explicitly, let us define the rescaled Hamiltonian  $H_{\lambda_0} = \lambda_0 H$ , where we introduced an additional scaling parameter  $\lambda_0$ . Then

$$\left( T \frac{\partial}{\partial T} + \lambda_0 \frac{\partial}{\partial \lambda_0} \Big|_{\lambda_0=1} \right) v_{xy}(\lambda_0, T) = 0. \quad (6.13)$$

Therefore we can define the  $T$ -component of the 1-form on the enlarged parameter space as follows:

$$\frac{dv_{xy}}{dT} = \frac{\partial}{\partial T} \left[ \beta^2 \int_0^{\infty} dt e^{-st} \langle \langle J^N(\delta f, t); J^Q(\delta g) \rangle \rangle + \beta U(\delta f, \delta g) \right] - \beta^2 \tau^N(\delta f \cup \delta g), \quad (6.14)$$

where  $\tau^N(\delta f \cup \delta g)$  is given by eq. (6.6) with  $\mu_{pqr}$  replaced with

$$\tau_{pqr}^N = \beta \langle \langle H_p; J_{qr}^N \rangle \rangle + \beta \langle \langle H_r; J_{pq}^N \rangle \rangle + \beta \langle \langle H_q; J_{rp}^N \rangle \rangle, \quad (6.15)$$

which is obtained from  $\mu^N$  by replacing  $dH_p$  with  $-H_p$ .

### Ettingshausen effect

One can derive a formula for the coefficient  $\eta_{xy}$  in a similar way. In this section, we will display only the key steps, since all arguments are the same.

In order to find the coefficient we deform the Hamiltonian density by

$$\Delta H_p = \epsilon e^{st} \widehat{g}(p) Q_p, \quad (6.16)$$

where  $\widehat{g}(p)$  is a hat-shaped function of  $y(p)$  as in Fig. 5.1b.

The change in the energy current across a vertical line  $x = a$  is

$$\Delta \langle J^E(\delta f) \rangle = \langle \Delta J^E(\delta f) \rangle + \epsilon \beta \int_0^\infty dt e^{-st} \langle \langle J^E(\delta f, t); J^N(\delta \widehat{g}) \rangle \rangle, \quad (6.17)$$

where  $f = \theta(a - x(p))$ . The explicit variation of the current is

$$\begin{aligned} \langle \Delta J^E(\delta f) \rangle &= \frac{i\epsilon}{2} \sum_{p,q \in \Lambda} \langle \widehat{g}(p) [H_q, Q_p] - \widehat{g}(q) [H_p, Q_q] \rangle (f(q) - f(p)) \\ &= \frac{\epsilon}{4} \sum_{p,q \in \Lambda} \langle J_{pq}^N \rangle (\widehat{g}(p) + \widehat{g}(q)) (f(q) - f(p)) - U(\delta f, \delta \widehat{g}). \end{aligned} \quad (6.18)$$

The first term can be expressed in terms of magnetization as in (6.4). We write  $\widehat{g}(p)$  as a difference  $\widehat{g}(p) = g_{II}(p) - g_I(p)$ , where  $g_{I,II}$  are translates of a smeared step-function  $g(p)$ . Then we rewrite the response as a difference of conductivities of different materials:

$$\begin{aligned} \delta \langle J^E(\delta f) \rangle &\approx \epsilon (\lambda_{II} - \lambda_I) \left\{ \frac{\partial}{\partial \lambda} \left[ \beta \int_0^\infty dt e^{-st} \langle \langle J^E(\delta f, t); J^N(\delta g) \rangle \rangle \right. \right. \\ &\quad \left. \left. - U(\delta f, \delta g) \right] + \mu_\lambda^N(\delta g \cup \delta f) \right\}. \end{aligned} \quad (6.19)$$

On the other hand, from the continuum phenomenological equation (2.2) one finds the current across the line  $x = a$  to be

$$-\epsilon \int_{-\infty}^\infty \eta_{xy} \partial_y g dy - \epsilon \mu \int_{-\infty}^\infty \sigma_{xy} \partial_y g dy = \epsilon \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \eta_{xy}}{\partial \lambda} d\lambda + \epsilon \mu \int_{\lambda_I}^{\lambda_{II}} \frac{\partial \sigma_{xy}}{\partial \lambda} d\lambda, \quad (6.20)$$

where the second term originates from the contribution of  $\phi \mathbf{j}^N$  to  $\mathbf{j}^E$ . Comparing it to (6.19) we find

$$d\eta_{xy} = d \left[ \beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle - U(\delta f, \delta g) \right] - \beta \mu^N(\delta f \cup \delta g). \quad (6.21)$$

This 1-form can be extended to include temperature as a parameter using the scaling relation

$$\left( T \frac{\partial}{\partial T} + \lambda_0 \frac{\partial}{\partial \lambda_0} \Big|_{\lambda_0=1} \right) \frac{\eta_{xy}(\lambda_0, T)}{T} = 0. \quad (6.22)$$

Therefore we can define the  $T$ -component of the 1-form on the enlarged parameter space as follows:

$$\frac{d}{dT} \frac{\eta_{xy}}{T} = \frac{\partial}{\partial T} \left[ \beta^2 \int_0^\infty dt e^{-st} \langle \langle J^Q(\delta f, t); J^N(\delta g) \rangle \rangle - \beta U(\delta f, \delta g) \right] - \beta^2 \tau^N(\delta f \cup \delta g), \quad (6.23)$$

where  $\tau^N$  is given by (6.15).

### Symmetric parts of transport coefficients

Note that the 1-forms  $\mu^N(\delta f \cup \delta g)$  and  $\tau^N(\delta f \cup \delta g)$  are formally skew-symmetric under the exchange of  $f$  and  $g$ . To make use of this symmetry, we need to argue that  $f$  can be replaced with a smeared step-function in the  $x$  direction. This can be argued as follows. Replacing  $f$  with a smeared step-function changes the operators  $J^N(\delta f)$  and  $J^E(\delta f)$  by  $J^N(\widehat{\delta f})$  and  $J^E(\widehat{\delta f})$ . The latter operators can be equivalently written as  $\frac{dQ(\widehat{f})}{dt}$  and  $\frac{dH(\widehat{f})}{dt}$ , where

$$Q(\widehat{f}) = \sum_p \widehat{f}(p) Q_p, \quad H(\widehat{f}) = \sum_p \widehat{f}(p) H_p, \quad (6.24)$$

and  $\widehat{f}(p)$  is a hat-shaped function which depends only on  $x(p)$ . The expectation value of these observables in the NESS that we are considering must be zero for any finite  $s$  and thus zero also in the limit  $s \rightarrow 0$ . Thus we can replace  $f$  with a smeared step-function in the  $x$ -direction without affecting  $\nu_{xy}$  or  $\eta_{xy}$ .

After this has been done, exchanging  $f$  and  $g$  is equivalent to exchanging  $x$  and  $y$ . Thus  $\mu^N(\delta f \cup \delta g)$  does not enter the microscopic formulas for the symmetrized

thermoelectric coefficients. These formulas then can be integrated, giving

$$\begin{aligned} v_{xy}^S = \frac{\beta^2}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left[ \langle\langle J^N(\delta f, t); J^Q(\delta g) \rangle\rangle + \langle\langle J^N(\delta g, t); J^Q(\delta f) \rangle\rangle \right] \\ + \beta U(\delta f, \delta g), \end{aligned} \quad (6.25)$$

$$\begin{aligned} \eta_{xy}^S = \frac{\beta}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left[ \langle\langle J^Q(\delta f, t); J^N(\delta g) \rangle\rangle + \langle\langle J^Q(\delta g, t); J^N(\delta f) \rangle\rangle \right] \\ - U(\delta f, \delta g). \end{aligned} \quad (6.26)$$

As we show in Appendix C.2, the two terms on the right-hand side of these equation are not separately invariant under Hamiltonian density redefinition, but the full transport coefficients are invariant. The correction term  $U(\delta f, \delta g)$  is zero for fermionic systems with only density-dependent interactions (see Appendix C.3 for more details).

### Skew-symmetric parts of transport coefficients

In a similar way one can find skew-symmetric parts of transport coefficients

$$\begin{aligned} dv^A = d \left[ \frac{\beta^2}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left( \langle\langle J^N(\delta f, t); J^Q(\delta g) \rangle\rangle - \langle\langle J^N(\delta g, t); J^Q(\delta f) \rangle\rangle \right) \right] \\ - \beta \mu^N(\delta f \cup \delta g), \end{aligned} \quad (6.27)$$

$$\begin{aligned} d\eta^A = d \left[ \frac{\beta}{2} \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \left( \langle\langle J^Q(\delta f, t); J^N(\delta g) \rangle\rangle - \langle\langle J^Q(\delta g, t); J^N(\delta f) \rangle\rangle \right) \right] \\ - \beta \mu^N(\delta f \cup \delta g). \end{aligned} \quad (6.28)$$

These formulas give only derivatives of transport coefficients with respect to parameters. Integration of these formulas over parameters or temperature gives the difference of relative transport coefficients at different values of parameters. It is natural to define relative transport coefficients of a trivial insulator to be zero. Determination of the relative transport coefficient in this case would correspond to integration over a path in the parameter space from a trivial insulator to the material of interest.

## 6.3 Discussion

In this chapter we have derived microscopic formulas for “transverse” thermoelectric coefficients of general 2d lattice systems. It was convenient to decompose them into

symmetric and anti-symmetric parts, since they have qualitatively different behavior: the former are absolute transport coefficients, while the latter are relative. Similar formulas for electric Hall conductivity and thermal Hall conductivity have already been derived in Chapter 5.

The usual Kubo formulas for transport coefficients require averaging the correlators of currents over the whole space. In contrast, our microscopic formulas involve net currents through two perpendicular lines. This is because a current on a 2d lattice is a function of a pair of points, and the natural observable associated to it is localized on a line rather than at a point. Despite this, after the limit  $s \rightarrow 0$  has been taken, our formula computes the same quantity as the usual continuum Kubo formula.

It is natural to ask whether longitudinal components of conductivity, thermal conductivity, and thermoelectric tensors of a 2d lattice system can be computed in a similar manner. This is easily achieved: one simply replaces two perpendicular lines with two lines making a nonzero angle  $\theta$ . It is easy to see determine from hydrodynamics which linear combination of components of the transport tensors describes the corresponding linear response. For example, if both currents involved are electric currents, one of the lines is given by  $y = 0$ , and the other one is  $y = x \cdot \tan \theta$ , then the correlator

$$\beta \lim_{s \rightarrow 0^+} \int_0^\infty e^{-st} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle dt \quad (6.29)$$

measures  $\sigma_{xy} - \frac{1}{\tan \theta} \sigma_{yy}$ . Thus by changing the functions  $f, g$  one can extract all four components of the conductivity tensor. The same is true about other transport coefficients.

In this chapter we focused on the case of 2d materials, but the 3d case can be accommodated as well. One can simply replace a lattice in  $\mathbb{R}^2$  with a lattice in  $\mathbb{R}^2 \times [0, L]$ , impose periodic boundary conditions in the third direction, divide all formulas by  $L$ , and take the limit  $L \rightarrow \infty$ . The functions  $f, g$  remain independent of the third coordinate. It should not matter whether the limit  $L \rightarrow \infty$  is taken before or after the limit  $s \rightarrow 0$ , since the problem is translationally invariant in the third direction.

In the 2d case, the quantity  $\nu^A(T)$  (normalized relative to the vacuum) is dimensionless, and Bloch's theorem implies that for gapped systems  $\nu^A(0)$  does not change under the variations of the Hamiltonian which do not close the gap. Thus if  $\nu^A(0)$  were nonzero, it would represent a new topological invariant of gapped 2d phases

of matter. However, we will show in the next chapter that on very general grounds  $\nu^A(0)$  vanishes for all gapped systems. By Onsager reciprocity, the  $T \rightarrow 0$  limit of  $\eta^A(T)/T$  also vanishes. Thus topological invariants of gapped 2d systems arise only from the Hall conductivity and the thermal Hall conductivity.

## NERNST AND ETTINGSHAUSEN EFFECTS IN GAPPED QUANTUM MATERIALS

### 7.1 Introduction

One of the most striking features of topological phases of matter is their unusual transport properties. Famously, 2D materials with broken time-reversal symmetry and a bulk energy or mobility gap can exhibit electric Hall conductance and thermal Hall conductance which are not exponentially suppressed at low temperatures. This can be attributed to chiral gapless edge modes which carry both electric and energy currents and are robust under arbitrary perturbations which do not close the gap. It is natural to ask whether other thermoelectric properties can exhibit similar anomalous behavior. In particular, can there be quantum Nernst and Ettingshausen effects by analogy with the quantum Hall and quantum thermal Hall effects? More generally, it is of interest to understand fundamental constraints on thermoelectric transport at low temperatures.

In the linear regime, the Nernst and Ettingshausen effects in 2D materials are usually described in terms of two coefficients  $\nu_{xy}$  and  $\eta_{xy}$  which enter the phenomenological expressions for net electric and heat currents<sup>1</sup>:

$$I_x^{el} = -\sigma_{xy}(T)\Delta_y\mu - \nu_{xy}(T)\Delta_yT, \quad (7.1)$$

$$I_x^{heat} = -\eta_{xy}(T)\Delta_y\mu - \kappa_{xy}(T)\Delta_yT. \quad (7.2)$$

Here  $\mu$  is the electrochemical potential (we are working in units where the electron charge  $e$  is set to 1),  $T$  is the temperature, and we assumed that  $\mu$  and  $T$  depend only on the  $y$ -coordinate. The coefficients  $\sigma_{xy}$  and  $\kappa_{xy}$  are the Hall conductance and the thermal Hall conductance, respectively. The coefficients  $\nu_{xy}$  and  $\eta_{xy}$  are usually called transverse thermoelectric coefficients; we will call them the Nernst and Ettingshausen coefficients, respectively.

The coefficients  $\sigma_{xy}$  and  $\nu_{xy}$  are dimensionless, while  $\eta_{xy}$  and  $\kappa_{xy}$  have the units of energy. Thus the quantum Nernst effect would mean that  $\nu_{xy}(T)$  approaches a

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<sup>1</sup>If time-reversal symmetry is present, Onsager reciprocity implies that  $\eta_{xy} = T\nu_{yx}$ , but in this chapter we are interested in situations where time-reversal symmetry is broken, either by an external magnetic field or spontaneously.



nonzero constant  $\nu_{xy}(0)$  at  $T = 0$ , while the quantum Ettingshausen effect would mean that  $\eta_{xy} = bT + \dots$ , where  $b$  is a nonzero constant and the dots denote terms which vanish faster than linearly (in a gapped material, presumably the dotted terms are exponentially suppressed). In a gapped material, there should be no appreciable bulk currents, and thus it should be possible to interpret the net currents (7.1-7.2) in terms of edge currents. Indeed, it is easy to see that if  $b = -\nu_{xy}(0)$ , then one can attribute (7.1-7.2) to chiral edge modes with equilibrium electric and energy currents

$$I_{edge}^{el} = -\sigma_{xy}(0)\mu - \nu_{xy}(0)T, \quad (7.3)$$

$$I_{edge}^E = -\sigma_{xy}(0)\frac{\mu^2}{2} - \nu_{xy}(0)T\mu - \frac{1}{2}cT^2. \quad (7.4)$$

Here we also assumed that  $\kappa_{xy}(T) = cT$  for some dimensionless constant  $c$ . F. Bloch's theorem [10, 60] and its energy counterpart of Chapter 4 prohibit equilibrium currents in genuine 1D systems, but not for edges of 2D systems.

For IQHE and FQHE systems, it was shown in 5 that both  $\sigma_{xy}(0)$  and  $c$  are nonzero and are topological invariants. If  $\nu_{xy}(0)$  were nonzero for some system, it would be a new topological invariant of gapped 2D materials. To see this, consider a strip of a 2D material infinitely extended in the  $x$  direction but having a finite extent in the  $y$  direction. Suppose that the parameters of the Hamiltonian are slowly varying in the  $y$  direction while maintaining a bulk gap. On the one hand, this system can be thought of as a 1D system, and therefore the net currents must vanish in equilibrium. Thus in equilibrium (that is, for constant  $T$  and  $\mu$ ) the edge currents must cancel between the two edges. On the other hand, the edge currents should be determined by the Hamiltonians near the respective edges. Thus  $\sigma_{xy}(0)$ ,  $\nu_{xy}(0)$ , and  $c$  do not change under the variations of the Hamiltonian which do not close the bulk energy gap.

It is well-known that if the edge modes are non-interacting fermions, both  $\nu_{xy}(T)$  and  $\eta_{xy}(T)/T$  vanish at  $T = 0$ . This follows from two observations: (1) systems of free fermions have approximate particle-hole symmetry which becomes exact at  $T = 0$ ; (2) under the particle-hole symmetry, the temperature and the energy current are even, while the electrochemical potential, the electric current, and the Nernst and Ettingshausen coefficients are odd. Thus a necessary condition for a nonzero  $\nu_{xy}(0)$  are strong interactions.

In the case when the edge modes are described by a 1+1d Conformal Field Theory, it is well-known that non-zero values of  $\sigma_{xy}(0)$  and  $c$  are related to  $U(1)$  and

gravitational anomalies, respectively, which can be cancelled by Chern-Simons and gravitational Chern-Simons terms in the bulk. By analogy one might expect that a nonzero value of  $\nu_{xy}(0)$  is related to topological terms in the bulk action involving both  $U(1)$  and gravitational fields. Since such terms cannot be constructed, the conclusion seems to be that the quantum Nernst and Ettingshausen effects do not exist either. However, this argument relies on the assumption that every anomaly of the edge modes can be cancelled by a term in the bulk effective action. This is not obvious and in fact is not true in certain non-unitary conformal field theories (CFTs). Specifically, ghost CFTs have mixed  $U(1)$ -gravitational anomalies [23]. In general, it is not understood which field theory anomalies can always be cancelled by bulk topological terms.

In this chapter we describe three arguments of varying generality showing that for gapped systems  $\nu_{xy}(0) = \lim_{T \rightarrow 0} \eta_{xy}(T)/T = 0$  and thus the quantum Nernst and Ettingshausen effects do not exist. In Section 7.2 we deduce the vanishing of  $\nu_{xy}(0)$  and  $\lim_{T \rightarrow 0} \eta_{xy}(T)/T$  from the Third Law of Thermodynamics. We also clarify the constraints imposed by the Third Law on the Seebeck and Peltier effects. In Section 7.3 we present another argument for the vanishing of  $\nu_{xy}(0)$  and  $\lim_{T \rightarrow 0} \eta_{xy}(T)/T$ , under the assumption that the edges are described by a *unitary* CFT. In Section 7.4 we present yet another argument for the vanishing of  $\nu_{xy}(T)$  at low temperatures, based on a flux insertion thought experiment. This argument does not require a unitary CFT structure for edge excitations, but it does invoke some reasonable but hard-to-prove physical assumptions. As part of the latter argument, we also show that there is no analog of the Thouless pump for entropy. We discuss our results in the concluding Section.

## 7.2 Thermoelectric coefficients of gapped materials and the Third Law

Consider a material with short-range interactions and either a bulk energy gap or a mobility gap.<sup>2</sup> If the temperature  $T$  is well below the bulk gap, the entropy production rate per unit volume should be exponentially small. From (2.6) we see that both  $\sigma^S(T)$  and  $\kappa^S(T)$  are exponentially small, while  $\eta_{mk}(T) \simeq -T\nu_{km}(T)$  up to exponentially small corrections.

Let us show that the Third Law of Thermodynamics implies  $\lim_{T \rightarrow 0} \eta^S(T)/T = \nu^S(0) = 0$ . One standard formulation of the Third Law ("the Nernst unattainability principle" [42]) states that it is impossible to lower the entropy of a body to its

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<sup>2</sup>The assumption about short-range interactions is made to exclude superconductors, where an energy gap arises only due to long-range Coulomb interactions.

zero-temperature value within a finite time. The Nernst unattainability principle prohibits creating a *perpetuum mobile* of the third kind (a Carnot engine where one of the heat baths is at  $T = 0$ ). Consider two heat baths at low  $T$  connected by a cylindrical “bridge” made of the material of interest. If one applies an electric field across the bridge, the entropy current density across the bridge is given by eq. (2.7). Since  $\kappa^S(T)$  is exponentially small, the magnitude of the entropy current is determined by  $\eta^S(T)/T$ . If  $\lim_{T \rightarrow 0} \eta^S(T)/T \neq 0$ , a nonzero amount of entropy  $\Delta S$  will be transported across the bridge per unit time even as  $T$  approaches zero. If the excess entropy of the “source” heat bath over its zero- $T$  value is  $S$ , it would take a finite time  $S/\Delta S$  to lower its entropy to its zero- $T$  value, in contradiction with the Nernst unattainability principle. Hence we must have  $\lim_{T \rightarrow 0} \eta^S(T)/T = 0$ . Then Onsager reciprocity (2.4) implies  $\nu^S(0) = 0$ . This argument is very robust and does not depend on the existence of the bulk gap.

To show that  $\lim_{T \rightarrow 0} \eta^A(T)/T = \nu^A(0) = 0$ , we make use of another common formulation of the Third Law: “the Nernst heat theorem”. It states that the  $T \rightarrow 0$  limit of the entropy of a body is finite and independent of the parameters of the Hamiltonian. It does not follow from the Nernst unattainability principle without additional assumptions [37] (for a recent discussion see [34]). For example, the ideal Boltzmann gas violates the Nernst heat theorem because its entropy diverges as  $T \rightarrow 0$ . Nevertheless, if one assumes that the  $T \rightarrow 0$  limit of the entropy is finite (“the Einstein principle”) and that the specific heat is strictly positive, one can deduce the Nernst heat theorem from the Nernst unattainability principle [37].

Consider a piece of material shaped as a cylindrical shell with caps on both ends. The shell is in contact with a heat bath at temperature  $T$ . Suppose there is a current-carrying solenoid inside the cylinder so that the two caps are subject to a magnetic field  $\pm B$ . We also assume that the material is not completely homogeneous and interpolates between a trivial insulator at one end and a gapped material of interest at the other end. At strictly zero  $T$  this might lead to a divergent correlation length at the interface between the two materials. However, at  $T > 0$  one expects such an interpolation to be possible while maintaining a finite correlation length throughout. For example, if the interface is described by a 1+1d CFT, the correlation length is of order  $1/T$ . This ensures that a hydrodynamic description is possible.

The main ingredient in the argument is the thermodynamic formula for the Nernst

coefficient [51]:

$$\nu^A(T) = \left( \frac{\partial m}{\partial T} \right)_\mu = \left( \frac{\partial s}{\partial B} \right)_\mu, \quad (7.5)$$

where  $m$  is magnetization per unit area and  $s$  is the entropy per unit area. Eq. (7.5) and a similar formula for the Hall conductance [52] are usually called Středa formulas, although they appeared already in [45]. Eq. (7.5) is not exact, but it becomes exact in gapped materials at low  $T$  if one assumes that in this limit only surface currents are non-zero [45, 52, 51]. This is discussed further in Appendix D.1.

According to the Nernst heat theorem, the entropy  $S$  of the cylinder must approach a  $B$ -independent constant at  $T = 0$ . On the other hand, we can compute the derivative of the entropy with respect to  $B$  using (7.5). The latter calculation gives

$$\left( \frac{\partial S}{\partial B} \right)_\mu = (\nu^A(T) - \nu_0^A(T))A, \quad (7.6)$$

where  $A$  is the area of the cap and  $\nu_0^A(T)$  is the Nernst coefficient of the trivial insulator. By the Nernst heat theorem, the l.h.s. of Eq. (7.6) approaches zero as  $T \rightarrow 0$ . Since the Nernst coefficient of the trivial insulator is zero, this implies  $\nu^A(0) = 0$ . Then Onsager reciprocity implies  $\lim_{T \rightarrow 0} \eta^A(T)/T = 0$ .

The above argument deserves a few comments. First, we should mention that we have made an implicit assumption, namely that the bulk energy (or mobility) gap remains open for sufficiently small  $B$ , where  $B$  is the magnetic field produced by the solenoid. This assumption is necessary to justify the Středa formula, Eq. (7.5).

Our second comment involves an interesting example, namely the  $\nu = 5/2$  FQH state. It was proposed by several authors [15, 61] that for this state, the gap  $\Delta_n$  for neutral bulk excitations might be much lower than the gap  $\Delta_c$  for charged excitations. If  $\Delta_n \ll T \ll \Delta_c$ , these neutral excitations have an extensive and  $B$ -dependent entropy, so that  $(\partial s/\partial B)_N$  is independent of  $T$  and nonzero. Given this  $B$  dependent entropy, one might think that the  $\nu = 5/2$  FQH state could have a nonzero Nernst coefficient  $\nu^A(T)$  at very low temperatures. However, this is *not* the case since the quantity that appears in Eq. (7.6) is  $(\partial s/\partial B)_\mu$  not  $(\partial s/\partial B)_N$ . Indeed, the results of [15, 61] imply that  $(\partial s/\partial B)_\mu = 0$  in this temperature range, and thus  $\nu^A(T) \simeq 0$ .

### 7.3 Equilibrium currents in a unitary CFT

In this section we show that if edge degrees of freedom of a 2D gapped material are described by a unitary 1+1d CFT with a  $U(1)$  symmetry, then the edge  $U(1)$

current is independent of  $T$ . Likewise, we show that the edge energy current has no  $\mu$  dependence except for the first term in Eq. (7.4). Translating these results into the language of transport coefficients, it follows that  $\nu^A(T)$  and  $\eta^A(T)/T$  are exponentially suppressed at low temperatures for any material of this kind.

By assumption, the edge excitations are described by a unitary CFT whose operator content includes a traceless symmetric conserved energy-momentum tensor  $T$  and a conserved  $U(1)$  current  $J$ . After performing the Wick rotation and introducing complex coordinates [18], the operator product expansions of the left-moving energy-momentum  $T(z) = \sum_n L_n z^{-n-2}$  and  $U(1)$  currents  $J(z) = \sum_n J_n z^{-n-1}$  are:

$$T(z)T(w) \sim \frac{c_L/2}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial T(w)}{(z-w)} + \text{reg}, \quad (7.7)$$

$$T(z)J(w) \sim \frac{\alpha_L}{(z-w)^3} + \frac{J(w)}{(z-w)^2} + \frac{\partial J(w)}{(z-w)} + \text{reg}, \quad (7.8)$$

$$J(z)J(w) \sim \frac{k_L}{(z-w)^2} + \text{reg}. \quad (7.9)$$

Analogous expressions are true for the right-moving currents  $\bar{T}$  and  $\bar{J}$ . This leads to the following transformation law under a conformal change of coordinates:

$$u'^2 \tilde{T}(u) = T(z) - \frac{c_L}{12} \left\{ \frac{u'''}{u'} - \frac{3}{2} \left( \frac{u''}{u'} \right)^2 \right\}, \quad (7.10)$$

$$u' \tilde{J}(u) = J(z) - \frac{\alpha_L}{2} \frac{u''}{u'}, \quad (7.11)$$

where  $u(z)$  is a conformal transformation and prime indicates derivatives with respect to  $z$ .

Under a gauge transformation  $\Omega(z)$  the currents change as follows:

$$\tilde{T} = T + \frac{\alpha_L}{2} (\ln \Omega)'' + \frac{k_L}{2} (\ln \Omega)'^2 - (\ln \Omega)' J(z), \quad (7.12)$$

$$\tilde{J} = J - k_L (\ln \Omega)'. \quad (7.13)$$

The energy and  $U(1)$  currents are given by

$$\langle j^E \rangle = \langle T_{tx} \rangle = \frac{1}{2\pi} \langle T - \bar{T} \rangle, \quad (7.14)$$

$$\langle j^N \rangle = \langle J_x \rangle = \frac{1}{2\pi} \langle J - \bar{J} \rangle, \quad (7.15)$$

where  $T_{tx}$  is time-space component of the standard energy-momentum tensor and  $J_x$  is the charge current. In the plane geometry the expectation values of  $j^E$  and  $j^N$

are equal zero due to conformal invariance. Expectation values of the currents at a finite temperature  $1/\beta$  can be found by a conformal transformation from a cylinder onto the plane [9, 2]:

$$u(z) = \exp \left[ \frac{2\pi i}{\beta} (\tau + ix) \right], \quad (7.16)$$

where  $z = \tau + ix$  is coordinate on a cylinder with periodic time  $\tau \sim \tau + \beta$  and  $u$  is a complex coordinate on the plane. Using the transformation law for the currents we find

$$\langle j^E \rangle_\beta = \frac{\pi}{12\beta^2} (c_L - c_R), \quad (7.17)$$

$$\langle j^N \rangle_\beta = \frac{i}{2\beta} (\alpha_L - \alpha_R). \quad (7.18)$$

In order to find the currents at non-zero electrochemical potential we can study the behavior of the operators under  $U(1)$  gauge transformations. One can see from eq. (7.12) that under a large gauge transformation

$$\Omega(z) = \exp(-\mu z) \quad (7.19)$$

the Hamiltonian  $H = \frac{1}{2\pi} (L_0 + \bar{L}_0)$  transforms as  $H \rightarrow H + \mu Q$  where  $Q = \frac{1}{2\pi} (J_0 + \bar{J}_0)$ . Therefore, a change in the electric potential can be mimicked by the gauge transformation (7.19). The currents change as follows:

$$\langle j^E \rangle_{\beta, \mu} = \frac{\pi}{12\beta^2} (c_L - c_R) + \frac{i\mu}{2\beta} (\alpha_L - \alpha_R) + \frac{(k_L - k_R) \mu^2}{2\pi} \frac{\mu^2}{2} \quad (7.20)$$

$$\langle j^N \rangle_{\beta, \mu} = \frac{i}{2\beta} (\alpha_L - \alpha_R) + \frac{k_L - k_R}{2\pi} \mu. \quad (7.21)$$

By considering two edges at slightly different temperatures and chemical potentials (or by comparing these expressions to (7.3) and (7.4)) we find the transport coefficients to be

$$\kappa^A = \frac{\pi}{6\beta} (c_R - c_L), \quad (7.22)$$

$$\nu^A = \frac{i}{2} (\alpha_R - \alpha_L), \quad (7.23)$$

$$\eta^A = \frac{iT}{2} (\alpha_R - \alpha_L), \quad (7.24)$$

$$\sigma^A = \frac{k_R - k_L}{2\pi}. \quad (7.25)$$

Now we will show that a non-zero value of either  $\alpha_L$  or  $\alpha_R$  contradicts the unitarity of the CFT. The operator product expansion (7.8) leads to the following commutation

relation for the modes of the energy-momentum tensor  $T(z) = \sum_n L_n z^{-n-2}$  and  $U(1)$  current  $J(z) = \sum_n J_n z^{-n-1}$ :

$$[L_n, J_m] = \alpha_L \frac{(n+1)n}{2} \delta_{n+m,0} - m J_{n+m}. \quad (7.26)$$

Using the fact that unitary CFT has a unique vacuum  $|0\rangle$  invariant under global conformal transformations  $L_{\pm 1}|0\rangle = L_0|0\rangle = 0$ , we find

$$0 = \langle [L_1, J_{-1}] \rangle + \langle [L_{-1}, J_1] \rangle = \alpha_L. \quad (7.27)$$

Similarly one can show that  $\alpha_R = 0$ .

#### 7.4 Flux insertion argument for vanishing of the Nernst coefficient

In this section, we present a flux insertion argument showing that the Nernst coefficient  $\nu^A(T)$  is exponentially small at low temperatures in any 2D gapped many-body system with short-range interactions and a  $U(1)$  symmetry. In the process, we also prove that there is no analog of a Thouless pump for entropy.

##### Statement of the main result

Consider a 2D gapped many-body system with short-range interactions and a  $U(1)$  symmetry, defined in a *cylinder* geometry. Consider a mixed state of the following form:

- The top edge of the cylinder is at temperature  $T_t$  and chemical potential  $\mu_t$ .
- The bottom edge of the cylinder is at temperature  $T_b$  and chemical potential  $\mu_b$ .
- The bulk of the cylinder is in one of a finite set of topologically degenerate ground states.

Here we assume that  $T_t, T_b \ll \Delta$  where  $\Delta$  is the bulk gap, and that  $\mu_t, \mu_b$  are in an appropriate range so that they are consistent with a bulk gap. Physically this mixed state can be prepared by starting the system in one of its ground states, coupling the system to appropriate baths at the two edges, and then decoupling the heat baths from the system.

We will denote the above mixed state by  $\rho_0$ . More generally, we let  $\rho_\theta$  denote the same kind of mixed state as above, but in the presence of magnetic flux  $\theta$  through the cylinder, where  $0 \leq \theta < 2\pi$ .

A few comments about the mixed states  $\rho_0$  and  $\rho_\theta$ : first, we should mention that  $\rho_0$  and  $\rho_\theta$  are only *approximately* stationary: if the system is initialized in one of these states, it will eventually relax to a fully equilibrated state in which the two edges are at the same temperatures and chemical potentials. We will mostly neglect this relaxation because it happens at very long time scales: the time scale for the relaxation process is set by dissipative transport coefficients which are exponentially small at low temperatures. Another comment about  $\rho_0$  and  $\rho_\theta$  is that these mixed states are not uniquely defined in the case where there are multiple topologically degenerate ground states. This ambiguity is not important for our purposes because we will only be interested in local observables, and all the different choices of  $\rho_\theta$  share the same expectation values for such observables.

We are now ready to state our main result. Define the “flux-averaged” current  $\bar{I}$  by

$$\bar{I} = \frac{1}{2\pi} \int_0^{2\pi} \text{Tr}(I\rho_\theta) d\theta, \quad (7.28)$$

where  $I$  is the  $U(1)$  current operator around the cylinder. Our main result is that  $\bar{I}$  is given by

$$\bar{I} = \sigma^A(0)(\mu_t - \mu_b) \quad (7.29)$$

up to an error term that is exponentially small for temperatures  $T_b, T_t \ll \Delta$ . Here,  $\sigma^A(0)$  denotes the zero temperature Hall conductance of the gapped many-body system.

We can go a step further if we make the “flux-averaging assumption” that  $\text{Tr}(I\rho_\theta)$  is independent of  $\theta$ . Under that assumption, Eq. (7.29) implies that

$$I = \sigma^A(0)(\mu_t - \mu_b), \quad (7.30)$$

where  $I$  is the expectation value of the current for any *fixed* value of flux, say  $\theta = 0$ .

The most important implication of these results is that  $\bar{I}$  and  $I$  do not depend on the temperature of the top or bottom edge, except for terms that are exponentially small for temperatures  $T_t, T_b \ll \Delta$ . This lack of temperature dependence means that the Nernst coefficient  $\nu^A(T) = \frac{dI}{dT}$  is also exponentially small for temperatures  $T \ll \Delta$ .

### Outline of the argument

Our argument is based on a flux insertion process similar to that of Laughlin [38]. We imagine initializing the system in the (zero flux) mixed state  $\rho_0$  described above.



We then imagine slowly inserting  $2\pi$  flux through the hole of the cylinder. Here when we say “slowly” we mean that the flux should be inserted over a time scale  $\mathcal{T}$  that is much longer than  $1/\Delta$  and also much longer than  $\tau$  where  $\tau$  is the relaxation time scale associated with the edge excitations. We will also assume that the flux insertion time scale  $\mathcal{T}$  is much *shorter* than the exponentially long time scale associated with equilibration between the two edges. This hierarchy of time scales is important because it guarantees that the flux insertion process is a “quasi-static” process, i.e. each edge remains in local thermal equilibrium throughout the process.

We make two claims about this flux insertion experiment which we will prove below. Our first claim is a finite temperature variant of one of the standard claims from Laughlin’s original flux insertion argument [38]:

**Claim 1** *The following identity holds:*

$$\bar{I} = \frac{\Delta E}{2\pi}, \quad (7.31)$$

where  $\Delta E$  is the change in the expectation value of the total energy of the cylinder when  $2\pi$  flux is inserted.

Our second claim is less familiar but can be derived from a basic thermodynamic inequality, together with locality properties of the flux insertion process:

**Claim 2** *The following inequalities hold:*

$$\Delta E_t \geq \mu_t \Delta N_t, \quad \Delta E_b \geq \mu_b \Delta N_b, \quad (7.32)$$

where  $\Delta E_t$  and  $\Delta N_t$  are the changes in the expectation values of the energy and number of particles near the top edge when  $2\pi$  flux is inserted through the cylinder, and  $\Delta E_b$  and  $\Delta N_b$  are defined similarly, but near the bottom edge.

Once we prove these claims, we can easily derive our main result, Eq. (7.29). The first step is to note that

$$\Delta E = \Delta E_t + \Delta E_b \quad (7.33)$$

since the flux insertion process does not change the energy density in the bulk (i.e. it returns the bulk to one of its ground states). Next, we note that the quantities  $\Delta N_t$  and  $\Delta N_b$  are related to the zero temperature Hall conductance  $\sigma^A(0)$  by

$$\Delta N_t = -\Delta N_b = 2\pi\sigma^A(0) \quad (7.34)$$

up to exponentially small corrections. Then, we combine (7.31), (7.32), (7.33), and (7.34) to deduce the inequality

$$\bar{I} \geq \sigma^A(0)(\mu_t - \mu_b). \quad (7.35)$$

Next, imagine rotating the cylinder by 180 degrees (exchanging the top and bottom of the cylinder). This operation changes  $\mu_b \leftrightarrow \mu_t$ , and replaces  $\bar{I} \rightarrow -\bar{I}$ , while preserving the Hall conductance  $\sigma^A(0)$ , so we deduce the inequality

$$-\bar{I} \geq \sigma^A(0)(\mu_b - \mu_t). \quad (7.36)$$

Combining the two inequalities (7.35), (7.36) proves the result (7.29).

In the next two sections we give physical arguments for Claims 1 and 2.

### Physical argument for Claim 1

To prove Claim 1, we directly compute the change in the expectation value of the energy of the cylinder,  $\Delta E$ .

First, we need to introduce some notation. Let  $H$  denote the initial Hamiltonian and let  $\theta(t)$  denote the flux through the cylinder at time  $t$ . We define the corresponding time dependent Hamiltonian  $H(t)$  as follows: we choose a branch cut that runs from one end of the cylinder to the other, and then we “twist” all the terms in  $H$  that straddle this branch cut by conjugating them by the unitary operator  $e^{i\theta(t)Q_+}$  where  $Q_+$  denotes the total  $U(1)$  charge on one side of the branch cut. A convenient feature of this gauge choice is that the initial and final Hamiltonians are the same, i.e.  $H(0) = H(\mathcal{T})$ , since  $\theta(\mathcal{T}) = 2\pi$ .

Next, let  $U(t)$  denote the unitary time evolution operator,

$$U(t) = \mathbf{T} \exp \left[ -i \int_0^t dt' H(t') \right]. \quad (7.37)$$

Finally, let  $U \equiv U(\mathcal{T})$  denote the time evolution operator for the whole flux insertion process.

With this notation the change in the expectation value of the energy is given by

$$\Delta E = \text{Tr}[HU\rho_0U^\dagger] - \text{Tr}(H\rho_0). \quad (7.38)$$

Rewriting this expression as an integral over  $t$  gives

$$\begin{aligned}
\Delta E &= \int_0^{\mathcal{T}} \frac{d}{dt} \text{Tr}[H(t)U(t)\rho_0U^\dagger(t)] dt \\
&= \int_0^{\mathcal{T}} \text{Tr} \left[ \frac{dH}{dt} U(t)\rho_0U^\dagger(t) \right] dt \\
&= \int_0^{\mathcal{T}} \text{Tr} \left[ \frac{\partial H}{\partial \theta} U(t)\rho_0U^\dagger(t) \right] \frac{d\theta}{dt} dt \\
&= \int_0^{\mathcal{T}} \text{Tr} [IU(t)\rho_0U^\dagger(t)] \frac{d\theta}{dt} dt. \tag{7.39}
\end{aligned}$$

Here, the third equality follows from the fact that the time dependence of  $H$  comes entirely from the time dependent flux  $\theta(t)$ , while the last equality follows from the fact that  $I = \frac{\partial H}{\partial \theta}$ .

So far everything is exact, but to proceed further we need to invoke physical arguments. The first step is to note that since the flux insertion process is *quasistatic*, the density matrix at time  $t$ , namely  $U(t)\rho_0U^\dagger(t)$ , shares approximately the same expectation values for local operators as a (local) equilibrium density matrix  $\rho_{eq}(t)$  of the following form:  $\rho_{eq}(t)$  describes a state where the top of the cylinder is at temperature  $T_t(t)$  and chemical potential  $\mu_t(t)$  and the bottom of the cylinder is at temperature  $T_b(t)$  and chemical potential  $\mu_b(t)$ , and where there is flux  $\theta(t)$  through the hole of the cylinder. In other words,

$$\text{Tr} [\mathcal{O}U(t)\rho_0U^\dagger(t)] \approx \text{Tr} [\mathcal{O}\rho_{eq}(t)] \tag{7.40}$$

for any local operator  $\mathcal{O}$ . Here the “ $\approx$ ” sign means that the error vanishes in the thermodynamic limit.

The next step is to note that the time-dependent temperatures and chemical potentials  $T_t(t), \mu_t(t), T_b(t), \mu_b(t)$  that appear in  $\rho_{eq}(t)$  only differ from their initial values  $T_t, \mu_t, T_b, \mu_b$  by an amount that vanishes in the thermodynamic limit. To see this, note that the flux insertion process can only change the energy/number of particles on a given edge by a quantity of at most order  $\mathcal{O}(1)$ , so it cannot affect the temperature or chemical potential of either edge when we take the thermodynamic limit. This means that we can replace  $\rho_{eq}(t) \rightarrow \rho_{\theta(t)}$  when computing expectation values, i.e.,

$$\text{Tr} [\mathcal{O}\rho_{eq}(t)] \approx \text{Tr} [\mathcal{O}\rho_{\theta(t)}] \tag{7.41}$$

for any local operator  $\mathcal{O}$ . Again, the “ $\approx$ ” sign means that the error vanishes in the thermodynamic limit.

Combining (7.40) and (7.41), and using  $O = I$ , we derive

$$\mathrm{Tr} [IU(t)\rho_0U^\dagger(t)] \approx \mathrm{Tr} [I\rho_{\theta(t)}], \quad (7.42)$$

where the error vanishes in the thermodynamic limit.<sup>3</sup>

With Eq. (7.42) in hand, the rest of the derivation follows from straightforward algebra. Substituting (7.42) into Eq. (7.39), we derive

$$\begin{aligned} \Delta E &= \int_0^{\mathcal{T}} \mathrm{Tr} [I\rho_{\theta(t)}] \frac{d\theta}{dt} dt \\ &= \int_0^{2\pi} \mathrm{Tr} [I\rho_\theta] d\theta \\ &= 2\pi\bar{I}. \end{aligned} \quad (7.43)$$

This completes our proof of Claim 1.

### Physical argument for Claim 2

We now give a physical argument for Claim 2. Our argument is based on two properties of the flux insertion process: (i) the flux insertion process does not create bulk excitations, and (ii) the flux insertion process takes a finite amount of time that does not scale with the length of the cylinder: that is, the unitary  $U$  that implements the flux insertion process can be written in the form

$$U = \mathbf{T} \exp \left( -i \int_0^{\mathcal{T}} H(t) dt \right), \quad (7.44)$$

where  $H(t)$  is a local Hamiltonian, and  $\mathcal{T}$  does not scale with the length of the cylinder.

In order to explain the argument we need to introduce some notation for labeling the low energy edge excitations of the cylinder (in the absence of flux): we label these states as  $|i, j, a\rangle$  where  $i$  labels the edge states at the bottom of the cylinder,  $j$  labels the edge states at the top, and  $a$  labels the topological sector of the system. Note that, despite the simple notation, each state  $|i, j, a\rangle$  is generally a complicated and highly entangled many-body wave function.

The topological sector  $a$  will not play an important role below, since we will assume that the cylinder is initialized in a single topological sector, and furthermore we will

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<sup>3</sup>Readers may object that  $I$  is not a local operator, but rather a sum of local operators along a branch cut, and hence Eq. (7.42) does not follow. However the crucial point is that  $I$  is a local operator in the *circumferential* direction. This locality in the circumferential direction is all that we need to justify (7.42).

assume that the flux insertion process does not change the topological sector.<sup>4</sup> Thus, the system will always be in the same sector throughout our discussion. For this reason, we will drop the “ $a$ ” index from now on and denote the low energy states by  $|i, j\rangle$ .

Next, we need to discuss the *quantum numbers* associated with each eigenstate  $|i, j\rangle$ . Because the two edges are well-separated, we assume that the energy of  $|i, j\rangle$  can be written as a sum of the form  $E_i^b + E_j^t$  for some real constants  $\{E_i^b\}, \{E_j^t\}$ , i.e.

$$H|i, j\rangle = (E_i^b + E_j^t)|i, j\rangle. \quad (7.45)$$

Likewise, we assume that the total particle number of  $|i, j\rangle$  is of the form  $N_i^b + N_j^t$ , i.e.

$$N|i, j\rangle = (N_i^b + N_j^t)|i, j\rangle. \quad (7.46)$$

With this notation, we can write down an explicit formula for the initial density matrix of the cylinder,  $\rho_0$ :

$$\begin{aligned} \rho_0 &= \sum_{i'j'} \rho_{ii'}^b \rho_{jj'}^t |i, j\rangle \langle i', j'|, \\ \rho_{ii'}^b &= \frac{1}{Z_b} e^{-(E_i^b - \mu_b N_i^b)/T_b} \delta_{ii'}, \quad \rho_{jj'}^t = \frac{1}{Z_t} e^{-(E_j^t - \mu_t N_j^t)/T_t} \delta_{jj'}. \end{aligned} \quad (7.47)$$

Next, consider the *final* density matrix,  $\rho_f = U\rho_0U^\dagger$ . Since the flux insertion process does not introduce any bulk excitations we know that  $\rho_f$  must be of the form

$$\rho_f = \sum_{i'j'} A_{ii'jj'} |i, j\rangle \langle i', j'| \quad (7.48)$$

for some coefficients  $A_{ii'jj'}$ . In fact, we can say more: using the fact that  $U$  is of the form given in Eq. (7.44) where  $\mathcal{T}$  does not scale with the length of the cylinder, it is possible to show that  $A_{ii'jj'}$  can be factored as

$$A_{ii'jj'} = \sigma_{ii'}^b \sigma_{jj'}^t, \quad (7.49)$$

where  $\sigma_{ii'}^b$  and  $\sigma_{jj'}^t$  are Hermitian matrices with the same eigenvalue spectrum as  $\rho_{ii'}^b$  and  $\rho_{jj'}^t$ :

$$\begin{aligned} \text{Spec}(\sigma^b) &= \text{Spec}(\rho^b), \\ \text{Spec}(\sigma^t) &= \text{Spec}(\rho^t). \end{aligned} \quad (7.50)$$

<sup>4</sup>We can guarantee the latter property by inserting  $2\pi m$  flux instead of  $2\pi$  flux, and taking  $m$  to be a multiple of  $1/e^*$ , where  $e^*$  is the smallest fractionally charged excitation.

We give the proof of Eqs. (7.49) and (7.50) in Appendix D.2.

To proceed further, we use the following result, which is a restatement of the well-known fact that the Gibbs state minimizes the free energy  $F = E - TS$ :

**Lemma 1** *Let  $H$  be a Hermitian matrix, and let  $\bar{\rho}$  be a matrix of the form*

$$\bar{\rho} = \frac{1}{Z} e^{-H/T}, \quad Z = \text{Tr}(e^{-H/T}) \quad (7.51)$$

*for some non-negative real  $T$ . Let  $\rho$  be another matrix of the same dimension as  $\rho$  such that  $\rho$  is positive semi-definite and  $\text{Tr}(\rho) = 1$ . Then*

$$\text{Tr}(H\rho + T\rho \log \rho) \geq \text{Tr}(H\bar{\rho} + T\bar{\rho} \log \bar{\rho}). \quad (7.52)$$

This inequality can be derived straightforwardly by minimizing the convex functional  $F[\rho] = \text{Tr}(H\rho + T\rho \log \rho)$ .

First we apply Lemma 1 with  $\rho = \sigma^t$ , and  $\bar{\rho} = \rho^t$  and with  $H$  being the diagonal matrix  $(E_i^t - \mu_t N_i^t) \delta_{ii'}$ . This gives the inequality

$$\sum_i (E_i^t - \mu_t N_i^t) \sigma_{ii}^t + T_t \cdot \text{Tr}(\sigma^t \log \sigma^t) \geq \sum_i (E_i^t - \mu_t N_i^t) \rho_{ii}^t + T_t \cdot \text{Tr}(\rho^t \log \rho^t). \quad (7.53)$$

Next, invoking Eq. (7.50), we can cancel the  $\text{Tr}(\sigma^t \log \sigma^t)$  and  $\text{Tr}(\rho^t \log \rho^t)$  terms on the two sides to obtain

$$\sum_i (E_i^t - \mu_t N_i^t) \sigma_{ii}^t \geq \sum_i (E_i^t - \mu_t N_i^t) \rho_{ii}^t. \quad (7.54)$$

Subtracting the right hand side from the left hand side gives the inequality

$$\Delta E_t - \mu_t \cdot \Delta N_t \geq 0, \quad (7.55)$$

where  $\Delta E_t, \Delta N_t$  denote the change in the expectation value of the energy and particle number at the top edge during the flux insertion process.

In the same way, we can apply Lemma 1 with  $\rho = \sigma^b$ , and  $\bar{\rho} = \rho^b$  and with  $H$  being the diagonal matrix  $(E_i^b - \mu_b N_i^b) \delta_{ii'}$  to derive

$$\Delta E_b - \mu_b \cdot \Delta N_b \geq 0, \quad (7.56)$$

This proves Claim 2.

### Impossibility of a Thouless pump for entropy

Using the thermodynamic identity,  $\Delta E = T\Delta S + \mu\Delta N$ , we can identify the two quantities  $\Delta E_t - \mu_t\Delta N_t$  and  $\Delta E_b - \mu_b\Delta N_b$  in the statement of Claim 2 with  $T_t\Delta S_t$  and  $T_b\Delta S_b$  where  $\Delta S_t$  and  $\Delta S_b$  are the change in entropy at the top and bottom edges. With these identifications, Claim 2 implies that

$$\Delta S_t \geq 0, \quad \Delta S_b \geq 0. \quad (7.57)$$

One implication of the above inequalities is that they rule out the possibility that the flux insertion process could pump entropy from one end of the cylinder to the other, i.e. the possibility that  $\Delta S_t = -\Delta S_b \neq 0$ . In fact, we can go a step further: since the proof of Claim 2 does not use any of the details of the flux insertion process, we can rule out the possibility of *any* adiabatic cycle consisting of local, quasi-1D Hamiltonians  $H(\theta)$  with a bulk energy gap that pumps a nonzero amount of entropy across the system at temperatures below the bulk gap. In other words, we deduce that it is impossible to construct an analog of the (1D) Thouless pump for entropy.

We note that a weaker<sup>5</sup> version of this no-go result can be derived directly from the Nernst unattainability principle. Specifically, the Nernst principle implies that for any adiabatic cycle  $H(\theta)$  of the above type, the amount of entropy  $\Delta S$  pumped across the system must vanish as  $T \rightarrow 0$ , i.e.  $\lim_{T \rightarrow 0} \Delta S = 0$ . To show this, we use the same argument in Sec. 7.2: if  $\Delta S$  remained nonzero in this limit, then we could use this adiabatic cycle to cool a finite heat bath to zero temperature in a finite number of cycles, which would contradict the Nernst unattainability principle.

### 7.5 Concluding remarks

It is often stated that the Third Law of Thermodynamics requires the tensors  $\nu_{km}(T)$  and  $\eta_{km}(T)/T$  to vanish at  $T = 0$ , see e.g. [28]. The discussion in this chapter shows that the relation between the Third Law and the behavior of thermoelectric coefficients near  $T = 0$  is rather subtle. On the one hand, the Nernst unattainability principle directly implies the vanishing of the symmetric tensor  $\eta^S(T)/T$  at  $T = 0$ . Applying this both to the original system and its time-reversal and using Onsager reciprocity, one concludes that  $\nu^S(0) = 0$  as well. On the other hand, a non-vanishing value of  $\eta^A(T)/T$  at  $T = 0$  is associated only with circulating entropy currents and does not directly conflict with the Nernst unattainability principle. For

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<sup>5</sup>The second version of the no-go result is weaker than the first because it only shows that  $\lim_{T \rightarrow 0} \Delta S = 0$ , while the first argument implies that  $\Delta S$  is exponentially small for  $T$  smaller than the bulk gap.

gapped systems, however, one can use the Středa formula to show that a nonzero value for  $\nu^A(0)$  is in conflict with the Nernst heat theorem (which follows from the Nernst unattainability principle and some standard assumptions). Then Onsager reciprocity implies the vanishing of  $\eta^A(T)/T$  at  $T = 0$  as well.

Among our arguments for the vanishing of  $\nu^A(0)$ , the one based on the Third Law of Thermodynamics is the most robust, but also the least informative. It shows that  $\nu^A(0) = 0$  but does not tell us anything about the magnitude of  $\nu^A(T)$  for small but nonzero  $T$ . The other arguments (Sections 7.3 and 7.4) rely on more assumptions but show that  $\nu^A(T)$  is exponentially small for  $T$  below the bulk gap.



## HIGHER-DIMENSIONAL GENERALIZATION OF THE BERRY CURVATURE

### 8.1 Introduction

Consider a quantum-mechanical system with a Hamiltonian depending on parameters, a unique ground state for all values of the parameters, and an energy gap to the lowest excited state. To these data one can associate a differential 2-form  $\Omega$  on the parameter space: the curvature of the Berry connection [8]. This 2-form is closed and quantized: its integrals over closed surfaces are integral multiples of  $2\pi$ . If the integral of  $\Omega$  over a surface  $\Sigma$  is non-zero,  $\Sigma$  must enclose points where the ground state is degenerate. Indeed, if the system were non-degenerate everywhere inside  $\Sigma$ , then by Stokes' theorem the integral of  $\Omega$  over  $\Sigma$  would vanish. Thus the Berry curvature can detect degeneracy points. Moreover, degeneracy points detected by the Berry curvature are stable against deformations of the Hamiltonian. Indeed, since the integral of the Berry curvature is quantized, it can only change discontinuously and thus any small deformation will not affect the value of the integral.

When we consider many-body Hamiltonians, the most direct analogs of Hamiltonians with a unique non-degenerate ground state are gapped systems in a trivial phase, or more generally systems in a Short-Range Entangled (SRE) phase. The analogs of degeneracy points are points where phase transitions occur. In view of the above discussion, it is natural to ask whether the presence of a phase transition (either continuous or discontinuous) can be detected by studying Short-Range Entangled systems in the neighborhood of the suspected phase transition. By analogy with the above discussion, one would hope to construct closed forms on the parameter space of Short-Range Entangled systems whose integrals over surfaces would serve as signatures of phase transitions.

A few years ago A. Kitaev proposed that for a family of SRE systems in spatial dimensions  $D$  one can define a closed  $(D + 2)$ -form on the parameter space. This form is a higher-dimensional generalization of the Berry curvature and can be used to detect phase transition loci in the parameter space. One difficulty in making this proposal concrete is that currently there is no useful definition of Short-Range Entangled systems, beyond the "negative" statement that these are systems which

exhibit neither spontaneous symmetry-breaking nor topological order.

Unlike the notion of a Short-Range Entangled system, the notion of a gapped system is straightforward to define. In this chapter we define and study higher-dimensional generalizations of the Berry curvature for gapped lattice systems on  $\mathbb{R}^D$ . For any gapped lattice Hamiltonian depending parameters we define a closed  $(D + 2)$ -form  $\Omega^{(D+2)}$  on the parameter space.<sup>1</sup> If an integral of this form over a  $(D+2)$ -dimensional surface in the parameter space is nonzero, then this surface cannot be contracted to a point within the space of gapped systems. Thus such integrals are able to detect the presence of phase transition loci completely surrounded by a gapped phase. The analogy with the Berry curvature is most complete in the case when this phase is Short-Range Entangled, as in Kitaev's proposal. In that case one can argue that the integral of  $\Omega^{(D+2)}$  over any  $(D + 2)$ -dimensional sphere is quantized (is an integral multiple of  $2\pi$ ).

In spatial dimension  $D > 0$ , it is natural to study boundaries or interfaces. It is well-known by now that an interface between two gapped systems in different phases may host gapless modes which are robust with respect to all deformations (or all deformations which do not break the symmetry, if one is dealing with Symmetry-Protected Topological phases).

If one considers an interface between two gapped systems in the same phase, then it is generically gapped. Even if there are gapless modes on a particular interface, a small deformation of the Hamiltonian can make them gapped. But the situation becomes more interesting if one considers families of trivially gapped systems and interfaces between them. Following the ideology of catastrophe theory [55], one might expect that sometimes perturbing the family cannot eliminate a gapless interface, it merely moves it to a different location in the parameter space. We show that the form  $\Omega^{(D+2)}$  can serve as a diagnostic for such families. Namely, suppose we are given a family of gapped  $D$ -dimensional Hamiltonians  $H(\lambda_1, \dots, \lambda_{D+2})$  continuously depending on  $D + 2$  parameters, such that the parameter space is a closed oriented  $(D + 2)$ -dimensional manifold. Fix a Hamiltonian  $H_0$  in the same phase as all the Hamiltonians in the family (for example, one can just let  $H_0$  be  $H(\lambda_1, \dots, \lambda_{D+2})$  for some specific values of the parameters). Now suppose we are given a family of interfaces between all the systems in the family and the system with the Hamiltonian  $H_0$ . We show that if all the interfaces have a gapped non-degenerate

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<sup>1</sup>For families of Euclidean lattice systems in  $D + 1$  dimensions with exponentially decaying correlations, A. Kitaev outlined a construction of a closed  $(D + 2)$ -form on the parameter space [33]. Our results can be viewed as a Hamiltonian version of this construction.

ground state, then the integral of  $\Omega^{(D+2)}$  over the parameter space must vanish. This is a form of bulk-boundary correspondence for families.

In view of the above, it is interesting to give examples of families of Hamiltonians where the forms  $\Omega^{(D+2)}$  and their integrals are non-zero. We will call such families topologically non-trivial. In general, computing the forms  $\Omega^{(D+2)}$  is a difficult task (this is also true for the Berry curvature). But in the case of translationally-invariant tight-binding free fermion Hamiltonians in 1d we show that the cohomology class of  $\Omega^{(D+2)}$  is determined by the curvature of the Berry-Bloch connection. We conjecture that this is true in any dimension. Free fermion systems thus can provide examples of families which exhibit gapless edge modes in families, despite being in a trivial phase for all values of the parameters.

Recently Cordova, Freed, Lam, and Seiberg studied field theories with "anomalies in the space of couplings" [16, 17]. Via the bulk-boundary correspondence, this subject is closely related to topologically-nontrivial families of gapped field theories in one dimension higher. It is natural to conjecture that there is a 1-1 correspondence between topological invariants of families of gapped field theories in  $(D + 1)$  space-time dimensions and topological invariants of families of gapped lattice models in  $D$  spatial dimensions some of which we study here.

## 8.2 Effective action considerations

The purpose of this section is to motivate the constructions in subsequent sections.

If a gapped system in  $D$  spatial dimensions is described by a trivial topological field theory at long distances, then its low-energy effective action is a well-defined function of background fields, such as the metric and the gauge fields which couple to global symmetries. If one deals with a family of such systems parameterized by a manifold  $M$ , one can let the parameters vary slowly from point to point, and the effective action is still a well-defined function of the background fields. The variation of the parameters can be described by a map  $\phi : X \rightarrow M$ , where  $X$  is the space-time. The effective action depends on  $\phi$  as well as other background fields.

Loosely speaking, topological terms in the action are those terms which survive when one re-scales the metric  $g_{\mu\nu} \mapsto e^\sigma g_{\mu\nu}$  and takes the limit  $\sigma \rightarrow +\infty$ . The simplest such terms are those which depend only on  $\phi$  and not on other background fields. For example, for  $D = 0$  (ordinary quantum mechanics) such a topological

term schematically has the form

$$S_{top}(X, \phi) = \int_X \omega_j^{(1)} \partial_t \phi^j dt = \int_X \phi^* \left( \omega^{(1)} \right), \quad (8.1)$$

where  $X$  is a one-dimensional manifold ( $S^1$  or  $\mathbb{R}$ ) and  $\omega^{(1)}$  is the 1-form on  $M$  representing the Berry connection. In a chart of  $M$  with coordinates  $\lambda^j$ , the 1-form is given by  $\omega^{(1)} = \sum_j \omega_j^{(1)} d\lambda^j$  and the Berry connection  $\omega_j^{(1)} = i \langle 0_\lambda | \frac{\partial}{\partial \lambda^j} | 0_\lambda \rangle$  where  $|0_\lambda\rangle$  is the ground state. The formula (8.1) is only schematic because in general the Berry connection on the parameter space can be represented by a 1-form  $\omega^{(1)}$  only locally on  $M$ . If the Chern class of the Berry curvature  $\Omega^{(2)}$  is non-trivial, then one cannot write  $\Omega^{(2)} = d\omega^{(1)}$  for a globally-defined 1-form  $\omega^{(1)}$ . Rather, one needs to cover the parameter space with charts, in each of which the connection is represented by a 1-form. On the overlaps of the charts these 1-forms are related by gauge transformations. To define  $S_{top}(X, \phi)$  properly, one needs to know both the locally-defined 1-forms and the gauge transformations connecting them.

If the space-time  $X$  is circle  $S^1$ , the geometric phase  $\exp(iS_{top}(X, \phi))$  represents the phase factor acquired by the ground state under adiabatic transformation around a loop  $\phi : S^1 \rightarrow M$  in the parameter space. It can be defined unambiguously, while the phase  $S_{top}(X, \phi)$  is defined only up to an integer multiple of  $2\pi$ . If the loop in the parameter space anchors a disk  $D$ , i.e. the map  $\phi : X \rightarrow M$  extends to a continuous map  $\tilde{\phi} : D \rightarrow M$ , then one can rewrite the geometric phase as integral of the Berry curvature over the surface bounded by the loop

$$S_{top} = \int_D \tilde{\phi}^* \left( \Omega^{(2)} \right). \quad (8.2)$$

This expression depends on the choice of  $\tilde{\phi}$ . But  $\exp(iS_{top}(X, \phi))$  is unambiguously defined since periods of  $\Omega^{(2)}$  are "quantized": the integral of  $\Omega^{(2)}$  over any 2-cycle on  $M$  is  $2\pi$  times an integer.

The geometric phase (8.2) depends on the dynamical detail of the system and can always be made trivial on any contractable submanifold of  $M$  by a suitable deformation of the Hamiltonian. A non-zero value of the integral of the Berry curvature over closed surface indicates a presence of gapless point inside of it. The latter serves as an obstruction for the contraction of this surface. More generally, any globally defined Berry connection can be made zero by a suitable deformation of the Hamiltonian preserving the gap. An equivalence class of a closed 2-form under the addition of the differential of a globally defined one-form is called the cohomology class of this form. Thus the cohomology class of the Berry curvature

$\Omega^{(2)}$  is a topological invariant under variations of the Hamiltonian which do not close the gap.

For  $D > 0$  the story is similar. A topological action which does not depend on fields other than  $\phi$  schematically has the form

$$S_{top}(X, \phi) = \int_X \phi^* \left( \omega^{(D+1)} \right) = \frac{1}{(D+1)!} \int_X \omega_{i_0 \dots i_D}^{(D+1)} (\partial_0 \phi^{i_0}) \dots (\partial_D \phi^{i_D}) dx^0 \dots dx^D, \quad (8.3)$$

where  $\omega^{(D+1)}$  is an  $(D+1)$ -form on  $M$  and  $X$  is a closed oriented  $(D+1)$ -manifold. If one takes this formula literally, then all such actions can be deformed to zero, since any  $(D+1)$ -form can be deformed to zero. But if one interprets  $\omega^{(D+1)}$  more creatively, as a sort of "higher connection", one can get more interesting actions which cannot be deformed to the trivial one. One way to find such a generalization is to note that the r.h.s. of the above equation does not change under  $\omega^{(D+1)} \mapsto \omega^{(D+1)} + d\lambda^{(D)}$ , where  $\lambda^{(D)}$  is an arbitrary  $D$ -form. Then it is natural to consider an object specified by locally-defined  $(D+1)$ -forms  $\omega_\alpha^{(D+1)}$ , where  $\alpha$  labels the charts. On the overlaps of charts these  $(D+1)$ -forms are related by  $D$ -form gauge transformations. The full story is rather complicated, since in order to be able to define "higher holonomy" along a  $(D+1)$ -dimensional submanifold one needs compatibility conditions for the gauge transformations which involve  $(D-1)$ -forms on triple overlaps, etc.

An alternative approach (first appearing of [13]) is to postulate the following natural property. If  $X = \partial Y$  for some  $(D+2)$ -manifold  $Y$ , and if  $\phi$  extends to a map  $\tilde{\phi} : Y \rightarrow M$ , then one must have

$$\exp(iS_{top}(X, \phi)) = \exp\left(i \int_Y \tilde{\phi}^* \left( \Omega^{(D+2)} \right)\right), \quad (8.4)$$

where  $\Omega^{(D+2)}$  is a  $(D+2)$ -form on  $M$ . For this formula to make sense,  $\Omega^{(D+2)}$  must be closed and its periods must be integer multiples of  $2\pi$ . For example, to see that  $\Omega^{(D+2)}$  must be closed, one can vary  $\tilde{\phi}$  infinitesimally while keeping its boundary value  $\phi$  fixed. It is easy to see that the r.h.s. will be unchanged only if  $d\Omega^{(D+2)} = 0$ . To see that  $\Omega^{(D+2)}$  must have periods which are integral multiples of  $2\pi$ , take  $X$  to be the empty manifold, and take  $Y$  to be any closed  $(D+2)$ -manifold.

Locally on  $M$  one can write  $\Omega^{(D+2)} = d\omega^{(D+1)}$ . If the cohomology class of  $\Omega^{(D+2)}$  is trivial, one can do it globally, and then  $S_{top}(X, \phi)$  can be defined by the simple formula (8.3). In general, one can show that given a closed  $(D+2)$ -form  $\Omega^{(D+2)}$  with "quantized" periods there exists an exponentiated action  $\exp(iS_{top}(X, \phi))$  satisfying

the above equation. It is unique up to a factor  $\exp(i \int_X \phi^*(\alpha))$ , where  $\alpha$  is a closed  $(D + 1)$ -form on  $M$ .

As in the case  $D = 0$ , this implies that the cohomology class of  $\Omega^{(D+2)}$  determines  $\exp(iS_{top}(X, \phi))$  up to a factor which can be deformed to 1. Thus one can say that deformation classes of such topological actions (known as Wess-Zumino-Witten terms) are classified by "quantized" cohomology classes of degree  $D + 2$ . There is also an interpretation of Wess-Zumino-Witten terms as holonomies of "higher connections" on "higher bundles" on  $M$ . Then the cohomology class of  $\Omega^{(D+2)}$  determines the topology of the corresponding "higher bundle". But since such an interpretation is quite abstract, we will not use it.

The conclusion is that given a family of trivial gapped systems in spatial dimension  $D$ , one should be able to obtain a closed  $(D + 2)$ -form on the parameter space with "quantized" periods. While the form itself depends on the dynamical details, its cohomology class is a topological invariant. It classifies possible deformation classes of Wess-Zumino-Witten terms on the parameter space.

The statement about quantization of periods needs some qualification in the case of fermionic systems. A fermionic path-integral depends on spin structure on  $X$  (i.e. choice of periodic/antiperiodic boundary condition for fermions going around each loop). For fermionic systems it is unreasonable to restrict attention to topological terms which depend only on the map  $\phi$ , one needs to study topological terms which depend both on  $\phi$  and the spin structure. Then one needs to generalize the Cheeger-Simons approach by requiring the manifolds  $X$  and  $Y$  to be spin manifolds. Such spin-structure-dependent Wess-Zumino-Witten terms were first considered in [19]. Alternatively, if one limits oneself to the case of systems on  $X = \mathbb{R}^{D+1}$  or its one-point compactification  $S^{D+1}$ , then one can always take  $Y = B^{D+2}$  ( $(D + 2)$ -dimensional ball). Then the quantization condition is relaxed: only integrals of the form

$$\int_{S^{D+2}} h^* \left( \Omega^{(D+2)} \right) \quad (8.5)$$

need to be integral multiples of  $2\pi$ . Here  $h : S^{D+2} \rightarrow M$  is any smooth map. We will call such an  $h$  a spherical cycle. Thus for fermionic systems only integrals of  $\Omega^{(D+2)}$  over spherical cycles are quantized. Of course, not all topological terms which are consistent on  $\mathbb{R}^{D+1}$  or  $S^{D+1}$  will remain consistent when considered on a general space-time. That is, quantization on spherical cycles is not enough to make the Wess-Zumino-Witten action well-defined on arbitrary spin manifolds.

### 8.3 Higher Berry curvature for gapped 1d systems

As explained in the previous section, given a family of trivial gapped theories on a  $D$ -dimensional lattice and assuming that the field theory description applies at each point in the parameter space  $M$ , there should be a way to construct a closed  $(D + 2)$ -form on  $M$  whose integrals over spherical cycles are quantized. The cohomology class of the form is a topological invariant of the family (cannot change under deformations). In this section we construct such a closed form  $\Omega^{(3)}$  on the parameter space for the case of gapped spin chains, that is, gapped lattice  $D = 1$  systems. We do not use the existence of the field theory limit. In Appendix E.1 we argue that integrals of  $\Omega^{(3)}$  over spherical 3-cycles are quantized. That is, integrals of the form  $\int_{S^3} h^* \Omega^{(3)}$ , where  $h$  is a map from  $S^3$  to  $M$ , are integer multiples of  $2\pi$ .

To begin with, let us recall how the Berry 2-form is defined for gapped 0d systems and why this definition does not work for  $D > 0$ . Let  $G = 1/(z - H)$  be the Green's function for a positive bounded Hamiltonian  $H$  which depends on some parameters. Assume that 0 is an isolated eigenvalue of  $H$  for all values of the parameters. Let

$$\Omega^{(2)} = \frac{i}{2} \oint \frac{dz}{2\pi i} \text{Tr}(G dHG^2 dH), \quad (8.6)$$

where  $\oint$  is the counterclockwise contour integral around  $z = 0$  and  $d$  denotes the exterior derivative on the parameter space  $M$ . That is,  $d = \sum_{\ell} d\lambda^{\ell} \frac{\partial}{\partial \lambda^{\ell}}$  where  $\lambda^{\ell}$  are parameters. The wedge product of forms  $\wedge$  is implicit in Eq. (8.6).  $\Omega^{(2)}$  is a closed 2-form on  $M$ . Indeed, since  $dG = G dHG$ , we compute

$$\begin{aligned} d\Omega^{(2)} &= \frac{i}{2} \oint \frac{dz}{2\pi i} \text{Tr}(G dHG dHG^2 dH - G dHG^2 dHG dH - G dHG dHG^2 dH) = \\ &= -\frac{i}{2} \oint \frac{dz}{2\pi i} \text{Tr}(G dHG^2 dHG dH) = \frac{i}{6} \oint \frac{dz}{2\pi i} \frac{\partial}{\partial z} \text{Tr}(G dHG dHG dH) = 0. \end{aligned} \quad (8.7)$$

$\Omega^{(2)}$  is the usual Berry curvature, as one can verify by inserting a complete set of states.

Suppose now  $H$  is a many-body Hamiltonian for an infinite 1d lattice system with an energy gap. Then  $H$  is unbounded, but one can still define a bounded operator  $G = 1/(z - H)$  for  $z$  which are away from the spectrum of  $H$ . We assume again that  $H$  is positive and that 0 is an isolated eigenvalue for all values of the parameters. Fixing  $p, q \in \Lambda$ , we can define a non-closed 2-form on the parameter space

$$\Omega_{pq}^{(2)} = \frac{i}{2} \oint \frac{dz}{2\pi i} \text{Tr}(G dH_p G^2 dH_q).$$

If the Hamiltonian  $H$  is gapped,  $\Omega_{pq}^{(2)}$  decays exponentially away from  $p = q$  (see [60]). The Berry curvature is formally given by

$$\Omega^{(2)} = \sum_{p,q \in \Lambda} \Omega_{pq}^{(2)},$$

but the contribution of the points near the diagonal,  $p \simeq q$ , is divergent for infinite-volume systems.

Instead of the ill-defined Berry curvature 2-form, consider the following 2-form depending on a site  $p$ :

$$F_p^{(2)} = \frac{i}{2} \oint \frac{dz}{2\pi i} \text{Tr}(G dH G^2 dH_p). \quad (8.8)$$

It is well-defined, but not closed. Instead one has an identity

$$dF_q^{(2)} = \sum_{p \in \Lambda} F_{pq}^{(3)}, \quad (8.9)$$

where the 3-form  $F_{pq}^{(3)}$  is given by

$$F_{pq}^{(3)} = \frac{i}{6} \oint \frac{dz}{2\pi i} \text{Tr}(G^2 dH G dH_p G dH_q - G dH G^2 dH_p G dH_q) - (p \leftrightarrow q).$$

The identity (8.9) can be verified by a straightforward computation. Note that  $F_{pq}^{(3)}$  decays exponentially away from the diagonal  $p = q$  thanks to the results of [60].

The identity (8.9) and other similar identities are key for defining topological invariants of families of gapped systems in one and higher dimensions. In the context of Euclidean lattice systems, analogous identities were first observed by A. Kitaev who used them to define invariants of families of such systems [33]. In this and next chapters we essentially derive Hamiltonian analogs of Kitaev's formulas.

Let  $f : \Lambda \rightarrow \mathbb{R}$  be a function which is 0 for  $p \ll 0$  and 1 for  $p \gg 0$ . For example, it could be simply 0 for  $p < a$  and 1 for  $p \geq a$ . Then we define a 3-form on the parameter space by

$$\Omega^{(3)}(f) = \frac{1}{2} \sum_{p,q \in \Lambda} F_{pq}^{(3)}(f(q) - f(p)). \quad (8.10)$$

It is well-defined because on the one hand  $F_{pq}^{(3)}$  decays exponentially for large  $|p - q|$ , and on the other hand  $f(q) - f(p)$  is non-zero only when  $p > a$  and  $q < a$ , or



the other way around. For the specific choice of  $f(p)$  equal 0 for  $p < a$  and 1 for  $p \geq a$ , the equation (8.10) takes a simple form

$$\Omega^{(3)}(f) = \sum_{\substack{p < a \\ q > a}} F_{pq}^{(3)}, \quad (8.11)$$

which makes its convergence more transparent.

Later we will show that

$$dF_{qr}^{(3)} = \sum_{p \in \Lambda} F_{pqr}^{(4)}, \quad (8.12)$$

where  $F_{pqr}^{(4)}$  is a function which is anti-symmetric in  $p, q, r$  and decays exponentially away from the diagonal  $p = q = r$ . We find

$$\begin{aligned} d\Omega^{(3)}(f) &= \frac{1}{2} \sum_{q,r \in \Lambda} (f(r) - f(q)) dF_{qr}^{(3)} = \frac{1}{2} \sum_{p,q,r \in \Lambda} (f(r) - f(q)) F_{pqr}^{(4)} \\ &= \frac{1}{6} \sum_{p,q,r \in \Lambda} (f(r) - f(q) + f(p) - f(r) + f(q) - f(p)) F_{pqr}^{(4)} = 0, \end{aligned} \quad (8.13)$$

where we have used the anti-symmetry of  $F_{pqr}^{(4)}$ . Therefore the 3-form  $\Omega^{(3)}(f)$  is closed.

Closedness of  $\Omega^{(3)}(f)$  implies that its cohomology class is a topological invariant of the family of gapped systems. Indeed, let us regard  $M$  as a submanifold in the space  $\mathfrak{M}_1$  of all gapped systems in dimension 1. Obviously, the form  $\Omega^{(3)}$  is a restriction of a closed form on  $\mathfrak{M}_1$  defined in exactly the same way. Deforming  $M$  within  $\mathfrak{M}_1$  can be thought of as a flow along a vector field on  $\mathfrak{M}_1$ . Since the Lie derivative of a closed form along any vector field is exact, deforming  $M$  cannot change the cohomology class of  $\Omega^{(1)}$ . In particular, whenever the integral over 3-sphere  $\int_{S^3} \Omega^{(3)}$  is non-zero there must be a gapless point inside of the region of the parameter space bounded by this 3-sphere.

The cohomology class of the 3-form  $\Omega^{(3)}(f)$  is independent of the choice of the function  $f$  as long as  $f(p) = 0$  for  $p \ll 0$  and  $f(p) = 1$  for  $p \gg 0$ . Indeed, any two such functions differ by a function  $g$  which is compactly supported, and for such a function we can write

$$\begin{aligned} \Omega^{(3)}(g) &= \frac{1}{2} \sum_{p,q \in \Lambda} (g(q) - g(p)) F_{pq}^{(3)} = \sum_{q \in \Lambda} g(q) \sum_{p \in \Lambda} F_{pq}^{(3)} \\ &= \sum_{q \in \Lambda} g(q) dF_q^{(2)} = d \sum_{q \in \Lambda} g(q) F_q^{(2)}. \end{aligned} \quad (8.14)$$

This means that  $\Omega^{(3)}(f+g)$  and  $\Omega^{(3)}(f)$  differ by a total derivative of a well-defined 2-form on  $M$  and therefore are in the same cohomology class.

This property implies that a family of systems parameterized by a closed 3-manifold  $\Sigma_3$  with a non-zero value of the integral  $\int_{\Sigma_3} \Omega^{(3)}(f)$  cannot have a gapped boundary condition which varies continuously over  $\Sigma_3$ . Indeed, a gapped boundary condition can be thought as an interpolation between this family for  $p \gg 0$  and a trivial system for  $p \ll 0$ . The above result means that the integral of the 3-form  $\Omega^{(3)}(f)$  will be the same regardless of whether  $a$  in  $f(p) = \theta(p - a)$  satisfies  $a \gg 0$  or  $a \ll 0$ . Since the formula for 3-form is local, for  $a \gg 0$  the integral of the 3-form coincides with  $\int_{\Sigma_3} \Omega^{(3)}(f)$  for the infinite system without the edge. On the other hand, for  $a \ll 0$  it is zero. Therefore, if  $\int_{\Sigma_3} \Omega^{(3)}(f) \neq 0$ , the family cannot have a continuously varying boundary condition which is gapped everywhere on  $M$ .

We note the following obvious properties of the 3-form  $\Omega^{(3)}(f)$ . It vanishes for constant families (i.e. families where the Hamiltonian is independent of parameters), and it is additive under stacking of families (with the same parameter space).

#### 8.4 Higher Berry curvature for gapped systems in any dimension

To construct analogs of Berry curvature in higher dimensions, the language of chains and cochains is very useful. For the relevant definitions and constructions see Appendix A.

Using this notation, we see that  $\Omega^{(3)}(f) = F^{(3)}(\delta f)$ , where  $F^{(3)}$  is a 1-chain with values in 3-forms on  $M$  with components  $F_{pq}^{(3)}$ . Furthermore, eq. (8.12) can be written as a relation between a 1-chain  $F^{(3)}$  valued in 3-forms and a 2-chain  $F^{(4)}$  valued in 4-forms:

$$dF^{(3)} = \partial F^{(4)}. \quad (8.15)$$

Then the computation leading to (8.13) can be shortened to

$$d\Omega^{(3)}(f) = dF^{(3)}(\delta f) = \partial F^{(4)}(\delta f) = F^{(4)}(\delta\delta f) = 0.$$

Similarly, the computation leading to (8.14) can be shortened to

$$\Omega^{(3)}(g) = F^{(3)}(\delta g) = \partial F^{(3)}(g) = dF^{(2)}(g).$$

Here  $g : \Lambda \rightarrow \mathbb{R}$  is supported on a finite set, therefore the application of the Stokes' theorem is legitimate.

Now we will generalize the construction of the previous section to arbitrary dimensions and define a closed  $(D+2)$ -form  $\Omega^{(D+2)}$  on the parameter space of a family of

gapped lattice systems in  $D$  spatial dimensions. For  $D > 1$  not all gapped systems can be continuously connected to the trivial one, thanks thanks to the possibility of topological order. Therefore we do not expect our  $(D + 2)$ -form to have quantized periods even on spherical cycles. Nevertheless we will argue in Appendix E.1 that for families of systems in an SRE phase its periods are quantized on spherical  $(D + 2)$ -cycles, as expected from the field theory analysis.

We will define higher Berry curvatures recurrently via the following "descent equation":

$$dF^{(n)} = \partial F^{(n+1)}, \quad (8.16)$$

where  $F^{(n)}$  is  $(n-2)$ -chain with values in  $n$ -forms on the parameter space. Analogous equations for families of Euclidean lattice systems were used in [33]. Starting from  $F^{(2)}$  defined in (8.9), we can find all its descendants. The result is

$$F_{p_0 \dots p_{n-2}}^{(n)} = \frac{i(-1)^n}{n(n-1)} \sum_{\sigma \in \mathcal{S}_{n-1}} \text{sgn}(\sigma) \oint \frac{dz}{2\pi i} \sum_{j=0}^{n-2} (n-j-1) \times \text{Tr} \left( G dH G dH_{p_{\sigma(0)}} G dH_{p_{\sigma(1)}} \dots G^2 dH_{p_{\sigma(j)}} \dots G dH_{p_{\sigma(n-2)}} \right). \quad (8.17)$$

For this to be a well-defined chain, it must decay exponentially when any two of the points  $p_0, \dots, p_{n-2}$  are separated by a large distance. For  $n = 3$  this was proved in [60], and we expect that the proof can be generalized to arbitrary  $n$ . Heuristically, exponential decay follows from the physical interpretation of the above correlators in terms of generalized local susceptibilities. For  $n = 2$  the correlator is a variation of the expectation value of a local operator  $dH_{p_0}$  with respect to an arbitrary infinitesimal variation of the Hamiltonian. That is, it is a local susceptibility. For  $n = 3$  it can be interpreted as a variation of a local susceptibility with respect to a variation of the Hamiltonian elsewhere. For  $n = 4$  it can be interpreted as a variation of a variation, etc. We expect all such quantities to decay exponentially for large spatial separations because the correlation length is finite for a gapped system at zero temperature.

In order to find a topological invariant of a family of gapped systems we need to contract this  $(n-2)$ -chain with an  $(n-2)$ -cochain. Let  $\alpha$  be an  $(n-2)$ -cochain, then  $\langle F^{(n)}, \alpha \rangle$  is an  $n$ -form on the parameter space. But in general it is not closed:

$$dF^{(n)}(\alpha) = \partial F^{(n+1)}(\alpha) = F^{(n+1)}(\delta\alpha). \quad (8.18)$$

In order for the integral of the  $n$ -form  $\int_{C_n} F^{(n)}(\alpha)$  to be independent of the deformation of the cycle  $C_n$ , the cochain  $\alpha$  must be closed,  $\delta\alpha = 0$ . On the other hand, if

the cochain  $\alpha$  is exact,  $\alpha = \delta\gamma$ , we find

$$F^{(n)}(\alpha) = F^{(n)}(\delta\gamma) = \partial F^{(n)}(\gamma) = dF^{(n-1)}(\gamma), \quad (8.19)$$

and all integrals  $\int_{C_n} F^{(n)}(\alpha)$  over cycles  $C_n$  will be zero.

We see that in order to get a non-trivial invariant of a family we need to contract the chain  $F^{(n)}$  with a cochain which is closed but not exact. Moreover, adding to such a cochain an exact cochain will not change the invariant. Thus we need to understand the space of closed cochains modulo the subspace of exact cochains, that is, the cohomology of the cochain complex  $(C^n(\Lambda), \delta)$ . If we omit the word "bounded" from the definition of cochains, then the cohomology of the corresponding complex is known in the mathematical literature as the coarse cohomology of  $\Lambda$  [48]. For physical applications, one may assume that  $\Lambda \subset \mathbb{R}^D$  uniformly fills the whole  $\mathbb{R}^D$ , in the sense that there exists  $\delta > 0$  such that each point of  $\mathbb{R}^D$  is within distance  $\delta$  of some point of  $\Lambda$ , and that  $\Lambda$  has no accumulation points. Then the  $n$ -th coarse cohomology group of  $\Lambda$  is isomorphic to the  $n$ -th cohomology group of  $\mathbb{R}^D$  with compact support [48]. The latter is non-trivial only for  $n = D$  and is one-dimensional. The generator of  $D$ -th coarse cohomology group can be taken to be  $\delta f_1 \cup \dots \cup \delta f_D$ , where  $f_\mu(p) = \theta(x^\mu(p))$  and  $x^\mu(p)$  is the  $\mu$ -coordinate of  $p$  and  $\theta(x)$  is theta function. More generally, one can choose  $f_\mu$  to be any function which depends only on  $x^\mu(p)$  and is 0 for  $x^\mu(p) \ll 0$  and 1 for  $x^\mu(p) \gg 0$ . Note that such cochains are bounded and thus also define a nontrivial cohomology class in the sense that we need. For a family of  $D$ -dimensional systems parameterized by  $M$  we therefore define a  $(D + 2)$ -form on  $M$ :

$$\Omega^{(D+2)}(f_1, \dots, f_D) = F^{(D+2)}(\delta f_1 \cup \dots \cup \delta f_D). \quad (8.20)$$

This  $(D + 2)$ -form is closed:

$$\begin{aligned} d\Omega^{(D+2)}(f_1, \dots, f_D) &= dF^{(D+2)}(\delta f_1 \cup \dots \cup \delta f_D) = \partial F^{(D+3)}(\delta f_1 \cup \dots \cup \delta f_D) \\ &= F^{(D+3)}\left(\delta(\delta f_1 \cup \dots \cup \delta f_D)\right) = 0. \end{aligned}$$

Its cohomology class is unchanged under the shift  $f_1 \rightarrow f_1 + g$  by a compactly-supported function  $g$  since

$$\begin{aligned} \Omega^{(D+2)}(g, f_2, \dots, f_D) &= F^{(D+2)}(\delta g \cup \delta f_2 \cup \dots \cup \delta f_D) \\ &= F^{(D+2)}\left(\delta(g \cup \delta f_2 \cup \dots \cup \delta f_D)\right) = \partial F^{(D+2)}(g \cup \delta f_2 \cup \dots \cup \delta f_D) \\ &= dF^{(D+1)}(g \cup \delta f_2 \cup \dots \cup \delta f_D) \end{aligned}$$

and analogously for other shifts  $f_\mu \rightarrow f_\mu + g$ .

In general, periods of  $\Omega^{(D+2)}(f_1, \dots, f_D)$  are not subject to quantization. In Appendix E.1 we argue that integrals over spherical cycles in the parameter space are quantized for families of SRE systems.

## 8.5 Discussion

In this chapter, we have constructed higher-dimensional generalizations of the Berry curvature starting from the ordinary Berry curvature for quantum-mechanical systems and solving the descent equation (8.16). In fact, this procedure of constructing higher-dimensional generalization of topological invariants from lower dimensional ones via descent equations is rather general. For example, the Thouless charge pump for 1d systems [56] and its higher-dimensional generalizations can be constructed from the ground-state charge of a quantum-mechanical system with a  $U(1)$  symmetry. This will be discussed in the next chapter.

When the usual Berry curvature of a family of gapped 0d systems is not exact, it is not possible to find a ground states for the whole family which depends continuously on the parameters. Similarly, we have shown that for a family of gapped  $D$ -dimensional systems the cohomology class of the form  $\Omega^{(D+2)}$  is an obstruction to having a continuously varying gapped boundary. Such a behavior is particularly striking when all the systems in the family are in a trivial phase. An example of a three-parameter family of 1d lattice systems in a trivial phase where  $\Omega^{(3)}$  is not exact is given in Appendix E.2, where we relate the 3-form  $\Omega^{(3)}(f)$  to the Berry-Bloch connection over the Brillouin zone.

For  $D = 0$  the cohomology class of the Berry curvature (regarded as an integral class) is the only topological invariant of the family. It is trivial if and only if the family can be deformed to a constant family without closing the gap. One can ask if the same is true for  $D > 0$  or if there are additional independent invariants. The existence of topological order for  $D > 1$  means that the answer will probably depend on which topological phase one considers. The case  $D = 1$  is special since all gapped 1d systems are Short-Range Entangled. Moreover, for  $D = 1$  it has been conjectured by A. Kitaev that a properly defined space of all gapped bosonic systems has the homotopy type  $K(\mathbb{Z}, 3)$ . That is, its only non-trivial homotopy group is in degree 3 and is isomorphic to  $\mathbb{Z}$ . If this is true, then all cohomology classes on the space of gapped bosonic 1d systems can be expressed as some complicated functions of the basic class which sits in degree 3. That is, for  $D = 1$  bosonic families there

are no further independent invariants beyond the one we constructed.

## HIGHER-DIMENSIONAL GENERALIZATIONS OF THE THOULESS CHARGE PUMP

### 9.1 Introduction

It has been argued by D. Thouless almost 40 years ago [56] that an adiabatic cycling of a gapped 1d system with a  $U(1)$  symmetry at zero temperature results in a quantized charge transport. This is now known as the Thouless charge pump. A simple example is obtained by taking an IQHE system in the cylinder geometry and adiabatically inserting one unit of magnetic flux. This results in a net transport of  $\nu$  units of electric charge, where  $\nu$  is the number of filled Landau levels. The original argument was stated for gapped systems of non-interacting electrons (possibly with disorder) but later was generalized by Niu and Thouless [43] to gapped 1d systems with interactions. They used it to argue that in an FQHE state with a filling fraction  $\nu$  the Hall conductance is  $\nu$  times  $e^2/h$ .

Two key properties of the Thouless charge pump are its integrality and topological invariance (invariance under deformations of the cycle which do not close the energy gap). When attempting to generalize it to higher dimensions, two difficulties present themselves. First, by analogy with the Quantum Hall Effect, one expects that in the presence of nontrivial topological order any topological invariant will be fractional. One expects integrality to hold only for Short-Range Entangled gapped systems. Second, the naive extension of the Thouless charge pump to  $D > 1$  dimensions is ill-defined, because the charge transported through a  $(D-1)$ -dimensional hyperplane under adiabatic cycling is typically infinite. If the system is periodic in the directions parallel to the hyperplane, one can consider the charge transported per unit cell. However, in this chapter we do not want to assume periodicity.

Even if the system is not strictly periodic, one expects uniformity on scales much larger than the correlation length. One can try to exploit this to define an analog of the Thouless charge pump in higher dimensions. Consider the case  $D = 2$  for concreteness and suppose we want to define quantized charge transport in the  $x$  direction. One can fix a real number  $b$ , take the region  $b \leq y \leq b + L$  for some  $L$  which is much larger than the correlation length, and repeat it periodically in the  $y$  direction with period  $L$ . This gives a system which is periodic in the  $y$  direction

but perhaps not gapped. Presumably one can fix this by modifying the system near the lines  $y = b + nL$  with  $n \in \mathbb{Z}$ . Assuming this is done, one can use the gradient expansion to estimate the net charge transported across  $x = 0$  per unit cell per one cycle as a function of  $L$ . One expects the leading terms in this expansion to be

$$Q(L) = AL + q + O(1/L). \quad (9.1)$$

For a macroscopically uniform system the coefficient  $A$  should be independent of  $b$  and of the way we modified the system to make it gapped, but it has dimensions of inverse distance and is not quantized. The dimensionless subleading term  $q$  is sensitive to edge effects, such as the choice of  $b$  and the details of the modification near  $y = b + nL$  and thus cannot be regarded as a characteristic of the original infinite system. It also has no reason to be quantized.

A possible way out is to consider families of gapped systems depending on  $D$  parameters instead of just one. In the above 2d example, suppose that we have a family of gapped systems which depends on two parameters  $\lambda_1$  and  $\lambda_2$  which both have period 1. Then we can make  $\lambda_1$  to be a function of time  $t$  such that  $\lambda_1(0) = 0$  and  $\lambda_1(T) = 1$  and make  $\lambda_2$  to be a function of  $y$  such that  $\lambda_2(b) = 0$  and  $\lambda_2(b + L) = 1$ . The charge transported per unit cell will have an expansion of the same form as when  $\lambda_2$  is fixed:

$$Q'(L) = AL + q' + O(1/L). \quad (9.2)$$

The coefficient  $A$  is expected to be the same, since the effective long-wavelength Hamiltonian differs from the one where  $\lambda_2$  is fixed only by terms which are of order  $1/L$ . The coefficient  $q'$  again depends on the choice of  $b$  and other details. But we claim that if all the systems in the family have a trivial topological order, the difference  $q' - q$  is quantized and is a topological invariant of the family. To see this, imagine stacking the family where  $\lambda_2$  varies with  $y$  with the time-reversal of the family where  $\lambda_2$  is fixed. On the one hand, the net charge transported per unit cell per cycle will be  $q' - q + O(1/L)$ . On the other hand, considering an  $L$ -periodic Short-Range Entangled system with a large  $L$  is essentially the same as compactifying it on a circle of radius  $L$ . By the usual quantization of the Thouless charge pump, the charge transported per cycle must be an integer topological invariant. Taking the limit  $L \rightarrow \infty$ , we conclude that  $q' - q$  is an integer topological invariant. Similarly, one can hope to assign an integer topological invariant to a family of Short-Range Entangled  $D$ -dimensional systems with a  $U(1)$  symmetry parameterized by a  $D$ -dimensional torus  $T^D$ .



The primary goal of this chapter is to define analogs of the Thouless charge pump for  $D$ -parameter families of gapped systems with  $U(1)$  symmetry in  $D$  dimensions. We take a more abstract approach and define topological invariants for families parameterized by arbitrary closed  $D$ -manifolds, not necessarily having the topology of  $T^D$ . While the physical interpretation of these topological invariants is not entirely clear, they are very natural from a mathematical standpoint. Let  $\mathfrak{M}_D^{U(1)}$  be the space of all gapped  $D$ -dimensional systems with a  $U(1)$  symmetry and a non-degenerate ground state. This is an infinite-dimensional space whose topology is of great interest. For example, its set of connected components is the set of gapped phases with  $U(1)$  symmetry in  $D$  dimensions. One can view the Thouless charge pump as a map which assigns an integer to a homotopy class of loops in  $\mathfrak{M}_1^{U(1)}$ . It is clear that this integer is additive under concatenation of loops, so one can view it as a homomorphism from the fundamental group of  $\mathfrak{M}_1^{U(1)}$  to  $\mathbb{Z}$ , or equivalently as an element of  $H^1(\mathfrak{M}_1^{U(1)}, \mathbb{Z})$ . The existence of cycles with a nonzero Thouless charge pump invariant shows that the space  $\mathfrak{M}_1^{U(1)}$  is not simply-connected. To probe higher homotopy or homology groups of spaces  $\mathfrak{M}_D^{U(1)}$ , it is natural to consider multi-parameter families of gapped systems.<sup>1</sup> In the context of systems of free fermions, higher-dimensional analogs of the Thouless charge pump have been considered by Teo and Kane [53]. The existence of higher-dimensional analogs of the Thouless charge pump for families of interacting systems was pointed out by A. Kitaev [32].

The original motivation for studying the Thouless charge pump was the Quantum Hall Effect (QHE) in 2d systems. By considering a 2d system in a cylinder geometry, one can reduce the study of flux insertion in 2d to the study of adiabatic variation of a parameter in 1d. In this special case Thouless charge pump is identified with the Hall conductivity at zero temperature [56, 43]. It is well known that a nonzero value for the zero-temperature Hall conductance of a 2d system implies the existence of gapless edge modes. We show that a similar statement holds for arbitrary 1d systems with a nonzero Thouless charge pump invariant. Namely, for at least one value of the parameters the system on a half-line must have gapless edge modes. This was recently observed numerically in 1d spin chains with a superlattice modulation of parameters [35].

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<sup>1</sup>To avoid possible misconception, we stress that we do not claim that the spaces  $\mathfrak{M}_D^{U(1)}$  are simply-connected for  $D > 1$ . We only claim that natural generalizations of the Thouless charge pump to  $D$  dimensions cannot detect topologically non-trivial loops in  $\mathfrak{M}_D^{U(1)}$  but can detect topologically nontrivial  $D$ -cycles.

## 9.2 Effective field theory

Consider a family of gapped 1d systems parameterized by a manifold  $M$ . If one allows the parameters to vary slowly with space-time coordinates, then the parameters become classical background fields on the two-dimensional space-time  $X$ . These fields are described by a map  $\phi : X \rightarrow M$ . Integrating out the gapped degrees of freedom, one gets an effective action for these fields. This action may contain topological terms, i.e. terms which do not depend on the metric on  $X$ . If all the gapped systems in the family have an on-site  $U(1)$  symmetry, they can also be coupled to a classical  $U(1)$  background gauge field  $A$ . Then the effective action depends both on  $\phi$  and  $A$ . When  $X$  is two-dimensional, gauge-invariance constrains these terms to have the form

$$S_{top}(X, \phi, A) = \int_X \epsilon^{\mu\nu} A_\mu \partial_\nu \phi^i \tau_i(\phi) d^2x + \dots = \int_X A \wedge \phi^* \tau + \dots, \quad (9.3)$$

where  $\tau^i(\phi)$  are components of a closed 1-form  $\tau$  on  $M$ ,  $\epsilon^{\mu\nu}$  denotes the anti-symmetric tensor density with  $\epsilon^{01} = 1$ , and dots denote terms independent of  $A$ . In addition, here and below Greek indices label coordinates on the space-time  $X$  while Roman indices label coordinates on the parameter space  $M$ . Varying the above action with respect to  $A$ , we find a topological term in the current

$$J_{top}^\mu(x^0, x^1) = \epsilon^{\mu\nu} \tau_i(\phi(x^0, x^1)) \partial_\nu \phi^i(x^0, x^1). \quad (9.4)$$

Such topological terms in the  $U(1)$  current have been discovered by Goldstone and Wilczek in their work on soliton charges [22]. If we now let  $\phi^i$  be independent of  $x^1$  and be periodic functions of  $x^0$  with period  $T$ , we find that the net topological charge per period transported through a section  $x^1 = a$  is given by

$$\Delta Q(a) = \int_0^T J_{top}^1(x^0, a) dx^0 = - \oint \tau_i(\phi) d\phi^i. \quad (9.5)$$

We see that the topological charge transport is independent of  $a$  and given by an integral of  $\tau$  along the corresponding loop in  $M$ . Such an integral is called a period of the 1-form  $\tau$ . A period of a closed 1-form does not change under continuous deformations of the loop, so  $\Delta Q(a)$  is a topological invariant.

To see that  $\Delta Q$  is quantized, one needs to exploit the invariance of the effective field theory under "large"  $U(1)$  gauge transformation which cannot be deformed to a constant. Such a transformation can be described by a continuous multi-valued function  $f : X \rightarrow \mathbb{R}$  whose values are defined up to an integer multiple of  $2\pi$ . Performing the gauge transformation  $A \mapsto A + df$ , we find that the action changes

by  $\int_X df \wedge \phi^* \tau$ . For  $e^{iS_{top}}$  to be unchanged, the change in the action must be an integral multiple of  $2\pi$ . This is satisfied for all conceivable  $f$  and  $\phi$  if and only if integrals of  $\tau$  over arbitrary 1-cycles on  $M$  (that is, all periods of  $\tau$ ) are integers. Therefore  $\Delta Q$  is also an integer.

In higher dimensions, gauge-invariance allows for a more complicated dependence of  $S_{top}$  on  $A$ . For example, quantum Hall response for 2d systems is described by the Chern-Simons action. However, if our goal is to generalize the Thouless charge pump to higher dimensions, we can focus on the terms which modify the current even when the gauge field strength vanishes. Such terms are linear in  $A$  and have the form

$$S_{top}(X, A, \phi) = \int_X A \wedge \phi^* \tau, \quad (9.6)$$

where  $X$  is  $(D + 1)$ -dimensional space-time,  $\phi : X \rightarrow M$  is a smooth map, and  $\tau$  is a closed  $D$ -form on  $M$ . Invariance with respect to "large" gauge transformations again imposes restrictions on periods of  $\tau$  (that is, integrals of  $\tau$  over  $D$ -cycles in  $M$ ). It is not entirely obvious what these restrictions are for general  $D$ . To see what the difficulty is, consider the current corresponding to the above action:

$$J_{top}^\mu = \epsilon^{\mu\nu_1 \dots \nu_D} \tau_{i_1 \dots i_D} \partial_{\nu_1} \phi^{i_1} \dots \partial_{\nu_D} \phi^{i_D}. \quad (9.7)$$

One effect of such a topological term in the current is to give charge to "skyrmions", i.e. topologically non-trivial configurations of fields  $\phi^i$ . Suppose the space-time has the form  $Y \times \mathbb{R}$ , where the spatial manifold  $Y$  is closed and oriented. Then the charge of a skyrmion is  $Q_Y(\phi) = \int_Y J = \int_Y \phi^* \tau$ . For  $Q_Y(\phi)$  to be integral,  $\tau$  must integrate to an integer over any  $D$ -cycle on  $M$  of the form  $\phi_*[Y]$ , where  $[Y]$  is the fundamental class of the  $D$ -manifold  $Y$ , and  $\phi_*$  denotes the pushforward map in homology. But for a general manifold  $M$  and a general  $D$  it is not true that any  $D$ -cycle in a manifold  $M$  can be realized as a pushforward of the fundamental homology class of some closed oriented  $D$ -manifold [54]. In the fermionic case the geometry of  $Y$  is even more restricted (it must be a  $Spin^c$  manifold [31]), so for general  $D$  the integrality of charge is not equivalent to the integrality of periods of  $\tau$ . Nevertheless, for sufficiently low  $D$  the integrality of charge does require the periods of  $\tau$  to be integral. In the bosonic case, this follows from the fact that for  $D \leq 6$  any  $D$ -cycle is a pushforward of the fundamental homology class of a closed oriented  $D$ -manifold [54]. Since any closed oriented  $D$ -manifold with  $D \leq 3$  has a spin structure, for fermionic systems in dimension  $D \leq 3$  the integrality of charge also requires the integrality of periods of  $\tau$ . Also, if the parameter space is

a  $D$ -dimensional sphere or a  $D$ -dimensional torus, one can set  $Y = S^D$  or  $Y = T^D$  both in the bosonic and fermionic cases. In this case  $\tau$  is a top-degree form, and the skyrmion charge is its integral over the whole  $M$ . Thus the integrality of charge requires the integral of  $\tau$  over  $S^D$  or  $T^D$  to be integral.

The argument for quantization of  $\tau$  in higher dimensions has an important loophole. If the gapped system of interest is in a topologically ordered phase, the effective field theory should really be a TQFT coupled to  $\phi$  and  $A$ . In this situation  $S_{top}$  written above need not be invariant under large gauge transformations by itself, and accordingly its integrals over  $D$ -cycles need not be integral.

### 9.3 Thouless charge pump for 1d lattice systems

Consider a lattice system in one spatial dimension, with a finite-dimensional on-site Hilbert space and an on-site  $U(1)$  symmetry. We also assume that there is a unique ground state, with a nonzero energy gap to excited states. If Hamiltonian  $H$  depends on a parameter  $\lambda$ , we will say that we have a one-parameter family of gapped  $U(1)$ -invariant 1d systems. We will assume that  $\lambda$  is periodically identified with period 1, so that our one-parameter family is a loop  $\Gamma$  in the space of gapped  $U(1)$ -invariant 1d systems.

Following Thouless [56], we consider slowly varying  $\lambda$  as a function of time  $t$ , so that  $\lambda(0) = 0$  and  $\lambda(T) = 1$  for some large time  $T$ . This will drive the system out of the ground state and create nonzero charge current. This current can be found as follows [43].

We can separate the density matrix into an instantaneous part and a small deviation:

$$\rho(t) = \rho_{inst}(\lambda(t)) + \Delta\rho(t), \quad (9.8)$$

where

$$\rho_{inst}(\lambda) = |0(\lambda)\rangle\langle 0(\lambda)| \quad (9.9)$$

and  $|0(\lambda)\rangle$  is the ground state of Hamiltonian  $H(\lambda)$ . We may always normalize the lowest eigenvalue to be 0, for all  $\lambda$ .

The equation of motion is

$$-i[H, \Delta\rho] = -i[H, \rho_{inst} + \Delta\rho] = \dot{\rho}_{inst} + \Delta\dot{\rho} \approx \dot{\rho}_{inst}, \quad (9.10)$$

where dot is derivative with respect to  $t$  and we have dropped  $\Delta\dot{\rho}$  since it is small in the adiabatic approximation. Sandwiching this equation between instantaneous

ground state  $|0(\lambda)\rangle$  with energy 0 and instantaneous excited state  $|n(\lambda)\rangle$  with energy  $E_n(\lambda)$ , we find

$$\langle 0|\Delta\rho|n\rangle = -\frac{i\langle\dot{0}|n\rangle}{E_n} = \frac{i\langle 0|\dot{H}|n\rangle}{E_n^2}. \quad (9.11)$$

Here in the last step we used the perturbation theory formula

$$|\dot{0}\rangle = \lambda \frac{\partial}{\partial\lambda}|0\rangle = -\lambda \frac{1}{H} P \frac{\partial H}{\partial\lambda}|0\rangle = -\frac{1}{H} P \dot{H}|0\rangle, \quad (9.12)$$

where  $P$  is the projector to the excited states.

Let  $J^N(a)$  be the operator corresponding to the current through a point  $a \in \mathbb{R}$

$$J^N(a) = \sum_{\substack{p>a \\ q<a}} J_{pq}^N. \quad (9.13)$$

The total charge passing through the point  $a$  over one period  $T$  is given by

$$\Delta Q = \int_0^T dt \left[ (1 + \Delta\rho_{00}) J^N(a)_{00} + \sum_{n \neq 0} (\Delta\rho_{0n} J^N(a)_{n0} + J^N(a)_{0n} \Delta\rho_{n0}) \right], \quad (9.14)$$

where we have dropped terms which are small in the adiabatic expansion. Due to Bloch's theorem [10, 59], the net current in a ground state is zero, hence  $J^N(a)_{00} = 0$ .

The remaining terms can be rewritten using (9.11) as

$$\Delta Q = i \int_0^T dt \left[ \langle \dot{H} \frac{P}{H^2} J^N(a) \rangle - \langle J^N(a) \frac{P}{H^2} \dot{H} \rangle \right] = i \int_0^T dt \oint \frac{dz}{2\pi i} \text{Tr} \left( G \dot{H} G^2 J^N(a) \right). \quad (9.15)$$

Here  $G = (z - H)^{-1}$  is the many-body Green's function, and the contour integral in the  $z$ -plane is taken along a loop surrounding only the lowest eigenvalue of  $H$ .

The integral over time  $t$  can be replaced with an integral in the parameter space. The result is that the total charge transported during periodic adiabatic variation is given by

$$\Delta Q = i \int_0^1 d\lambda \oint \frac{dz}{2\pi i} \text{Tr} \left( G \frac{dH}{d\lambda} G^2 J^N(a) \right). \quad (9.16)$$

#### 9.4 A static formula for the Thouless charge pump

As explained in [56], Hall conductance can be viewed as a special case of the charge pump. For Hall conductance, there are two types of formulas: the Streda formula [51] and various versions of the Kubo formula (see e.g. [43]). The Streda formula

at zero temperature involves only static linear response. The Kubo formula involves dynamic response even if one specializes to zero temperature and is more subtle. In this section we derive a formula for the Thouless charge pump, which involves only static linear response and thus is analogous to the zero-temperature Streda formula. It turns out to be a more convenient starting point for higher-dimensional generalizations.

As a warm-up, consider a family of gapped 0d quantum-mechanical systems with a  $U(1)$  symmetry and a non-degenerate ground state parameterized by a manifold  $M$ . We will collectively denote the parameters  $\lambda^\ell$  as  $\lambda$ . The charge operator  $Q$  has integer eigenvalues and is assumed to be independent of the parameters. This is because the symmetry action on the Hilbert space is fixed. The Hamiltonian  $H$  is a Hermitian operator continuously depending on the parameters  $\lambda$ . By adding to  $H(\lambda)$  a scalar depending on  $\lambda$ , one can normalize the ground-state energy to be zero for all  $\lambda$ . The ground-state charge  $Q^{(0)} = \langle Q \rangle$  is independent of  $\lambda$  because it is an integer and varies continuously with  $\lambda$ . One can also prove this without using integrality:

$$d\langle Q \rangle = -\left\langle dH \frac{P}{H} Q \right\rangle - \left\langle Q \frac{P}{H} dH \right\rangle = -Q^{(0)} \left\langle dH \frac{P}{H} \right\rangle - Q^{(0)} \left\langle \frac{P}{H} dH \right\rangle = 0. \quad (9.17)$$

Here  $P$  is the projector to excited states,  $d = \sum_\ell d\lambda^\ell \frac{\partial}{\partial \lambda^\ell}$  is the exterior differential on  $M$ , and the angular brackets denote ground-state average.

Turning to gapped many-body systems in dimension  $D > 0$ , we note that the Goldstone theorem implies that the  $U(1)$  symmetry is unbroken, and thus expectation values of the form  $\langle [Q_{tot}, A] \rangle$  vanish for all local operators  $A$ . Here  $Q_{tot} = \sum_p Q_p$  as before. This does not mean, however, that the ground-state is annihilated by  $Q_{tot}$ . The operator  $Q_{tot}$  is unbounded, and its ground-state expectation value is typically ill-defined. The change in the expectation value of  $Q_{tot}$  under variation of  $\lambda$  is typically ill-defined too.

For  $D = 1$  one can hope that the change in the expectation of the charge on the half-line  $p > a$  is finite. Indeed, one expects this to be equal to the charge which flows from the region  $p < a$  to the region  $p > a$  as one changes parameters. Since the current operator  $J^N(a)$  is bounded for  $D = 1$ , the change in the charge should be well-defined. Some regularization might be needed though.

The infinitesimal change in the expectation value of the charge  $Q_q$  at site  $q$  can be

computed using static linear response theory:

$$d\langle Q_q \rangle = \oint \frac{dz}{2\pi i} \text{Tr} (G dH G Q_q). \quad (9.18)$$

Here we used an integral representation of the projector to the ground state  $1 - P$ :

$$1 - P = \oint \frac{dz}{2\pi i} \frac{1}{z - H}. \quad (9.19)$$

The expression (9.18) is well-defined because one can write it as an absolutely convergent sum of correlators of local observables:

$$d\langle Q_q \rangle = \sum_{p \in \Lambda} \oint \frac{dz}{2\pi i} \text{Tr} (G dH_p G Q_q). \quad (9.20)$$

Indeed, the terms in this sum decay exponentially with  $|p - q|$  [60]. On the other hand, the sum  $\sum_{q>a} d\langle Q_q \rangle$  has no reason to be absolutely convergent and its value is ambiguous. To make sense of it, we first of all rewrite eq. (9.18) as follows:

$$d\langle Q_q \rangle = \sum_{p \in \Lambda} T_{pq}^{(1)}, \quad (9.21)$$

where

$$T_{pq}^{(1)} = \oint \frac{dz}{2\pi i} \text{Tr} (G dH_p G Q_q - G dH_q G Q_p). \quad (9.22)$$

The second term in  $T_{pq}^{(1)}$  gives zero contribution to  $d\langle Q_q \rangle$ , since

$$- \oint \frac{dz}{2\pi i} \text{Tr} (G dH_q G Q_{tot}) = - \oint \frac{dz}{2\pi i} \text{Tr} (G^2 dH_q Q_{tot}) = \oint \frac{dz}{2\pi i} \frac{\partial}{\partial z} \text{Tr} (G dH_q Q_{tot}) = 0. \quad (9.23)$$

Introducing  $f(p) = \theta(p - a)$  and using the skew-symmetry of  $T_{pq}^{(1)}$ , one can formally write

$$\sum_{q>a} d\langle Q_q \rangle = \sum_{p, q \in \Lambda} f(q) T_{pq}^{(1)} = \frac{1}{2} \sum_{p, q \in \Lambda} (f(q) - f(p)) T_{pq}^{(1)}. \quad (9.24)$$

The rightmost sum is absolutely convergent because  $T_{pq}^{(1)}$  decays exponentially when  $|p - q|$  is large [60], while  $f(q) - f(p)$  is nonzero only when  $q > a$  and  $p < a$  or  $q < a$  and  $p > a$ . To make the convergence more obvious one can write the rightmost sum more explicitly as  $\sum_{\substack{p < a \\ q > a}} T_{pq}^{(1)}$ .

Let us therefore define a 1-form  $Q^{(1)}(f)$  on the parameter space of gapped 1d systems with a  $U(1)$  symmetry

$$Q^{(1)}(f) = \frac{1}{2} \sum_{p, q \in \Lambda} (f(q) - f(p)) T_{pq}^{(1)}. \quad (9.25)$$

It will be convenient to allow  $f$  to be an arbitrary real function on the lattice  $\Lambda$  such that  $f(p) = 0$  for  $p \ll 0$  and  $f(p) = 1$  for  $p \gg 0$ . Convergence still holds, as can be easily verified. In the case  $f(p) = \theta(p - a)$  the 1-form  $Q^{(1)}(f)$  has the meaning of the regularized differential of the charge on the half-line  $p > a$ .

We are now going to relate  $Q^{(1)}(f)$  to the Thouless charge pump. Eq. (9.16) expresses the net charge pumped during one cycle as an integral of a 1-form on the parameter space. We would like to compare this 1-form with the 1-form  $Q^{(1)}(f)$ . The first step is to generalize the 1-form appearing in (9.16) by allowing dependence on a function  $f : \Lambda \rightarrow \mathbb{R}$ . This is achieved by replacing the current operator  $J^N(a)$  with a smeared current operator

$$-J^N(\delta f) = -\frac{1}{2} \sum_{p,q \in \Lambda} (f(q) - f(p)) J_{pq}^N. \quad (9.26)$$

If we assume  $f(p) = 1$  for  $p \gg 0$  and  $f(p) = 0$  for  $p \ll 0$ , then this expression is well-defined. If we set  $f(p) = \theta(p - a)$ , it reduces to  $J^N(a)$ . Ignoring convergence issues, one can formally write  $J^N(\delta f) = \sum_{p,q} f(q) J_{pq}^N$ . Upon using the conservation law (3.2), this becomes  $-dQ(f)/dt$ , where  $Q(f) = \sum_q f(q) Q_q$  is the smeared charge on a half-line. Of course, these manipulations are formal, since for  $f$  as above both the operator  $Q(f)$  and its time-derivative is unbounded, and so is its time-derivative. In any case, replacing  $J^N(a)$  with  $-J^N(\delta f)$  we get a 1-form on the parameter space

$$\tilde{Q}^{(1)}(f) = -i \oint \frac{dz}{2\pi i} \text{Tr} \left( G dH_q G^2 J^N(\delta f) \right). \quad (9.27)$$

We provisionally denoted this 1-form  $\tilde{Q}^{(1)}(f)$ , but in fact it coincides with  $Q^{(1)}(f)$ . Indeed, their difference is

$$\begin{aligned} & \frac{1}{2} \sum_{p,q \in \Lambda} (f(q) - f(p)) \oint \frac{dz}{2\pi i} \text{Tr} \left( G dH_p G Q_q - G dH_q G Q_p + i G dH G^2 J_{pq}^N \right) \\ &= \frac{1}{2} \sum_{p,q,r \in \Lambda} (f(q) - f(p)) \oint \frac{dz}{2\pi i} \text{Tr} \left( i G dH_p G^2 J_{qr}^N + i G dH_q G^2 J_{rp}^N + i G dH_r G^2 J_{pq}^N \right) \\ &= \frac{1}{6} \sum_{p,q,r \in \Lambda} (f(q) - f(p) + f(r) - f(q) + f(p) - f(r)) \\ & \quad \times \oint \frac{dz}{2\pi i} \text{Tr} \left( i G dH_p G^2 J_{qr}^N + i G dH_q G^2 J_{rp}^N + i G dH_r G^2 J_{pq}^N \right) = 0. \end{aligned} \quad (9.28)$$

Thus we proved a new formula for the Thouless charge pump:

$$\Delta Q = \int Q^{(1)}(f). \quad (9.29)$$



Here  $Q^{(1)}(f)$  is a 1-form on the parameter space  $M$  and the integration is over a loop in  $M$  specifying the periodic family of Hamiltonians we are interested in. In principle one should set  $f(p) = \theta(p - a)$ . In fact, this expression is independent of  $f$ , provided the asymptotic behavior is as required above. Indeed, given any other such function  $f'$ , the difference  $g = f' - f$  is compactly supported. Therefore

$$Q^{(1)}(f') - Q^{(1)}(f) = \frac{1}{2} \sum_{p,q} (g(q) - g(p)) T_{pq}^{(1)} = \sum_{p,q} g(q) T_{pq}^{(1)} = d\langle Q(g) \rangle. \quad (9.30)$$

Here  $Q(g) = \sum_q g(q) Q_q$ . Since the difference of these two 1-forms is exact, their integrals over any loop are the same. In particular, the value of  $\Delta Q$  is independent of  $a$  (the location of the point where the current is measured).

This last result immediately implies that a family of systems with a non-zero value of  $\Delta Q$  cannot have an edge which is gapped and varies continuously with the loop parameter. Indeed, such an edge would be the same as a gapped interpolation between our family of systems for  $p \gg 0$  and a trivial system (i.e. a gapped system with a product ground state which is independent of parameters) for  $p \ll 0$ . The above result means that we can choose  $a$  to be in either of these regions and the result will be unaffected by the choice. Since the formula for  $\Delta Q$  is local, we conclude that  $\Delta Q$  computed for  $a \gg 0$  will coincide with  $\Delta Q$  computed for the infinite system without an edge. For the same reason, for  $a \ll 0$  we find  $\Delta Q = 0$ , since the system is trivial there. Therefore, if  $\Delta Q \neq 0$ , such an edge does not exist and there must be gapless edge modes for some values of the loop parameter. The appearance of gapless edge modes in 1d spin chains depending on a parameter has been numerically observed in [35].

We note the following useful properties of the 1-forms  $T_{pq}^{(1)}$  and  $Q^{(1)}(f)$ . Suppose we replace each  $H_p$  with its complex-conjugate  $H_p^*$ . Physically this corresponds to time-reversal. Using the Hermiticity of  $H_p$  and  $Q_p$ , it is easy to see that this operation maps  $T_{pq}^{(1)}$  to  $T_{qp}^{(1)}$  and thus reverses the sign of  $Q^{(1)}(f)$ . This agrees with the intuition that time-reversal flips the sign of the Thouless charge pump. Another useful fact is when we stack together two independent families of systems, the corresponding 1-forms  $T_{pq}^{(1)}$  and  $Q^{(1)}(f)$  add up. This is not easy to see from the above formulas. However, it follows from the physical interpretation of the Thouless charge pump and can be shown formally by re-writing the above formulas in terms of Kubo's canonical correlation function.

The new formula is a convenient starting point to for proving that the Thouless charge pump is a topological invariant, i.e. that it does not change under continuous

deformations of the loop in the parameter space. The integral of a 1-form does not vary under continuous changes of the contour if and only if the 1-form is closed. As we will show later in the chapter, there exists a 2-form  $T_{pqr}^{(2)}$  which is skew-symmetric in  $p, q, r$ , decays exponentially when any of the pairwise distances between  $p, q, r$  are large, and satisfies

$$dT_{qr}^{(1)} = \sum_{p \in \Lambda} T_{pqr}^{(2)}. \quad (9.31)$$

This can be used to show that  $dQ^{(1)}(f) = 0$ :

$$\begin{aligned} dQ^{(1)}(f) &= \frac{1}{2} \sum_{p, q \in \Lambda} (f(q) - f(p)) dT_{pq}^{(1)} = \frac{1}{2} \sum_{p, q, r \in \Lambda} (f(q) - f(p)) T_{pqr}^{(2)} \\ &= \frac{1}{6} \sum_{p, q, r \in \Lambda} (f(q) - f(p) + f(r) - f(q) + f(p) - f(r)) T_{pqr}^{(2)} = 0. \end{aligned} \quad (9.32)$$

Putting the above observations together, we conclude that  $Q^{(1)}(f)$  defines a degree-1 cohomology class on the parameter space which does not depend on the choice of  $f$ . The Thouless charge pump for any loop is the evaluation of this cohomology class on the homology class of the loop. This makes the topological nature of the Thouless charge pump completely explicit. In Appendix F.1 we argue that the integral of  $Q^{(1)}(f)$  over any loop in the parameter space is an integer. So in fact the cohomology class of  $Q^{(1)}(f)$  is integral and  $\Delta Q$  is quantized.

## 9.5 Descendants of the Thouless charge pump

Trying to keep the same level of transparency in formulas is hard when passing to higher dimensions. The formulas tend to be clumsy and computations become cumbersome. However, introduction of some straightforward and natural notations makes the equations look elegant and cumbersome computations become a simple routine. In this section, we will use notations and definitions explained in Appendix A.

We have seen that the Thouless charge pump of a 1d system can be expressed as an integral of a 1-form on the parameter space. This 1-form represents a suitably regularized differential of the ground-state charge on a half-line. The ground-state charge of the whole 1d system as well as its differential are ill-defined in the infinite volume limit. In a sense, the Thouless charge pump is a 1d descendant of the ground-state charge. Mathematically, this statement is encapsulated by eq. (9.21). Using the chain notation, it can be written as

$$dT^{(0)} = \partial T^{(1)}, \quad (9.33)$$

where  $T^{(0)}$  is a 0-chain with components  $\langle Q_p \rangle$ ,  $T^{(1)}$  is 1-chain with components  $T_{pq}^{(1)}$ ,  $d$  is the exterior differential on the parameter space, and  $\partial$  is the boundary operator on chains. Note that the chain  $T^{(0)}$  takes values in 0-forms on the parameter space while the chain  $T^{(1)}$  takes values in 1-forms on the parameter space. If we say that the total degree of an  $n$ -chain with values in  $m$ -forms is  $n - m$ , then both  $T^{(0)}$  and  $T^{(1)}$  have total degree 0. Both  $d$  and  $\partial$  increase the total degree by 1.

Generalising this we can consider a more general “descent equation”:

$$dT^{(n)} = \partial T^{(n+1)}, \quad (9.34)$$

with  $T^{(n)}$  is an  $n$ -chain with value in  $n$ -forms on the parameter space. This descent equations was first proposed by A. Kitaev [33, 32]. Using the 0-chain  $T^{(0)}$  with components  $\langle Q_p \rangle$  as initial condition, a solution to this equation can be found to be

$$T_{p_0 \dots p_n}^{(n)} = \sum_{\sigma \in \mathcal{S}_{n+1}} (-1)^{\text{sgn} \sigma} \oint \frac{dz}{2\pi i} \text{Tr} \left( G dH_{p_{\sigma(0)}} G dH_{p_{\sigma(1)}} \dots G dH_{p_{\sigma(n-1)}} G Q_{p_{\sigma(n)}} \right), \quad (9.35)$$

where  $\mathcal{S}_{n+1}$  is the permutation group on  $n + 1$  objects and wedge product of forms  $\wedge$  is implicit. For  $n = 2$  the expression  $T_{pqr}^{(2)}$  decays exponentially when  $|p - q|$ ,  $|q - r|$ , or  $|p - r|$  are large [60]. The physical interpretation is that static linear response of a gapped system to perturbations near a point  $p$  is insensitive to variations of the Hamiltonian far from  $p$ . We expect that the method of [60] can be used to show that  $T^{(n)}$  for any  $n$  decays exponentially when any two of the points  $p_0, \dots, p_n$  are far apart. This means that  $T^{(n)}$  is a well-defined  $n$ -chain. Physically, such a decay means that the all-order non-linear static response of a gapped system to perturbations near a point  $p$  is insensitive to variations of the Hamiltonian far from  $p$ .

Note that the descent equation for  $n = 2$  was used by us to argue that the 1-form  $Q^{(1)}(f)$  is closed. Now that we know that a solution to the  $n = 2$  descent equation exists, our proof that  $Q^{(1)}(f)$  is closed is complete.

To get an  $n$ -form on  $M$  it is natural to consider expressions of the form  $T^{(n)}(\alpha)$  for some  $n$ -cochain  $\alpha$ . An  $n$ -form can be integrated over a closed  $n$ -manifold in the parameter space, or more generally over an  $n$ -cycle in the parameter space. Such an integral is a topological invariant (unchanged under deformations of the cycle) if and only if the  $n$ -form  $T^{(n)}(\alpha)$  is closed. Using the descent equation we get:

$$dT^{(n)}(\alpha) = \partial T^{(n+1)}(\alpha) = T^{(n+1)}(\delta\alpha). \quad (9.36)$$

Thus we want the cochain  $\alpha$  to be closed,  $\delta\alpha = 0$ . Also, for exact cochain  $\alpha = \delta\gamma$  we find

$$T^{(n)}(\alpha) = T^{(n)}(\delta\gamma) = \partial T^{(n)}(\gamma) = dT^{(n-1)}(\gamma) = dT^{(n-1)}(\gamma). \quad (9.37)$$

This means that integral of such a form over any cycle will be zero.

Combining these two facts we see that in order to get a non-trivial topological invariant one has to contract the  $n$ -chain  $T^{(n)}$  with an  $n$ -cochain  $\alpha$  which is closed but not exact. As explained in [48], such cochains are controlled by the coarse geometry of  $\Lambda$ . If  $\Lambda \subset \mathbb{R}^D$  is coarsely equivalent to  $\mathbb{R}^D$  (in the sense that there exists some  $R > 0$  such that any point of  $\mathbb{R}^D$  is within distance  $R$  of some point of  $\Lambda$ ), then one can construct closed but not exact cochains of degree  $D$ , but not in other degrees. Moreover, the space of closed  $D$ -cochains modulo exact  $D$ -cochains (that is, degree- $D$  cohomology) is one-dimensional, so up to an overall scaling  $\alpha$  is essentially unique. One can take it to be  $\delta f_1 \cup \dots \cup \delta f_D$  where  $f_\mu = \theta(x^\mu(p))$  with  $x^\mu(p)$  being the  $\mu$ -coordinate of cite  $p$ , and  $\cup$  is a product operation on cochains.

The conclusion is that one can define a topological invariant of  $D$ -parameter families of gapped  $D$ -dimensional systems as an integral of a  $D$ -form  $Q^{(D)}(f_1, \dots, f_D)$  on the parameter space. This  $D$ -form is given by

$$Q^{(D)}(f_1, \dots, f_D) = T^{(n)}(\delta f_1 \cup \dots \cup \delta f_D). \quad (9.38)$$

The integral of this  $D$ -form over a  $D$ -cycle in the parameter space is invariant under deformations of the cycle. It is also invriant under changes of the functions  $f_\mu(p)$ , provided they have the same asymptotic behavior as  $\theta(x^\mu(p))$ . Thus integrals of  $Q^{(D)}$  over  $D$ -cycles in the parameter space are a natural generalization of the Thouless charge pump to dimension  $D$ .

We argue in Appendix F.1 that the form  $Q^{(D)}$  is properly normalized, in the sense that for familes of Short-Range Entangled systems its integrals over spherical cycles are integer.

## 9.6 Physical interpretation of the 2d Thouless charge pump

Our approach to defining higher-dimensional analogs of the Thouless charge pump was rather formal. In this section we are going to clarify their physical meaning in the case when the system is two-dimensional and the parameter space is a torus of dimension two. As proposed in the introduction, the physical interpretation involves making the parameters of the Hamiltonian slowly varying functions of both time and spatial coordinates.

As a warm-up, let us discuss an alternative interpretation of the usual Thouless charge pump for gapped 1d systems. As discussed in Section 2, the same term in the effective action gives rise to the Thouless charge pump and gives charge to 1d skyrmions. A skyrmion is defined as a topologically nontrivial map  $\phi$  from  $\mathbb{R}$  to the parameter space  $M$  which approaches the same point both at  $x = -\infty$  and  $x = +\infty$ . Such a map is topologically the same as a loop in the parameter space with a basepoint corresponding to the value of the parameters at  $x = \pm\infty$ . It follows from eq. (9.4) that the topological invariant  $\Delta Q = \int \phi^* \tau$  attached to a loop can be interpreted in two different ways: as minus the net charge pumped through  $x = 0$  when the loop parameter is a slowly-varying function of time and as the charge of a skyrmion corresponding to the loop. From the point of view of lattice models, it is far from obvious that the same topological invariant controls both quantities. Our first goal is to show that this is indeed the case.

Let us consider the parameter space  $M$  given by a loop  $S^1$  parameterized by a variable  $\lambda \in [0, 1]$  such that both 0 and 1 correspond to the basepoint. Thus we have a one-parameter family of gapped  $U(1)$ -invariant Hamiltonians

$$H(\lambda) = \sum_p H_p(\lambda) \quad (9.39)$$

such that  $H_p(0) = H_p(1)$ . We assume that all these Hamiltonians have a unique ground state and denote by  $\xi$  the supremum of the correlation lengths of these ground states.

Let  $g : \mathbb{R} \rightarrow [0, 1]$  be a continuous function defined as follows:

$$g(x) = \begin{cases} 0, & x < L \\ \frac{x}{L} - 1, & L \leq x \leq 2L \\ 1, & x > 2L. \end{cases} \quad (9.40)$$

The "skyrmion" Hamiltonian  $H^s$  is obtained by making  $\lambda$  depend on  $p$ :

$$H^s = \sum_p H_p^s = \sum_p H_p(g(p)). \quad (9.41)$$

Thus  $H_p^s = H_p(0)$  if  $p < L$  or  $p > 2L$ .

To proceed, we need to make a technical assumption. Suppose we are given a family of gapped Hamiltonians depending on some parameters which live in a compact parameter space  $\mathcal{R}$ . Suppose also that all these Hamiltonians have a unique ground state and let  $\xi$  be the supremum of the correlation lengths of all the ground states.

Now suppose we make the parameters slowly varying functions of coordinates. By a slow variation we mean that the parameters vary appreciably over a scale  $L$  which is much larger than  $\xi$ . Our technical assumption will be that the new Hamiltonian is still gapped, has a unique ground state, and its correlation length is of order  $\xi$  and thus is still much smaller than  $L$ . Essentially, this is the same as assuming that derivative expansion makes sense for gapped systems with a unique ground state.

Assuming this, we can apply the results of [60] on the insensitivity of the expectation values of local observables on the behavior of the Hamiltonian far from the support of the observable. In particular, the expectation values of observables supported at  $x < 0$  or  $x > 3L$  in the ground state of  $H^s$  are exponentially close to the expectation values of the same observables in the ground state of  $H(0)$ . Therefore we can define the skyrmion charge as follows:

$$Q^s = \lim_{L \rightarrow \infty} \sum_p (\langle Q_p \rangle_s - \langle Q_p \rangle_0), \quad (9.42)$$

where  $\langle \dots \rangle_s$  and  $\langle \dots \rangle_0$  denote expectation values in ground states of  $H^s$  and  $H(0)$ , respectively. The sum over  $p$  is converging exponentially fast away from  $L < p < 2L$ , so we can write

$$Q^s = \sum_p \langle Q_p \rangle_s h(p) - \sum_p \langle Q_p \rangle_0 h(p) + O(L^{-\infty}), \quad (9.43)$$

where  $h(x) = \theta(x) - \theta(x - 3L)$ .

To compute the r.h.s. of eq. (9.43) we need a family of gapped Hamiltonians interpolating between  $H(0)$  and  $H^s$ . Since the loop used to define  $H^s$  is assumed to be non-contractible, such an interpolation does not exist if we require the asymptotic behavior at  $x = \pm\infty$  to be fixed. But if we relax this constraint, the difficulty disappears. We are going to use the following one-parameter family:

$$\tilde{H}(\mu) = \sum_p \tilde{H}_p(\mu) = \sum_p H_p(g_\mu(p)), \quad (9.44)$$

where  $\mu \in [0, 1]$  and the continuous function  $g_\mu : \mathbb{R} \rightarrow [0, 1]$  is defined as follows:

$$g_\mu(x) = \begin{cases} g(x), & x < L(1 + \mu), \\ \mu, & x \geq L(1 + \mu). \end{cases} \quad (9.45)$$

Obviously,  $\tilde{H}(0) = H(0)$  and  $\tilde{H}(1) = H^s$ . Also, if  $p < L$ , then  $\tilde{H}_p(\mu) = H_p(0)$  regardless of the value of  $\mu$ , while for  $p > 2L$   $\tilde{H}_p(\mu) = H_p(\mu)$ . By our basic

assumption, the Hamiltonian  $\tilde{H}(\mu)$  is gapped for all  $\mu$ , has a unique ground state, and its correlation length is of order  $\xi$ . We can write:

$$Q^s = \sum_q h(q) \int_0^\mu d\mu \frac{d}{d\mu} \langle Q_q \rangle_\mu + O(L^{-\infty}), \quad (9.46)$$

where  $\langle \dots \rangle_\mu$  denotes the expectation value in the ground-state corresponding to  $\tilde{H}(\mu)$ .

On the other hand, for the one-parameter family  $\tilde{H}(\mu)$  we have an identity

$$d\langle Q_q \rangle_\mu = \sum_p \tilde{T}_{pq}^{(1)}. \quad (9.47)$$

Here the 1-form  $\tilde{T}_{pq}^{(1)}$  on  $[0, 1]$  is given by

$$\tilde{T}_{pq}^{(1)} = \oint \frac{dz}{2\pi i} \text{Tr} (\tilde{G} d\tilde{H}_p \tilde{G} Q_q - \tilde{G} d\tilde{H}_q \tilde{G} Q_p), \quad (9.48)$$

and  $\tilde{G} = (z - \tilde{H})^{-1}$ . It is skew-symmetric under the interchange of  $p, q$  and decays exponentially when  $|p - q|$  is large. Using this, we can re-write the skyrmion charge as follows:

$$Q^s = \frac{1}{2} \int_0^1 \sum_{pq} (h(q) - h(p)) \tilde{T}_{pq}^{(1)} + O(L^{-\infty}). \quad (9.49)$$

Now note that since the function  $h(x) = \theta(x) - \theta(x - 3L)$  is constant on the scale  $\xi$  everywhere except near  $x = 0$  and  $x = 3L$ , only the neighborhoods of  $p = q = 0$  and  $p = q = 3L$  may contribute appreciably to the double sum over  $p, q$ . One can make this explicit by writing

$$Q^s = Q_0^s - Q_{3L}^s + O(L^{-\infty}), \quad (9.50)$$

where  $Q_a^s$  is obtained from the r.h.s. of eq. (9.49) by replacing  $h(x)$  with  $\theta(x - a)$ .

Now, since  $\tilde{H}_p(\mu)$  is independent of  $\mu$  for  $p < L$ , the 1-forms  $\tilde{T}_{pq}^{(1)}$  are identically zero when both  $p$  and  $q$  are in the neighborhood of  $x = 0$ . Therefore  $Q_0^s$  is exponentially small for  $L \gg \xi$ . Further, when both  $p$  and  $q$  are in the neighborhood of  $x = 3L$ , the 1-forms  $\tilde{T}_{pq}^{(1)}$  are exponentially close to the 1-forms  $T_{pq}^{(1)}$  for the Hamiltonian  $H(\mu)$ . This follows from the insensitivity of the correlators of the form

$$\oint \frac{dz}{2\pi i} \text{Tr}(G A G B) \quad (9.51)$$

to the Hamiltonian far from the support of  $A$  and  $B$  [60]. Thus

$$Q^s = -\frac{1}{2} \int \sum_{p,q} (\theta(q - 3L) - \theta(p - 3L)) T_{pq}^{(1)} + O(L^{-\infty}). \quad (9.52)$$

Comparing with eq. (9.25) and taking the limit  $L \rightarrow \infty$ , we conclude that the skyrmion charge is minus the value of the Thouless charge pump for the corresponding loop.

Now we use the same approach to understand the physical meaning of the Thouless charge pump invariant for 2d systems. We start with a family of  $U(1)$ -invariant gapped 2d Hamiltonians parameterized by  $S^1 \times S^1$ :

$$H(\lambda, \sigma) = \sum_p H_p(\lambda, \sigma). \quad (9.53)$$

Here  $\lambda$  and  $\sigma$  are periodically identified with period 1. We are going to associate to this two-parameter family two one-parameter families. The first one is simply

$$H^0(\lambda) = \sum_p H_p(\lambda, 0). \quad (9.54)$$

To define the second one, we need to choose a strip  $\mathcal{S}$  on  $\mathbb{R}^2$  of width  $3L$  much larger than the correlation length. We choose coordinates on  $\mathbb{R}^2$  so that the strip is given by the inequalities  $0 \leq y \leq 3L$ . Let us also denote by  $\mathcal{S}_0$  the strip of width  $L$  which in this coordinate system is given by  $L \leq y \leq 2L$ . Obviously,  $\mathcal{S}_0 \subset \mathcal{S}$ . We define

$$H^s(\lambda) = \sum_p H_p^s(\lambda) = \sum_p H_p(\lambda, g(y(p))), \quad (9.55)$$

where  $g$  is defined in (9.40). Thanks to the periodicity in  $\sigma$ ,  $H_p^s(\lambda)$  coincides with  $H_p(\lambda, 0)$  outside of the strip  $\mathcal{S}_0$ . Also, both families are  $U(1)$ -invariant and periodic in  $\lambda$  with period 1. By our basic technical assumption, for sufficiently large  $L$  the Hamiltonians  $H^s(\lambda)$  are gapped for all  $\lambda$ .

Now consider adiabatically varying  $\lambda$  as a function of time. As one varies  $\lambda$  from 0 to 1, the charge flows across the line  $x = 0$ . The net charge transport across  $x = 0$  will be infinite both for  $H^0(\lambda)$  and  $H^s(\lambda)$ . However, their difference is finite. This is because outside the strip  $\mathcal{S}_0$  the two Hamiltonians coincide, and thus outside the horizontal strip  $\mathcal{S}$  correlators of the form (9.51) are the same up to terms which are exponentially suppressed far from  $\mathcal{S}$ . The difference of net charges transported across  $x = 0$  is

$$\Delta Q^s - \Delta Q^0 = \frac{1}{2} \int_0^1 \sum_{pq} (f(q) - f(p)) \left( T_{pq}^{s(1)}(\lambda) - T_{pq}^{(1)}(\lambda, 0) \right), \quad (9.56)$$

where  $f(p) = \theta(x(p))$ , and  $T_{pq}^{s(1)}(\lambda)$  and  $T_{pq}^{(1)}(\lambda, 0)$  are the 1-forms (9.22) on  $[0, 1]$  for Hamiltonian families  $H^s(\lambda)$  and  $H^0(\lambda)$ , respectively. The above expression for



$\Delta Q^s - \Delta Q^0$  can be interpreted in more physical terms by stacking the family  $H^s(\lambda)$  with the time-reversal of the family  $H^0(\lambda)$ . This gives a family of 2d systems for which the Thouless charge pump across the line  $x = 0$  is finite, because the charge transport cancels out outside the strip  $\mathcal{S}$ .

Next we introduce a cut-off function  $h(p) = \theta(y(p)) - \theta(3L - y(p))$  and write

$$\Delta Q^s - \Delta Q^0 = \frac{1}{2} \int_0^1 \sum_{pq} (f(q) - f(p)) h(q) \left( T_{pq}^{s(1)}(\lambda) - T_{pq}^{(1)}(\lambda, 0) \right) + O(L^{-\infty}). \quad (9.57)$$

Using the chain-cochain notation, this can also be written as

$$\Delta Q^s - \Delta Q^0 = \int_0^1 T_{pq}^{s(1)}(\lambda; \delta f \cup h) - \int_0^1 T^{(1)}(\lambda, 0; \delta f \cup h) + O(L^{-\infty}). \quad (9.58)$$

The advantage of introducing the cut-off function  $h$  is that now both terms in eq. (9.58) are separately well-defined.

To compute the r.h.s. of (9.58) we construct a two-parameter family of gapped Hamiltonians  $\tilde{H}(\lambda, \mu)$  which interpolates between the family  $H^s(\lambda)$  and the family  $H^0(\lambda)$ . We define

$$\tilde{H}(\lambda, \mu) = \sum_p \tilde{H}_p(\lambda, \mu) = \sum_p H_p(\lambda, g_\mu(y(p))), \quad (9.59)$$

where  $g_\mu : \mathbb{R} \rightarrow [0, 1]$  is defined by eq. (9.45). After the same kind of manipulations that lead from (9.43) to (9.49) we get

$$\Delta Q^s - \Delta Q^0 = - \int \tilde{T}^{(2)}(\delta f \cup \delta h) + O(L^{-\infty}), \quad (9.60)$$

where the integration is over the square  $[0, 1]^2$  in the  $\lambda - \mu$  plane. The contraction of a 2-chain with a 2-cochain involves a triple sum over  $p, q, r \in \Lambda$ . Now we note that only the terms where all three points  $p, q, r$  are close to the lines  $y = 3L$  or  $y = 0$  contribute appreciably to the sum. The contribution of  $y = 0$  is of order  $O(L^{-\infty})$ , because  $\tilde{H}_p(\lambda, \mu)$  does not depend on  $\mu$  there and thus the 2-form  $\tilde{T}_{pqr}^{(2)}$  is exponentially small. When evaluating the contribution of  $y = 3L$ , one can replace  $\tilde{T}^{(2)}$  with  $T^{(2)}$  while making an error of order  $O(L^{-\infty})$ . Thus we get

$$\Delta Q^s - \Delta Q^0 = \int T^{(2)}(\delta f \cup \delta h_{3L}) + O(L^{-\infty}), \quad (9.61)$$

where  $h_{3L}(p) = \theta(y(p) - 3L)$ . Taking the limit  $L \rightarrow \infty$  we conclude that  $\Delta Q^s - \Delta Q^0$  is the topological invariant of the family  $H(t, \sigma)$ .

### 9.7 Higher Thouless charge pump for systems of free fermions in 2d

In this section we compute the descendant of the Thouless charge pump for a family of systems of free fermions in two spatial dimensions (that is, for families of 2d insulators of class A). The two-form  $T_{p_0 p_1 p_2}^{(2)}$  can be found from (9.35) to be

$$T_{p_0 p_1 p_2}^{(2)} = \sum_{\sigma \in \mathcal{S}_3} (-1)^{\text{sgn } \sigma} \oint \frac{dz}{2\pi i} \text{Tr} \left( G dH_{p_{\sigma(0)}} G dH_{p_{\sigma(1)}} G Q_{p_{\sigma(2)}} \right). \quad (9.62)$$

We will compute this expression for the following many-body Hamiltonian density

$$H_p = \frac{1}{2} \sum_{m \in \Lambda} \left( a_p^\dagger h(p, m) a_m + a_m^\dagger h(m, p) a_p \right), \quad (9.63)$$

where  $h(p, q)$  is an infinite Hermitian matrix  $h(p, q)^* = h(q, p)$  whose rows and columns are labeled by  $\Lambda$ , and  $a_p, a_p^\dagger, p \in \Lambda$ , are fermionic operators satisfying anticommutation relation

$$\begin{aligned} \{a_p^\dagger, a_q\} &= \delta_{p,q}, \\ \{a_p, a_q\} &= \{a_p^\dagger, a_q^\dagger\} = 0, \end{aligned} \quad (9.64)$$

with  $\delta_{p,q}$  being the Kronecker delta. We define the conserved charge density to be

$$Q_p = a_p^\dagger a_p. \quad (9.65)$$

Expanding the many-body operators in eq. (9.62), we find that it can be reduced to a single-particle correlation function

$$T_{p_0 p_1 p_2}^{(2)} = \sum_{\sigma \in \mathcal{S}_3} (-1)^{\text{sgn } \sigma} \oint \frac{dz}{2\pi i} \text{tr} \left( g d h_{p_{\sigma(0)}} g d h_{p_{\sigma(1)}} g \delta_{p_{\sigma(2)}} \right), \quad (9.66)$$

where the contour of integration encloses filled states below the Fermi level and the trace is taken over the single-particle Hilbert space  $\ell^2(\Lambda)$ . Lowercase letters denote single-particle operators acting on the single-particle Hilbert space and functions on  $\Lambda$  are thought of as multiplication operators on  $\ell^2(\Lambda)$ . In particular  $h$  should be thought as an operator with matrix elements  $h(p, q)$ , its resolvent is  $g = (z - h)^{-1}$ , the Hamiltonian density is  $h_p = \frac{1}{2}(\delta_p h + h \delta_p)$ , and the charge density operator is the Kronecker delta function  $\delta_p$  which is equal to 1 on cite  $p$  and 0 on all other cites.

After contracting this expression with the 2-cochain  $\delta f_1 \cup \delta f_2$ , we find

$$\begin{aligned} T^{(2)}(\delta f_1 \cup \delta f_2) &= \frac{1}{4} \oint \frac{dz}{2\pi i} \text{tr} \left( 2g^2 [h, f_1] g d h g [h, f_2] g d h + g^2 [h, f_1] g [d h, f_2] g d h \right. \\ &\quad \left. - g [d h, f_1] g [h, f_2] g^2 d h - (f_1 \leftrightarrow f_2) \right). \end{aligned} \quad (9.67)$$

Both  $f$  and  $h$  are not trace class operators and it is not obvious that trace in the above expression exists. If we choose  $f_1(p) = \theta(x^1(p))$  and  $f_2(p) = \theta(x^2(p))$ , the operators  $[h, f_1]$  and  $[h, f_2]$  are supported on vertical and horizontal lines with a finite intersection. Since the matrix elements of  $g = (z - h)^{-1}$  decay faster than any power of the distance, the trace is convergent and well-defined.

Up to this point we have not imposed any additional condition on the Hamiltonian besides being free and charge-conserving. If in addition we choose  $\Lambda = \mathbb{Z}^2$  and impose a symmetry under lattice translations, then there is another natural topological invariant one can attach to a two-parameter family of such systems. Consider a translationally-invariant fermionic system depending on two parameters  $\lambda_1, \lambda_2$  which are local coordinates on some closed surface  $\Sigma$ . We assume that the gap between valence bands and conduction bands does not close for any values of the parameters. Then Bloch wavefunctions of the valence bands form a vector bundle over the product of the Brillouin zone  $S^1 \times S^1$  and the parameter space  $\Sigma$ . One can define a non-Abelian Bloch-Berry connection with curvature  $\mathcal{F}$  on this bundle. The integral of the degree 4 component of the Chern character of this connection over the product of Brillouin zone and the parameter space

$$\int_{S^1 \times S^1 \times \Sigma} \text{Ch}(\mathcal{F}) = -\frac{1}{8\pi^2} \int_{S^1 \times S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}) \quad (9.68)$$

is a topological invariant of this family.

This invariant can be expressed as non-linear response coefficient (see Sec. IIIA in [46])

$$\begin{aligned} -\frac{1}{8\pi^2} \int_{S^1 \times S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}) &= \frac{\pi^2}{15} \epsilon^{\mu\nu\rho\sigma\tau} \oint \frac{dz}{2\pi i} \int_{S^1 \times S^1} \frac{d^2 k}{(2\pi)^2} \int_{\Sigma_2} \frac{d^2 \lambda}{(2\pi)^2} \\ &\quad \text{tr}' \left[ \left( g \frac{\partial g^{-1}}{\partial q^\mu} \right) \left( g \frac{\partial g^{-1}}{\partial q^\nu} \right) \left( g \frac{\partial g^{-1}}{\partial q^\rho} \right) \left( g \frac{\partial g^{-1}}{\partial q^\sigma} \right) \left( g \frac{\partial g^{-1}}{\partial q^\tau} \right) \right], \end{aligned} \quad (9.69)$$

where  $q^\mu = (z, k_1, k_2, \lambda_1, \lambda_2)$ , the first integral encloses the energies of the valence bands, the second integral is over the Brillouin zone, and the last integral is over the two-dimensional parameter space  $\Sigma$ . Here the trace  $\text{tr}'$  is taken over the space of valence-band Bloch wavefunctions with a fixed quasi-momentum. In order to relate this formula to (9.67) we should interpret the integral over the Brillouin zone as a

part of the trace  $\text{tr}$  and replace  $\frac{\partial g^{-1}}{\partial k_i}$  with  $i[h, f_i]$ . We find

$$\begin{aligned} & -\frac{1}{8\pi^2} \int_{S^1 \times S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}) = -\frac{1}{6} \oint \frac{dz}{2\pi i} \int_{\Sigma_2} \text{tr} \left[ g^2[h, f_1]g[h, f_2]gdhgdh \right. \\ & -g^2[h, f_1]gdhgdh[h, f_2]gdh + g^2[h, f_1]gdhgdhg[h, f_2] + g^2dhg[h, f_1]g[h, f_2]gdh \\ & \left. -g^2dhg[h, f_1]gdhg[h, f_2] + g^2dhgdhg[h, f_1]g[h, f_2] - (f_1 \leftrightarrow f_2) \right], \end{aligned} \quad (9.70)$$

where  $dh = \sum_{\ell} \frac{\partial h}{\partial \lambda^{\ell}} d\lambda^{\ell}$ . The integrand of this expression differs from (9.67) by a total derivative

$$\frac{1}{12} d \left[ \oint \frac{dz}{2\pi i} \text{tr} \left( g^2[h, f_1]g[h, f_2]gdh - g[h, f_1]g[h, f_2]g^2dh - (f_1 \leftrightarrow f_2) \right) \right]. \quad (9.71)$$

Therefore for the free fermions the 2d Thouless charge pump integrated over  $\Sigma$  is equal to  $\int_{S^1 \times S^1 \times \Sigma} Ch(\mathcal{F})$ . Since  $\Sigma$  is arbitrary, this proves that the cohomology class of  $Q^{(2)}(f_1, f_2)$  is the cohomology class of the degree-4 component of the Chern character integrated over the Brillouin zone.

One can construct an example with a non-trivial  $Q^{(2)}$  by taking the 4d Chern insulator (see sec. IIIB of [46]) and declaring two components of the quasi-momentum to be parameters. The parameter space is a torus  $T^2$  in this case. In this way one gets the following Hamiltonian:

$$H = \sum_{k_x, k_y} \psi_{\vec{k}}^{\dagger} d_a(\vec{k}, \vec{\lambda}) \Gamma^a \psi_{\vec{k}}, \quad (9.72)$$

where  $\Gamma^a$  are five-dimensional Dirac matrices satisfying the Clifford algebra and

$$d_a(\vec{k}, \vec{\lambda}) = \left[ (m + c + \cos k_x + \cos k_y + \cos \lambda_1 + \cos \lambda_2), \sin k_x, \sin k_y, \sin \lambda_1, \sin \lambda_2 \right]. \quad (9.73)$$

It was shown in [46] that for a particular choice of  $m$  and  $c$  this model has a nontrivial integral of the Chern class  $Ch(\mathcal{F})$  over  $T^4 = T^2 \times T^2$ .

## 9.8 Discussion

We have shown how to attach topological invariants to  $D$ -parameter families of  $U(1)$ -invariant gapped Hamiltonians in  $D$  dimensions. In agreement with field theory, we found that they can be encoded in a closed  $D$ -form on the parameter space. The form itself depends on some additional choices, but its cohomology

class does not. Thus integrals of this  $D$ -form over  $D$ -cycles in parameter space are independent of any choices.

All these topological invariants arise from the ground-state charge via the "descent" equations proposed by Kitaev [33, 32]. This is analogous to how the Berry curvature of 0d systems gives rise to Wess-Zumino-Witten-type invariants of families of  $D$ -dimensional gapped systems without symmetries of Chapter 8. In general, one expects that every topological invariant of a gapped Hamiltonian in dimension  $D$  gives rise to a topological invariant of a  $k$ -dimensional family of gapped Hamiltonians in dimension  $D + k$ . In particular, Hall conductance for 2d gapped systems with a  $U(1)$  symmetry gives rise to a topological invariant of one-parameter families of 3d gapped systems with a  $U(1)$  symmetry. We plan to discuss this invariant in a future publication.

Topological invariants of families of gapped systems of free fermions were previously discussed by Teo and Kane [53]. They interpreted the parameter space as the complement of a gapless defect in an otherwise gapped system. Thus the parameter space was homotopically equivalent to a sphere of dimension  $D - k - 1$ , where  $k$  is the dimension of the defect. Note that the dimension of the parameter space is strictly less than  $D$ , so this situation is distinct from the one considered here. But Ref. [53] also considered a situation where the Hamiltonian depends on an additional periodic parameter  $t$ , so that the total parameter space is  $S^{D-k-1} \times S^1$ . For  $k = 0$  (point-like defects) this has dimension  $D$  and thus can be compared with our construction. Indeed, for systems of class A Ref. [53] assigns to such a family an integer topological invariant and interprets it as the net charge pumped towards the defect as the system undergoes an adiabatic cycle in the variable  $t$ . From the effective field theory perspective, considering a point-like defect in  $\mathbb{R}^D$  is the same as compactifying the system on  $S^{D-1}$ . Then the topological invariant discussed in Ref. [53] is the Thouless charge pump of the resulting 1d system. One can regard the results obtained in this chapter as a generalization of Ref. [53] in two distinct directions: to the case of interacting  $U(1)$ -invariant systems and to the case of  $D$ -dimensional parameter spaces of arbitrary topology. The interpretation in terms of point-like defects is lost when one considers parameter spaces which are not of the form  $S^{D-1} \times S^1$ . It is desirable to find a physical interpretation of the higher Thouless charge pump invariant for arbitrary parameter spaces. Field theory suggests that it can be interpreted as the ground-state charge of the system compactified on a topologically non-trivial space and deformed by spatially-varying parameters.

Unfortunately, it is difficult to make sense of this in the world of lattice models, with the exception of the case when the spatial manifold is a torus.

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*Appendix A*

## SOME MATHEMATICAL CONSTRUCTIONS

### Chains and cochains

In this thesis we have encountered local operators  $H_p$  and  $Q_p$  which depend on a lattice point  $p \in \Lambda$ , operators  $J_{pq}^N$  and  $J_{pq}^E$  which depend on a pair of points, and energy magnetization  $M_{pqr}^E$  which depends on three points. It is useful to introduce a suitable terminology for such objects. Let  $n$  be a non-negative integer. Consider a quantity  $A_{p_0, \dots, p_n}$  which depends on  $n + 1$  points of  $\Lambda$ , is skew-symmetric under the exchange of points, and decays rapidly when the distance between any two points becomes large. Given an ordered set of points  $p_0, \dots, p_n \in \Lambda$ , let  $[p_0, \dots, p_n]$  denote an abstract oriented  $n$ -simplex with vertices  $p_0, \dots, p_n$ . Then one can consider a formal linear combination of simplices

$$A = \frac{1}{(n+1)!} \sum_{p_0, \dots, p_n} A_{p_0, \dots, p_n} [p_0, \dots, p_n]. \quad (\text{A.1})$$

Such a linear combination is called an  $n$ -chain, or a chain of degree  $n$ . For example, the operators  $J_{pq}^N$  form an operator-valued 1-chain  $J^N$ .

The simplest decay condition one can impose is to require  $A_{p_0, \dots, p_n}$  to vanish whenever any two of its arguments are separated by more than some finite distance  $\epsilon$ . This distance may be different for different chains. In the body of the thesis such chains are called finite-range. In the mathematical literature they are called controlled chains [48]. The current 1-chain  $J^N$  is finite-range, or controlled, because  $[H_p, Q_q] = 0$  for  $|p - q| > R$ .

Another natural decay condition is to require  $A_{p_0, \dots, p_n}$  to satisfy

$$\sum_{p_0, p_1, \dots, p_n} \|A_{p_0, \dots, p_n}\| < \infty. \quad (\text{A.2})$$

Here  $\|\cdot\|$  denotes operator norm if  $A$  is operator-valued and absolute value if  $A$  is real-valued or complex-valued. We will call such chains summable. For example, the real-valued 2-chain defined in eq. (3.20) is summable if  $\frac{dH_p}{d\lambda}$  is nonzero only for  $p$  in a finite subset and the Kubo pairings of local operators decay rapidly with distance.

There is an operation  $\partial$  on chains which lowers the degree by 1:

$$(\partial A)_{p_1, \dots, p_n} = \sum_{q \in \Lambda} A_{q, p_1, \dots, p_n}. \quad (\text{A.3})$$

Although the sum is infinite, the operation is well-defined for  $n > 0$  since we assumed rapid decay when  $q$  is far away from any of the points  $p_1, \dots, p_n$ . This operation satisfies  $\partial \circ \partial = 0$ . It maps controlled chains to controlled chains, and summable chains to summable chains. The chain  $\partial A$  is called the boundary of the chain  $A$ . A cycle is a chain whose boundary is zero. Using this notation, the conservation equation (3.4) can be written as

$$\frac{dQ}{dt} = -\partial J^N. \quad (\text{A.4})$$

Dually, an  $n$ -cochain is a function of  $n + 1$  points of  $\Lambda$  which is skew-symmetric, but need not decay when one of the points is far from the rest. We will only consider real-valued cochains. A natural operation on cochains is

$$(\delta \alpha)(p_0, \dots, p_{n+1}) = \sum_{j=0}^{n+1} (-1)^j \alpha(p_0, \dots, p_{j-1}, p_{j+1}, \dots, p_{n+1}). \quad (\text{A.5})$$

It increases the degree by 1 and satisfies  $\delta \circ \delta = 0$ . The cochain  $\delta \alpha$  is called the coboundary of the cochain  $\alpha$ . A cocycle is a cochain whose coboundary is zero. The evaluation of an  $n$ -chain  $A$  on an  $n$ -cochain  $\alpha$  is formally defined as

$$A(\alpha) = \frac{1}{(n+1)!} \sum_{p_0, \dots, p_n} A_{p_0, \dots, p_n} \alpha(p_0, \dots, p_n). \quad (\text{A.6})$$

This definition is formal because without some constraints on the cochain  $\alpha$  the infinite sum will not be absolutely converging. An example of a 1-cochain is a function  $\eta(p, q)$  which appears in (3.8), then the operator  $J(\eta)$  is simply the evaluation of the operator-valued 1-chain  $J$  on a 1-cochain  $\eta$ .

Suppose all our chains are controlled. Then the problematic contribution in (A.6) arises from the region where all points  $p_0, \dots, p_n$  are nearby but otherwise can be anywhere in  $\Lambda$ . We will call such a region in the  $(n + 1)$ -fold Cartesian product of  $\Lambda$  with itself a thickened diagonal. To make the evaluation well-defined, it is natural to impose the following requirement on  $\alpha$ : the intersection of the support of  $\alpha$  with any thickened diagonal must be finite. In the mathematical literature such cochains are called cocontrolled [48]. For example, if we regard  $\chi_B$  as a 0-cochain, then  $\eta = \delta \chi_B$  is cocontrolled if either  $A$  or  $B$  are compact. One can evaluate an

arbitrary complex-valued controlled  $n$ -chain on a cocontrolled  $n$ -cochain and get a well-defined number. Or, when one evaluates an operator-valued controlled chain on a cocontrolled cochain, one gets a bounded operator.

If our chains are summable, then it is natural to require  $n$ -cochains to be bounded functions on the  $(n+1)$ -fold Cartesian product of  $\Lambda$  with itself. The space of bounded cochains is the Banach-dual of the space of summable chains, where the norms are the obvious ones. Thus the evaluation of a chain on a cochain is well-defined and is a continuous function of both the chain and the cochain.

With this said, we can state a kind of "Stokes' theorem"

$$A(\delta\beta) = \partial A(\beta). \quad (\text{A.7})$$

It applies to any controlled  $n$ -chain  $A$  and any cocontrolled  $(n-1)$ -cochain  $\beta$ . It also applies to any summable  $n$ -chain and a bounded  $(n-1)$ -cochain. In the special case  $A = J$  and  $\beta = \chi_B$  for some finite set  $B$ , combining (A.7) and the conservation equation (A.4) we get that the current through the boundary of  $B$  (represented by the 1-cocycle  $\delta\chi_B$ ) is equal to minus the rate of change of the total charge in  $B$ .

Given an  $n$ -cochain  $\alpha$  and an  $m$ -cochain  $\gamma$  one can define an  $(n+m)$ -cochain  $\alpha \cup \gamma$  by

$$\begin{aligned} (\alpha \cup \gamma)(p_0, \dots, p_{n+m}) &= \frac{1}{(n+m+1)!} \\ &\times \sum_{\sigma \in \mathcal{S}_{n+m+1}} (-1)^{\text{sgn } \sigma} \alpha(p_{\sigma(0)}, \dots, p_{\sigma(n)}) \gamma(p_{\sigma(n)}, \dots, p_{\sigma(n+m)}), \end{aligned} \quad (\text{A.8})$$

where  $\mathcal{S}_{n+m+1}$  is the permutation group on  $n+m+1$  objects. This operation satisfies

$$\alpha \cup \gamma = (-1)^{nm} \gamma \cup \alpha, \quad \delta(\alpha \cup \gamma) = \delta\alpha \cup \gamma + (-1)^n \alpha \cup \delta\gamma. \quad (\text{A.9})$$

The operations  $\delta$  and  $\cup$  on cochains are analogous to operations  $d$  and  $\wedge$  on differential forms. In the body of the thesis we apply these formulas in the case when  $\alpha = \delta f$  and  $\gamma = \delta g$ , where  $f$  is a "smeared step-function" in the  $x$ -direction, and  $g$  is a "smeared step-function" in the  $y$ -direction. The chains  $\alpha$  and  $\gamma$  are bounded, and so is  $\alpha \cup \gamma$ . Hence if  $\frac{dH_p}{d\lambda}$  is nonzero only for a finite subset of  $\Lambda$ , the evaluation of the summable chain (3.20) on the bounded cochain  $\delta f \cup \delta g$ . More generally, we may consider uniform deformations such that  $\frac{dH_p}{d\lambda}$  is bounded, but does not vanish at infinity. Then the chain (3.20) is only locally summable. Nevertheless, its evaluation on  $\delta f \cup \delta g$  is still well-defined because  $\delta f \cup \delta g$  is cocontrolled as well as bounded.

Finally, we note that if an  $n$ -chain  $A_{p_0, \dots, p_n}$  is nonzero only if  $|p_i - p_j| \leq \delta$  for all  $i, j$ , then its contraction with an  $n$ -cochain  $\alpha$  is well-defined even if  $\alpha(p_0, \dots, p_n)$  is only defined for  $|p_i - p_j| \leq \delta$ . We will make occasional use of such partially-defined cochains below.

## Applications

In this section we discuss some physical application of the machinery of chains and cochains. As discussed above, electric current is a operator-valued controlled 1-chain satisfying (A.4). A natural solution is given by (3.3), but there is an obvious ambiguity (3.5). In the language of chains, it amounts to  $J^N \mapsto J^N + \partial U$ , where  $U$  is an operator-valued controlled 2-chain. This ambiguity does not affect quantities like  $J^N(\eta)$ , where  $\eta$  is a cocontrolled 1-cycle. Indeed, using the Stokes' theorem, we get  $(J^N + \partial U)(\eta) = J^N(\eta) + U(\delta\eta) = J^N(\eta)$ . Similarly, while the energy current (3.11) has an obvious ambiguity (3.13), it does not affect quantities like  $J^E(\eta)$ , where  $\eta$  is a cocontrolled 1-cocycle. A special case of this is the electric or energy current from region  $B$  to region  $A$  which is denoted  $J^N(A, B)$  or  $J^E(A, B)$  in the body of the thesis. This is a physically measurable quantity and it is not affected by this ambiguity.

A more subtle question is whether there are other ambiguities in the definition of currents. This is equivalent to asking whether the equation  $\partial \Delta J^N = 0$  has solutions other than  $\Delta J^N = \partial U$ . To answer this question we need to know the homology of the complex of controlled chains in degree 1. More generally, one might want to know the homology of the complex of controlled chains in all degrees. It turns out that under natural assumptions on the lattice  $\Lambda \subset \mathbb{R}^d$  the controlled homology in degree  $n$  is independent of  $\Lambda$  and equal to the locally-finite (Borel-Moore) homology of  $\mathbb{R}^d$  [27]. The latter is equal to 0 for  $n \neq d$  and isomorphic to  $\mathbb{R}$  for  $n = d$ . The condition on  $\Lambda$  is, roughly speaking, that it fills the whole  $\mathbb{R}^d$  uniformly. More precisely, there should exist a number  $r > 0$  such that any point of  $\mathbb{R}^d$  is within distance  $r$  of some point of  $\Lambda$ . In the terminology of [48], this implies that  $\Lambda$  is coarsely equivalent to  $\mathbb{R}^d$ .

Given this result, we see that for  $d > 1$  the only solutions to  $\partial \Delta J^N = 0$  have the form  $\Delta J^N = \partial U$ , where  $U$  is a controlled operator-valued chain. In other words, our formulas for  $J_{pq}^N$  and  $J_{pq}^E$  are essentially unique. The case  $d = 1$  is a bit different, since the degree 1 homology of controlled chains is nontrivial. In the case  $d = 1$  points of  $\Lambda$  can be naturally labeled by integers, and a nontrivial solution



to  $\partial\Delta J^N = 0$  has the form  $\Delta J_{pq}^N = J_0^N(\delta_{p,q-1} - \delta_{q,p-1})$ , where  $J_0^N$  is a fixed local operator. However, if we make a natural assumption that  $J_0^N$  must be supported in some fixed-size neighborhood of the points  $p, q$  for all  $p, q$ , then  $J_0^N$  must be proportional to the identity operator. The same applies to the energy current. Thus for  $d = 1$  system currents are unique up to an addition of a constant c-number. This c-number, if present, would violate the conclusion of Bloch's theorem [10] or its energy counterpart. It would lead to an unphysical electric or energy current even at  $T = \infty$ , when all degrees of freedom are in a maximally-mixed state. If we normalize the currents so that their expectation values vanish at  $T = \infty$ , we eliminate this ambiguity even for  $d = 1$ . With this normalization, both Bloch's theorem and its energy counterpart hold for all temperatures.

Another application is the definition of magnetization and energy magnetization. The equilibrium expectation value of the electric current satisfies

$$\partial\langle J^N \rangle = 0. \quad (\text{A.10})$$

An obvious solution has the form

$$\langle J^N \rangle = \partial M^N, \quad (\text{A.11})$$

where  $M^N$  is a real-valued 2-chain. This is a lattice analog of of the continuum equation

$$\langle J_k^N(\mathbf{r}) \rangle = -\epsilon_{kj} \partial_j M^N(\mathbf{r}) \quad (\text{A.12})$$

which defines magnetization  $M^N(\mathbf{r})$ . Thus one can regard the real-valued 2-chain  $M_{pqr}^N$  as a lattice analog of magnetization.

In order for the magnetization 2-chain to exist, eq. (A.11) must be the most general solution of (A.10). Thus magnetization exists if the homology of  $\partial$  in degree 1 is trivial, or more generally, if the homology class of the 1-chain  $\langle J^N \rangle$  is zero. Since the 1-chain  $\langle J_{pq}^N \rangle$  is controlled, it is sufficient to look at the homology of controlled chains. If  $\Lambda$  is coarsely equivalent to  $\mathbb{R}^d$  and  $d > 1$ , the controlled homology in degree 1 is trivial, as explained above. Thus magnetization exists. It is not unique, of course, since there is always an ambiguity  $M^N \mapsto M^N + \partial P$ , where  $P$  is any real-valued controlled 3-chain. This is a harmless ambiguity since physical expressions involve expressions like  $M^N(\zeta)$ , where  $\zeta$  is a cocontrolled 2-cochain and are unaffected. A more serious ambiguity arises if controlled homology of  $\Lambda$  in degree 2 is non-trivial. This is the case if  $\Lambda$  is coarsely equivalent to  $\mathbb{R}^2$ . Given any magnetization 2-chain, one can get another acceptable magnetization 2-chain by

adding to it a controlled 2-cycle. Thus magnetization has an unavoidable ambiguity for 2d lattices, but not for lattices of higher dimensions. The same remarks apply verbatim to energy magnetization.

The case  $d = 1$  is again a bit special. Controlled homology in degree 1 is nontrivial, but  $\langle J^N(\eta) \rangle = 0$  for any cocontrolled 1-cochain thanks to Bloch's theorem. Hence the homology class of  $\langle J^N \rangle$  is trivial, and magnetization still exists. The same applies to the energy current and energy magnetization.

Finally, the homology of summable chains is trivial in degree higher than 0 for any lattice  $\Lambda$ . This is proved by exhibiting a contracting homotopy for the summable chain complex. Therefore if  $\frac{dH_p}{d\lambda}$  is supported on a finite set, the chain (3.20) is unique up to a replacement  $\mu^E \mapsto \mu^E + \partial N$ , where  $N$  is a summable 3-cochain. This shows that our expression for  $\mu^E$  is essentially unique for deformations of the Hamiltonian which are supported on a finite set. Since a general bounded deformation can be written as an (infinite) sum of these, we conclude that our formula for  $\mu^E$  is essentially unique.

*Appendix B*

APPENDICES TO CHAPTER V

**B.1 Kubo canonical pairing**

Kubo canonical pairing of two operators  $A, B$  is defined as follows [57]:

$$\langle\langle A; B \rangle\rangle = \frac{1}{\beta} \int_0^\beta \langle A(-i\tau)B \rangle d\tau - \langle A \rangle \langle B \rangle. \quad (\text{B.1})$$

Here  $\langle \dots \rangle$  denotes average over a Gibbs state at temperature  $T = 1/\beta$  (or more generally, over a state satisfying the Kubo-Martin-Schwinger condition), and  $A(-i\tau) = e^{H\tau} A e^{-H\tau}$ . Kubo pairing determines static linear response: if the Hamiltonian is perturbed by  $\lambda B$ , where  $\lambda$  is infinitesimal, then the change in the equilibrium expectation value of  $A$  is

$$\Delta \langle A \rangle = \langle \Delta A \rangle - \beta \lambda \langle\langle A; B \rangle\rangle + O(\lambda^2). \quad (\text{B.2})$$

Here the first term is due to the possible explicit dependence of  $A$  on the Hamiltonian, while the second term is the change in the expectation value of  $A$  due to the change in the equilibrium state.

Kubo pairing is symmetric,  $\langle\langle A; B \rangle\rangle = \langle\langle B; A \rangle\rangle$ , and satisfies

$$\beta \langle\langle i[H, A]; B \rangle\rangle = \langle i[B, A] \rangle. \quad (\text{B.3})$$

In finite volume, one can write it in terms of the energy eigenstates as follows:

$$\langle\langle A; B \rangle\rangle = Z^{-1} \sum_{n,m} \langle n | \bar{A} | m \rangle \langle m | \bar{B} | n \rangle \frac{e^{-\beta E_m} - e^{-\beta E_n}}{\beta(E_n - E_m)}, \quad (\text{B.4})$$

where  $\bar{A} = A - \langle A \rangle$ , and  $\bar{B} = B - \langle B \rangle$ .

**B.2 Dynamic response**

Consider the following perturbation of the Hamiltonian

$$\Delta H = \epsilon e^{st} B, \quad (\text{B.5})$$

where  $\epsilon$  is infinitesimal parameter and the variable  $s$  controls how fast the perturbation is turned on.

The change of the state of the system can be found from Liouville equation as follows. The density matrix

$$\rho(t) = \rho_0 + \Delta\rho(t) \quad (\text{B.6})$$

satisfies Liouville equation

$$\Delta\rho = -i[H, \rho_0] + \dots, \quad (\text{B.7})$$

where  $\rho_0$  is equilibrium density matrix at  $t = -\infty$  and dots represent higher order terms in  $\epsilon$ . The solution to this equation is

$$\Delta\rho(t=0) = -\rho_0 \int_0^\infty dt \int_0^\beta d\tau \Delta\dot{H}(-t - i\tau). \quad (\text{B.8})$$

The change of the observable  $A$  can be found to be

$$\Delta\langle A \rangle = \langle \Delta A \rangle - \beta \int_0^\infty dt \langle \langle A; \Delta\dot{H}(-t) \rangle \rangle, \quad (\text{B.9})$$

where we used Kubo pairing notation (see Appendix B.1) and  $\Delta A$  is explicit variation of the operator. Using explicit form of the perturbation (B.5) and properties of the Kubo pairing we can rewrite this formula as

$$\Delta\langle A \rangle = \langle \Delta A \rangle - \epsilon\beta \int_0^\infty dt e^{-st} \langle \langle A(t); \dot{B} \rangle \rangle, \quad (\text{B.10})$$

where we neglected term proportional to small  $s$ .

### B.3 Exponential decay of certain correlators in a gapped phase

Let  $A$ ,  $B$ , and  $C$  be local operators such that the supports of  $A$  and  $B$  are separated by at least  $L$ . Let  $G = (z - H)^{-1}$  be the Green's function of a gapped Hamiltonian, and let  $E_0$  be the energy of the ground state. For the time being we assume that the ground state is unique and comment on the more general case later. We are going to prove that the correlator

$$\oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} ([A, GBG] GCG), \quad (\text{B.11})$$

is exponentially suppressed for large  $L$ . Note that the support of the operator  $C$  is not required to be separated from the supports of  $A$  and  $B$ . By performing the  $z$

integration we get

$$\begin{aligned}
\oint \frac{dz}{2\pi i} \text{Tr} ([A, GBG] GCG) &= \langle AG_0BG_0^2C \rangle + \langle BG_0^2CG_0A \rangle - \langle CG_0^2AG_0B \rangle \\
&\quad - \langle CG_0AG_0^2B \rangle + \langle BG_0^2AG_0C \rangle + \langle BG_0AG_0^2C \rangle - \langle AG_0CG_0^2B \rangle \\
&\quad - \langle CG_0^2BG_0A \rangle + 2 \left( \langle CG_0^3B \rangle - \langle BG_0^3C \rangle \right) \langle A \rangle \\
&\quad + \left( \langle AG_0^3B \rangle - \langle BG_0^3A \rangle \right) \langle C \rangle + \left( \langle CG_0^3A \rangle - \langle AG_0^3C \rangle \right) \langle B \rangle,
\end{aligned} \tag{B.12}$$

where  $\langle \dots \rangle$  denotes the average over the ground state and we have introduced the notation

$$G_0 = \sum_{n \neq 0} \frac{|n\rangle\langle n|}{E_0 - E_n}. \tag{B.13}$$

Now we use the following facts from [60] and other similar identities:

$$\begin{aligned}
\langle O_1 G_0^n O_2 G_0^m O_3 \rangle &= \langle O_1 G_0^{n+m} O_3 \rangle \langle O_2 \rangle + O(e^{-L/\xi}), \\
\langle O_2 G_0^n O_1 G_0^m O_3 \rangle &= O(e^{-L/\xi}), \\
\langle O_1 G_0^n O_2 \rangle &= O(e^{-L/\xi}),
\end{aligned} \tag{B.14}$$

if  $n, m > 0$  and the support of operator  $O_2$  is at least  $L$  distance away from the supports of  $O_1$  and  $O_3$ . Here  $\xi > 0$  is a scale parameter which is finite for gapped systems. See [60] for the derivation of these identities.

Using these we can simplify the first term in (B.12). Separating  $C$  (which is by assumption a sum of local operators) into two parts  $C = C_A + C_B$  where the support of  $C_A$  is far away from  $B$  and the support of  $C_B$  is far away from  $A$ , we get

$$\begin{aligned}
\langle AG_0BG_0^2C \rangle &= \langle AG_0BG_0^2C_A \rangle + \langle AG_0BG_0^2C_B \rangle \\
&= \langle AG_0^3C_A \rangle \langle B \rangle + O(e^{-L/\xi}) = \langle AG_0^3C \rangle \langle B \rangle + O(e^{-L/\xi}).
\end{aligned} \tag{B.15}$$

Similarly, we have

$$\langle BG_0^2 CG_0 A \rangle = \langle BG_0^3 A \rangle \langle C \rangle + O(e^{-L/\xi}), \quad (\text{B.16})$$

$$-\langle CG_0^2 AG_0 B \rangle = -\langle CG_0^3 B \rangle \langle A \rangle + O(e^{-L/\xi}), \quad (\text{B.17})$$

$$-\langle CG_0 AG_0^2 B \rangle = -\langle CG_0^3 B \rangle \langle A \rangle + O(e^{-L/\xi}), \quad (\text{B.18})$$

$$\langle BG_0^2 AG_0 C \rangle = \langle BG_0^3 C \rangle \langle A \rangle + O(e^{-L/\xi}), \quad (\text{B.19})$$

$$\langle BG_0 AG_0^2 C \rangle = \langle BG_0^3 C \rangle \langle A \rangle + O(e^{-L/\xi}), \quad (\text{B.20})$$

$$-\langle AG_0 CG_0^2 B \rangle = -\langle AG_0^3 B \rangle \langle C \rangle + O(e^{-L/\xi}), \quad (\text{B.21})$$

$$-\langle CG_0^2 BG_0 A \rangle = -\langle CG_0^3 A \rangle \langle B \rangle + O(e^{-L/\xi}). \quad (\text{B.22})$$

These eight terms exactly cancel the remaining six terms in (B.12). Putting everything together, we get

$$\oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr} ([A, GBG] GCG) = O(e^{-L/\xi}). \quad (\text{B.23})$$

We have assumed a single ground state in the above derivation. However, as noted in [60], exactly the same arguments work for a  $q$ -fold degenerate ground state assuming that they are indistinguishable by local operators, i.e. if

$$\langle p|O|q \rangle = \delta_{pq} \langle p|O|p \rangle + O(L^{-\infty}), \quad (\text{B.24})$$

where  $|p\rangle, |q\rangle$  are ground states,  $O$  is a local operator, and  $L$  is the size of the system.

#### B.4 On the path-independence of the relative thermal Hall conductance

In this section we give a more detailed argument showing that the relative thermal Hall conductance is independent of the choice of the path connecting two points in the parameter space of 2d systems with finite correlation length. As explained in the body of the thesis, it is sufficient to show that the 1-form  $\mu^E(\delta f \cup \delta g)$  is exact. Here  $f(p)$  and  $g(p)$  are smeared step-functions in the  $x$  and  $y$  directions. Let  $f(p)$  be constant except for  $x(p) \simeq a$ , and  $g(p)$  be constant except for  $y(p) \simeq b$ .

The first step is to make the  $y$  direction periodic with period  $L$ , thereby replacing  $\mathbb{R}^2$  with a cylinder  $\mathbb{R}_x \times S_y^1$ . For  $L$  much larger than the correlation length this will change local quantities such as  $\mu_{pqr}^E$  by an amount of order  $L^{-\infty}$ . One complication is that the function  $g(p)$  is not periodic in the  $y$  direction and thus does not descend to  $\mathbb{R}_x \times S_y^1$ . We deal with this by reinterpreting  $(\delta g)(p, q) = g(q) - g(p)$  as a function on  $\Lambda \times \Lambda$  defined only for  $|p - q| < L/2$ . To make the evaluation of  $\mu^E$  on  $\delta f \cup \delta g$  well-defined, we truncate  $\mu_{pqr}^E$  to zero whenever any two of the points

$p, q, r$  are farther apart than  $L/2$ . Let us denote the truncated energy magnetization by  $\tilde{\mu}_{pqr}^E$ . Because of truncation, we now have  $d\langle J_{pq}^E \rangle = \sum_r \tilde{\mu}_{pqr}^E + O(L^{-\infty})$ . Or using the notation of Appendix A,

$$d\langle J^E \rangle = \partial \tilde{\mu}^E + O(L^{-\infty}). \quad (\text{B.25})$$

Naively, one can deduce the desired result using the Stokes' theorem (A.7):

$$\int_{\Gamma} \tilde{\mu}^E(\delta f \cup \delta g) = \int_{\Gamma} d\langle J^E \rangle(f \cup \delta g) + O(L^{-\infty}) = O(L^{-\infty}). \quad (\text{B.26})$$

This argument is not correct because the 1-cochain  $f \cup \delta g$  is not cocontrolled (because  $(f \cup \delta g)(p, q)$  does not vanish when  $x(p) \simeq x(q)$  and both  $x(p)$  and  $x(q)$  are large and negative), and the evaluation of  $d\langle J^E \rangle$  on such a 1-cochain is not well-defined. To fix this, we first modify the Hamiltonian for  $x < a - L$  by scaling it to zero. Since there are no phase transitions in 1d systems, the correlation length remains finite, and therefore the effect of such a modification on  $\tilde{\mu}^E(\delta f \cup \delta g)$  will be of order  $L^{-\infty}$ . Then the operator-valued chain  $J^E$  also becomes zero for  $x \ll a$ , and the application of the Stokes' theorem becomes legitimate. This concludes the argument.

Since by definition  $\mu^E(\delta f \cup \delta g)$  is the differential of energy magnetization in the neighborhood of the point  $(a, b)$ , this result means that energy magnetization exists as a globally-defined function on the parameter space. This function is defined up to an additive constant.

### B.5 The low-temperature behavior of the 1-form $\Psi$ in a gapped system

In this appendix we analyze the properties of the 1-form  $\Psi(f, g)$  whose integral defines the relative invariant of gapped 2d systems. We will have to use estimates on the behavior of certain correlation functions at low but non-zero temperature. More precisely, we will assume that if the  $T \rightarrow 0$  limit of a correlator is well-defined, then at sufficiently low temperature deviations from the  $T = 0$  value are of order  $O(e^{-T^*/T})$  for some  $T^* > 0$ . Physically, this is what one expects for a Hamiltonian with a gap for localized excitations.

One could try to prove it by putting the system on a torus of finite size  $L$ . Then for a correlation function  $C(T)$  one can construct a finite-size analog  $C(T, L)$  such that  $C(T) = \lim_{L \rightarrow \infty} C(T, L)$ . The correlation function  $C(T, L)$  can be rewritten in terms of many-body Green's function  $G = (z - H)^{-1}$ . For example, one can write

$$\int_0^\beta \langle A(-i\tau)B \rangle_L d\tau = Z^{-1} \oint e^{-\beta z} \frac{dz}{2\pi i} \text{Tr}(GAGB), \quad (\text{B.27})$$

where  $Z$  is the partition function, and the contour surrounds all the eigenvalues of  $H$ . Now if we deform the contour into a pair of contours, one surrounding  $z = E_0$  and the other surrounding all other eigenvalues, we see that for low  $T$  the contribution of the first contour is exponentially close to its  $T \rightarrow 0$  limit, while the contribution of the second one is exponentially small at low  $T$ . Thus  $C(T, L) - C(0, L)$  is exponentially small at low  $T$ . If we assume that the order of limits  $T \rightarrow 0$  and  $L \rightarrow \infty$  can be interchanged, we can conclude that  $C(T)$  is exponentially small at low  $T$ . These arguments are at best heuristic, since it is far from clear when interchanging the order of limits is legitimate.

For simplicity of presentation we will work on  $\mathbb{R}^2$  and simply assume that correlation functions in gapped phase at non-zero temperature are exponentially closed to their zero-temperature expectation value. Also, we will consider the system at a fixed non-zero temperature  $T$  and will vary only the Hamiltonian. As was explained in Section 5.3, rescaling the temperature is equivalent to rescaling the Hamiltonian. Finally, let us fix some  $L > 0$  which is much larger than the correlation length and define the  $L$ -support of a 1-cochain  $\alpha$  to be the set of points  $p \in \Lambda$  such that  $\alpha(p, q) \neq 0$  for at least for one  $q$  such that  $|p - q| < L$ .

Consider the integral of  $\Psi(f, g)$  along a path connecting two zero-temperature phases  $\mathcal{M}$  and  $\mathcal{M}'$ :

$$I(\mathcal{M}, \mathcal{M}') = \int_{\mathcal{M}}^{\mathcal{M}'} \Psi(f, g). \quad (\text{B.28})$$

We will argue that it converges, does not change under the shift of the end points  $\mathcal{M}, \mathcal{M}'$  as long as they do not cross zero-temperature phase transitions, and does not change under suitable deformations of  $f, g$ .

Let us start with the last property. We consider adding to  $f$  a function of  $x(p)$  which has compact support (as a function of  $x$ ). We need to show that

$$\int_{\mathcal{M}}^{\mathcal{M}'} \Psi(f_0, g) = 0, \quad (\text{B.29})$$

where  $f_0$  is as in Fig 5.1b. Since the path in the parameter space is away from phase transitions, the correlation length is finite everywhere along the path. Truncating  $f_0$  to zero a distance  $L$  away from the  $L$ -support of  $\delta g$  will introduce error of order  $L^{-\infty}$ . Denote the truncated cochain  $\tilde{f}_0$ . It has compact support, and therefore we



can rewrite the magnetization term as

$$\mu^E(\delta\tilde{f}_0 \cup \delta g) = \partial\mu^E(\tilde{f}_0 \cup \delta g) = d\langle J^E(\tilde{f}_0 \cup \delta g) \rangle = -\frac{1}{2}d\langle i[H(\tilde{f}_0), H(g)] \rangle, \quad (\text{B.30})$$

where in the last step we have used the definition of  $J^E$  and cup product. The Kubo term, on the other hand, can be rewritten as

$$\begin{aligned} \kappa_{xy}^{\text{Kubo}}(\tilde{f}_0, g) &= -\beta^2 \lim_{s \rightarrow 0^+} \int_0^\infty dt e^{-st} \langle \langle \frac{dH(\tilde{f}_0, t)}{dt}; J^E(\delta g) \rangle \rangle \\ &= \beta^2 \langle \langle H(\tilde{f}_0); J^E(\delta g) \rangle \rangle + \beta^2 \lim_{s \rightarrow 0^+} s \int_0^\infty dt e^{-st} \langle \langle H(\tilde{f}_0, t); J^E(\delta g) \rangle \rangle. \end{aligned} \quad (\text{B.31})$$

The last term is in general non-zero since  $\langle \langle H(\tilde{f}_0, t); J^E(\delta g) \rangle \rangle$  does not have to converge to zero as  $t \rightarrow \infty$ . However, at zero temperature and for a gapped Hamiltonian one can explicitly check that this term is zero. Indeed, expanding the expression in the energy eigenbasis we get

$$\begin{aligned} &\lim_{s \rightarrow 0^+} s \int_0^\infty dt e^{-st} \langle \langle H(\tilde{f}_0, t); J^E(\delta g) \rangle \rangle \\ &= -i \lim_{s \rightarrow 0^+} s \sum_{n>0} \frac{\langle 0|H(\tilde{f}_0)|n \rangle \langle n|J^E(\delta g)|0 \rangle - \langle 0|J^E(\delta g)|n \rangle \langle n|H(\tilde{f}_0)|0 \rangle}{(E_0 - E_n)^2} = 0. \end{aligned}$$

Therefore at small but non-zero temperature we expect the second term in (B.31) to be exponentially suppressed. The remaining term can be rewritten as

$$\beta^2 d\langle \langle H(\tilde{f}_0); J^E(\delta g) \rangle \rangle = \beta^2 d\langle \langle H(\tilde{f}_0); -i[H, H(g)] \rangle \rangle = -\beta d\langle i[H(\tilde{f}_0), H(g)] \rangle. \quad (\text{B.32})$$

This term cancels the energy magnetization contribution (B.30). Therefore  $\Psi(\tilde{f}_0, g)$  is a differential of a function which is exponentially small for  $T \rightarrow 0$ . Hence the integral of  $\Psi(\tilde{f}_0, g)$  along a path connecting two gapped zero-temperature systems is zero. Therefore the integral of  $\Psi(f_0, g)$  along the same path is of order  $L^{-\infty}$ . Since  $L$  is arbitrary, we can take the limit  $L \rightarrow \infty$  and conclude that the integral of  $\Psi(f_0, g)$  along this path is zero. Similarly, one can prove that  $I(\mathcal{M}, \mathcal{M}')$  does not change if we add to  $g$  a compactly supported function of  $y$ .

It is tempting to use the same argument with  $f_0$  replaced with  $f$  to show that  $I(\mathcal{M}, \mathcal{M}')$  is zero. But the argument cannot be carried through because it is impossible to truncate  $f$  and make its support compact in such a way that the

support of  $\delta f \cup \delta g$  coincides with the support of  $\delta \tilde{f} \cup \delta g$ . There will necessarily be additional intersections.

In order to show that the integral (B.28) defining  $I(\mathcal{M}, \mathcal{M}')$  converges and is independent of the precise choice of endpoints, consider a variation of the Hamiltonian supported in a quadrant of  $\mathbb{R}^2$ . A general perturbation can be decomposed into a sum of four such perturbations. As discussed in Section 5.3, in order to show that  $I(\mathcal{M}, \mathcal{M}')$  is independent of endpoints and converges it is sufficient to show that all components of the 1-form  $\Psi(f, g)$  are exponentially small as  $T \rightarrow 0$ . Following the same logic as before, we can shift  $f, g$  in  $\Psi(f, g)$  away from the support of the variation introducing an error which is exponentially small in temperature. Recall that the 1-form  $\Psi$  is defined as

$$\Psi(f, g) = \beta^2 \left[ d \int_0^\infty \beta e^{-st} \langle \langle J^E(\delta f, t); J^E(\delta g) \rangle \rangle dt - 2\mu^E(\delta\alpha \cup \delta\gamma) \right]. \quad (\text{B.33})$$

Using the same arguments as in Section 5.2, one can show that expression in square brackets is zero at  $T = 0$ . Therefore, it is exponentially small at zero temperature, and the same applies to  $\Psi(f, g)$ .

## B.6 Free fermion systems

### Definitions and correlation functions

In this appendix we will specialize our microscopic formula for thermal Hall coefficient to free fermionic systems. The Hamiltonian is taken to be

$$H = \sum_{p, q \in \Lambda} a_p^\dagger h(p, q) a_q, \quad (\text{B.34})$$

where an infinite matrix  $h(p, q)$  is Hermitian  $h(p, q)^* = h(q, p)$ , and  $a_p^\dagger, a_p$  are fermionic creation-annihilation operators satisfying the standard anti-commutation relations

$$a_p a_q^\dagger + a_q^\dagger a_p = \delta_{p, q}, \quad a_p a_q + a_q a_p = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = 0. \quad (\text{B.35})$$

We define the Hamiltonian density on site  $p$  to be

$$H_p = \frac{1}{2} \sum_m \left( a_p^\dagger h(p, m) a_m + a_m^\dagger h(m, p) a_p \right). \quad (\text{B.36})$$

The charge operator on site  $p$  is defined as

$$Q_p = a_p^\dagger a_p. \quad (\text{B.37})$$

The electric current can be found from the conservation equation:

$$J_{pq}^N = i(a_q^\dagger h(q, p)a_p - a_p^\dagger h(p, q)a_q). \quad (\text{B.38})$$

The net current through a section defined by  $\delta f(p, q) = f(q) - f(p)$  is

$$J(\delta f) = -ia^\dagger [h, f]a,$$

where a bounded function  $f \in \ell^2(\Lambda)$  is understood as an operator acting on the one-particle Hilbert space  $\ell^2(\Lambda)$  by multiplication. Summation over sites is implicit.

The energy current operator is

$$\begin{aligned} J_{pq}^E = \frac{-i}{4} \sum_{m \in \Lambda} & \left( a_p^\dagger h(p, q)h(q, m)a_m - a_q^\dagger h(q, p)h(p, m)a_m \right. \\ & - a_m^\dagger h(m, q)h(q, p)a_q + a_m^\dagger h(m, p)h(p, q)a_q \\ & \left. + a_p^\dagger h(p, m)h(m, q)a_q - a_q^\dagger h(q, m)h(m, p)a_p \right). \quad (\text{B.39}) \end{aligned}$$

The net energy current is

$$J^E(\delta f) = -\frac{i}{2}a^\dagger [h^2, f]a.$$

The state of the system at a temperature  $T = 1/\beta$  is defined via Wick's theorem and Gibbs distribution

$$\langle a_p(t)a_q^\dagger \rangle = \left\langle p \left| \frac{e^{-iht}}{1 + e^{-\beta h}} \right| q \right\rangle, \quad (\text{B.40})$$

$$\langle a_p(t)^\dagger a_q \rangle = \left\langle q \left| \frac{e^{iht}}{1 + e^{\beta h}} \right| p \right\rangle, \quad (\text{B.41})$$

where  $a_p(t)$  are operators in the Heisenberg picture.

Using these formulas we find

$$\langle J^N(\delta f, t)J^N(\delta g) \rangle = -\text{Tr} \left( [h, f] \frac{e^{-iht}}{1 + e^{-\beta h}} [h, g] \frac{e^{iht}}{1 + e^{\beta h}} \right),$$

where the trace is over the 1-particle Hilbert space  $\ell^2(\Lambda)$ , and the functions  $f : \Lambda \rightarrow \mathbb{R}$  and  $g : \Lambda \rightarrow \mathbb{R}$  are operators on this Hilbert space. The operators  $[h, f]$  and  $[h, g]$  have support on a vertical strip and a horizontal strip, respectively.

Switching to the energy basis, substituting  $t \rightarrow t - i\tau$ , and integrating from 0 to  $\beta$  over  $\tau$  we find

$$\begin{aligned} \langle \langle J^N(\delta f, t); J^N(\delta g) \rangle \rangle &= \frac{-1}{\beta} \sum_{n, m} \langle n | [h, f] | m \rangle \langle m | [h, g] | n \rangle e^{i(\varepsilon_n - \varepsilon_m)t} \\ &\quad \times \frac{e^{\beta\varepsilon_n} - e^{\beta\varepsilon_m}}{(1 + e^{\beta\varepsilon_n})(1 + e^{\beta\varepsilon_m})(\varepsilon_n - \varepsilon_m)}, \end{aligned}$$

where  $\varepsilon_n$  are 1-particle Hamiltonian energy eigenvalues.

Multiplying this by  $e^{-st}$  and integrating over  $t$ , we arrive at

$$\sigma_{xy} = i \lim_{s \rightarrow 0} \sum_{n,m} \frac{\langle n|[h, f]|m\rangle \langle m|[h, g]|n\rangle \mathfrak{f}(\varepsilon_n) - \mathfrak{f}(\varepsilon_m)}{\varepsilon_n - \varepsilon_m + is} \frac{\mathfrak{f}(\varepsilon_n) - \mathfrak{f}(\varepsilon_m)}{\varepsilon_n - \varepsilon_m},$$

where  $\mathfrak{f}(\varepsilon) = \frac{1}{1+e^{\beta(\varepsilon)}}$  is the Fermi-Dirac distribution. We absorb the chemical potential into a shift of the Hamiltonian.

The above expressions assume a discrete energy spectrum and thus can only be used for finite-volume systems. To get an expression applicable to infinite-volume systems, let us rewrite it in terms of the one-particle Green's functions  $G_{\pm}(z) = 1/(z - h \pm i0)$ . Some of the useful formulas are

$$\begin{aligned} \langle a^\dagger Aa \rangle &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left( [G_+ - G_-] A \right), \\ -\beta \langle \langle a^\dagger Aa; a^\dagger Ba \rangle \rangle &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left( [G_+ - G_-] A G_+ B + G_- A [G_+ - G_-] B \right) \\ &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left( G_+ A G_+ B - G_- A G_- B \right), \end{aligned} \quad (\text{B.42})$$

where we have dropped  $z$  for  $G_{\pm}(z)$ . Here  $A$  and  $B$  are operators acting on the one-particle Hilbert space, and in the second formula we assumed in addition that their average is zero:  $\langle a^\dagger Aa \rangle = \langle a^\dagger Ba \rangle = 0$ . Note also that

$$hG_{\pm} = G_{\pm}h = zG_{\pm} - 1, \quad [G_{\pm}, A] = G_{\pm}[h, A]G_{\pm}.$$

Using this notation the formula for the electric conductivity takes the form

$$\sigma_{xy} = -\frac{1}{2\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left\{ [h, f] G_+^2 [h, g] (G_+ - G_-) - [h, f] (G_+ - G_-) [h, g] G_-^2 \right\}, \quad (\text{B.43})$$

where the integration is over the real axis in the  $z$ -plane.

## Magnetization

The value of energy magnetization  $\mu^E$  on a 2-cochain  $\delta f \cup \delta g$  can be found to be

$$\begin{aligned} \mu^E(\delta f \cup \delta g) &= \frac{1}{16\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left( G_+ dh G_+ \left\{ [[h, f], [h, g]] + [h^2, f] G_+ [h, g] \right. \right. \\ &\left. \left. + [h, f] G_+ [h^2, g] - [h^2, g] G_+ [h, f] - [h, g] G_+ [h^2, f] \right\} \right) - (G_+ \rightarrow G_-), \end{aligned} \quad (\text{B.44})$$

where  $dh$  is the variation of the 1-particle Hamiltonian. In the translationally invariant case, one can replace  $f$  and  $g$  with momentum derivatives.

Using the above formulas, it is straightforward to compute the 1-form  $\Psi$  for any free system. Let us demonstrate this by computing the  $T$ -component of the 1-form  $\Psi$ .

For a global re-scaling of the Hamiltonian we have  $dh = h$ , and eq. (C.37) can be simplified

$$\begin{aligned} \tau^E(\delta f \cup \delta g) = & -\frac{1}{16\pi} \int_{-\infty}^{\infty} dz \operatorname{Tr} \left\{ 2\check{f}(z) G_-^2[h^2, f](G_+ - G_-)[h^2, g] \right. \\ & - 2\check{f}(z)(G_+ - G_-)[h^2, f] G_+^2[h^2, g] + 4\check{f}'(z) h^2 (G_+ - G_-)[h, f] G_+[h, g] \\ & \left. - 4\check{f}'(z) G_-[h, f] h^2 (G_+ - G_-)[h, g] - \check{f}'(z) h (G_+ - G_-)[[h, f], [h, \beta]] \right\}. \quad (\text{B.45}) \end{aligned}$$

Variation of  $\kappa_{xy}^{\text{Kubo}}(f, g)$  contains two pieces:

$$\begin{aligned} & -\frac{\beta}{8\pi} d \left( \int_{-\infty}^{\infty} dz \check{f}(z) \operatorname{Tr} \left\{ [h^2, f] G_+^2[h^2, g](G_+ - G_-) \right\} \right) = \frac{\beta}{8\pi} \int_{-\infty}^{\infty} dz \\ & \times \operatorname{Tr} \left\{ -2\check{f}(z)[h^2, f] G_+^2[h^2, g](G_+ - G_-) - 4\check{f}'(z)[h, f] G_+^2[h, g] h^3 (G_+ - G_-) \right. \\ & \left. + 4\check{f}'(z)[h, f] G_+[h, g] h^2 (G_+ - G_-) - \check{f}'(z)[h, f][h, g] h (G_+ - G_-) \right\} \quad (\text{B.46}) \end{aligned}$$

and

$$\begin{aligned} & \frac{\beta}{8\pi} d \left( \int_{-\infty}^{\infty} dz \check{f}(z) \operatorname{Tr} \left\{ [h^2, g] G_-^2[h^2, f](G_+ - G_-) \right\} \right) = \frac{\beta}{8\pi} \int_{-\infty}^{\infty} dz \\ & \times \operatorname{Tr} \left\{ 2\check{f}(z)[h^2, g] G_-^2[h^2, f](G_+ - G_-) + 4\check{f}'(z)[h, g] G_-^2[h, f] h^3 (G_+ - G_-) \right. \\ & \left. - 4\check{f}'(z)[h, g] G_-[h, f] h^2 (G_+ - G_-) + \check{f}'(z)[h, g][h, f] h (G_+ - G_-) \right\}. \quad (\text{B.47}) \end{aligned}$$

Inserting these three contributions into eq. (5.41) we arrive at

$$\begin{aligned} \frac{d}{dT} \left( \frac{\kappa_{xy}(f, g)}{T} \right) = & \frac{1}{2\pi T^3} \int_{-\infty}^{\infty} dz \operatorname{Tr} \left\{ \check{f}'(z)[h, f] G_+^2[h, g] z^3 (G_+ - G_-) \right. \\ & \left. - \check{f}'(z)[h, g] G_-^2[h, f] z^3 (G_+ - G_-) \right\}. \quad (\text{B.48}) \end{aligned}$$

The right-hand side looks very similar to the electric conductance (B.43). Indeed, integrating it over temperature from 0 to  $\infty$  and using the formula

$$\int_0^{\infty} \frac{dT}{T^3} \check{f}'(z) = -\frac{\pi^2}{6|z|^3} = -\frac{\pi^2}{3z^3} \left( \check{f}(z) \Big|_{T=\infty} - \check{f}(z) \Big|_{T=0} \right) \quad (\text{B.49})$$

gives

$$\frac{\kappa^A}{T}\Big|_{T=\infty} - \frac{\kappa^A}{T}\Big|_{T=0} = \frac{\pi^2}{3} \left( \sigma^A\Big|_{T=\infty} - \sigma^A\Big|_{T=0} \right). \quad (\text{B.50})$$

Since at infinite temperature the electric Hall conductance vanishes, while the thermal Hall conductance can be defined to vanish, we arrive at the Wiedemann-Franz law.

## APPENDICES TO CHAPTER VI

**C.1 Onsager reciprocity revisited**

Derivations of Onsager relations are based on the analysis of hydrodynamic fluctuations, so it might seem that they should put constraints only on those transport coefficients which enter the hydrodynamic equations of motion. On closer inspection, one finds [12] that the derivation involves net currents which measure the rate of change of conserved quantities in a finite volume and thus require understanding boundary contributions. As a result, Onsager reciprocity constrains both absolute transport coefficients and relative transport coefficients defined relative to the vacuum. Equivalently, it imposes conditions on the derivatives of relative transport coefficients with respect to parameters. To illustrate how this works, let us discuss the constraints imposed by Onsager reciprocity on relative transport coefficients of time-reversal-invariant 2d systems. For the skew-symmetric thermal conductivity  $\kappa^A$ , time-reversal-invariance implies

$$\frac{\partial}{\partial \lambda} \kappa^A = 0, \quad (\text{C.1})$$

where  $\lambda$  is a parameter of the Hamiltonian. Thus  $\kappa^A$  can be a function of temperature only. Further, if we treat  $T$  as a parameter, then scaling analysis gives

$$\frac{\partial}{\partial T} \frac{\kappa^A}{T} = 0. \quad (\text{C.2})$$

Hence  $\kappa^A(T) = aT$ , where  $a$  does not depend on parameters. The parameter  $a$  has no physical significance, but it is natural to set it to zero, so that the vacuum has zero thermal Hall conductivity. Thus we reach the standard conclusion that for a system with time-reversal invariance  $\kappa^A = 0$ .

The case of thermoelectric coefficients is slightly different. Usually one says that Onsager reciprocity requires  $v_{km} = T^{-1} \eta_{mk}$ , which implies  $v^A + T^{-1} \eta^A = 0$  [36]. Since both  $v^A$  and  $\eta^A$  are relative transport coefficients, one should interpret this as

$$\frac{\partial}{\partial \lambda} (v^A + T^{-1} \eta^A) = 0. \quad (\text{C.3})$$

Hence  $v^A + T^{-1} \eta^A$  can depend only on the temperature. If we treat temperature as a parameter, then the scaling analysis gives

$$\frac{\partial}{\partial T} (v^A + T^{-1} \eta^A) = 0. \quad (\text{C.4})$$

Hence  $\nu^A + T^{-1}\eta^A = a$ , where  $a$  is a constant which is independent of any parameters or temperature and has no physical significance. One can choose it to be zero. Then  $\nu^A = -T^{-1}\eta^A$ . So for a time-reversal-invariant 2d system there is only one independent skew-symmetric thermoelectric transport coefficient, namely  $\nu^A$ .

## C.2 Invariance under Hamiltonian density redefinition

For a given Hamiltonian, there are many ways to define a Hamiltonian density. A typical example of this is the ambiguity in splitting an interaction term between two sites  $p$  and  $q$  into  $H_p$  and/or  $H_q$ . In this appendix, we will show that our microscopic formulas for physically observable transport coefficients are independent of the choice of the Hamiltonian density, even though individual terms in the microscopic formulas are not invariant. For some systems this can be used to simplify the microscopic formulas.

### Invariance of the electric current

Consider the following change of the Hamiltonian density

$$H_p \rightarrow H_p + \sum_{r \in \Lambda} A_{rp}, \quad (\text{C.5})$$

where  $A_{rp}$  is skew-symmetric in  $r, p$ . We want the final Hamiltonian to be  $U(1)$ -invariant. Therefore, we have to impose

$$[Q, \sum_{r \in \Lambda} A_{rp}] = 0. \quad (\text{C.6})$$

For a general choice of  $A_{pq}$  a stronger condition

$$[Q, A_{pq}] = 0, \quad (\text{C.7})$$

will not hold. However, one can always redefine  $A_{pq}$  (by subtracting the  $U(1)$ -non-invariant part) in such a way that (C.7) holds without affecting  $H_p$ . In the following we will assume this was done and (C.7) is true.

Under the transformation (C.5) the electric current changes as

$$J_{pq}^N \rightarrow J_{pq}^N + i \sum_{r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]). \quad (\text{C.8})$$

Even though the current density changes, the net current through any section is invariant. Indeed,

$$J^N(\delta f) \rightarrow J^N(\delta f) + \frac{i}{2} \sum_{p, q, r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]) (f(q) - f(p)), \quad (\text{C.9})$$



and the last term is zero since

$$\begin{aligned}
& \sum_{p,q,r \in \Lambda} ([A_{rq}, Q_p] - [A_{rp}, Q_q]) (f(q) - f(p)) \\
&= \sum_{p,q,r \in \Lambda} ([A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]) (f(q) - f(p)) \\
&= \frac{1}{3} \sum_{p,q,r \in \Lambda} ([A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]) \\
&\quad \times (f(q) - f(p) + f(p) - f(r) + f(r) - f(q)) = 0, \quad (\text{C.10})
\end{aligned}$$

where we have used (C.7) and the skew-symmetry of  $[A_{rq}, Q_p] + [A_{pr}, Q_q] + [A_{qp}, Q_r]$ .

### Covariance of the energy current

Let us now consider the effect of the redefinition of the Hamiltonian density on the energy current. Imposing an energy analog of (C.6) or (C.7)

$$[H, \sum_{r \in \Lambda} A_{rp}] \stackrel{?}{=} 0, \quad \text{or} \quad [H, A_{pq}] \stackrel{?}{=} 0, \quad (\text{C.11})$$

is far too restrictive, since it would only allow changes of the Hamiltonian density by conserved quantities. For example, the difference between putting the interaction term between the two sites  $p$  and  $q$  either into  $H_p$  or into  $H_q$  corresponds to  $A_{pq}$  equal to the interaction term. Obviously, interaction terms are not integrals of motion in general. Because of this we will not impose either of the equations in (C.11).

Under the redefinition of the Hamiltonian density (C.5) the energy current changes as

$$J_{pq}^E \rightarrow J_{pq}^E + i \sum_{r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]), \quad (\text{C.12})$$

while the net current transforms as

$$J^E(\delta f) \rightarrow J^E(\delta f) + \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]) (f(q) - f(p)). \quad (\text{C.13})$$

The last term can be rewritten as

$$\begin{aligned}
& \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [H_q, A_{rp}]) (f(q) - f(p)) \\
&= \frac{i}{2} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [A_{pr}, H_q] + [A_{qp}, H_r]) (f(q) - f(p)) \\
& - \frac{i}{2} \sum_{p,q,r \in \Lambda} [A_{qp}, H_r] (f(q) - f(p)) = \frac{i}{6} \sum_{p,q,r \in \Lambda} ([A_{rq}, H_p] + [A_{pr}, H_q] + [A_{qp}, H_r]) \\
& \times (f(q) - f(p) + f(p) - f(r) + f(r) - f(q)) - \frac{i}{2} \sum_{p,q \in \Lambda} [H, A_{pq}] (f(q) - f(p)) \\
&= -\dot{A}(\delta f),
\end{aligned}$$

where we have defined

$$A(\delta f) = \frac{1}{2} \sum_{p,q \in \Lambda} A_{pq} (f(q) - f(p)). \quad (\text{C.14})$$

We find that the net energy current transforms as follows under a redefinition of the Hamiltonian density:

$$J^E(\delta f) \rightarrow J^E(\delta f) - \dot{A}(\delta f). \quad (\text{C.15})$$

But this should be expected since a redefinition of the energy density changes how we define the energy of sub-regions and therefore should affect the net energy current. Indeed, one can see that (C.13) is exactly the transformation needed in order to satisfy the energy conservation law

$$\dot{H}_p = - \sum_{q \in \Lambda} J_{pq}^E \quad \rightarrow \quad \dot{H}_p + \sum_{q \in \Lambda} \dot{A}_{qp} = - \sum_{q \in \Lambda} J_{pq}^E + \sum_{q \in \Lambda} \dot{A}_{qp} \quad (\text{C.16})$$

for the new energy density  $H_p + \sum_{q \in \Lambda} A_{qp}$ . By summing this transformation law over  $p$  weighted by a function  $f(p)$  with a compact support we find that

$$\dot{H}(f) = -J^E(\delta f) \quad \rightarrow \quad \dot{H}_p + \dot{A}(\delta f) = -J^E(\delta f) + \dot{A}(\delta f), \quad (\text{C.17})$$

which reproduces (C.15). Here we used an identity

$$\sum_{p,q \in \Lambda} A_{pq} f(q) = \frac{1}{2} \sum_{p,q \in \Lambda} A_{pq} (f(q) - f(p)) = A(\delta f) \quad (\text{C.18})$$

which is true for any  $f$  with a compact support.

From the above discussion, one can see that energy current is not invariant but covariant under energy density redefinitions. If we choose  $f(p)$  to be 1 when  $p$  is in some compact set  $B$  and zero otherwise, the physical meaning of (C.15) is very clear. It corresponds to ambiguities in the energy currents due to interaction terms along the boundary of  $B$ . Depending on how we distribute the interaction terms among  $H_p$  we can change the energy stored in the region  $B$  as well as energy current through its boundary.

### Invariance of the microscopic formulas for thermoelectric coefficients

In this section we will show that the coefficients  $\nu_{xy}$  and  $\eta_{xy}$  are invariant under a redefinition of the Hamiltonian density. We will start with skew-symmetric coefficients

$$d\nu^A = \frac{1}{2}d\left(\nu^{\text{Kubo}}(\delta f, \delta g) - \nu^{\text{Kubo}}(\delta g, \delta f)\right) - \beta^2\mu^N(\delta f \cup \delta g), \quad (\text{C.19})$$

$$d\eta^A = \frac{1}{2}d\left(\eta^{\text{Kubo}}(\delta f, \delta g) - \eta^{\text{Kubo}}(\delta g, \delta f)\right) - \beta\mu^N(\delta f \cup \delta g). \quad (\text{C.20})$$

Here we defined the Kubo parts as

$$\nu^{\text{Kubo}}(\delta f, \delta g) = \beta^2 \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle\langle J^N(\delta f, t); J^Q(\delta g) \rangle\rangle, \quad (\text{C.21})$$

$$\eta^{\text{Kubo}}(\delta f, \delta g) = \beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle\langle J^Q(\delta f, t); J^N(\delta g) \rangle\rangle. \quad (\text{C.22})$$

Under Hamiltonian density redefinition the Kubo parts transform as

$$\begin{aligned} \nu^{\text{Kubo}}(\delta f, \delta g) &\rightarrow \nu^{\text{Kubo}}(\delta f, \delta g) - \beta^2 \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle\langle J^N(\delta f, t); \dot{A}(\delta g) \rangle\rangle \\ &= \nu^{\text{Kubo}}(\delta f, \delta g) - \beta^2 \langle\langle J^N(\delta f); A(\delta g) \rangle\rangle, \end{aligned} \quad (\text{C.23})$$

$$\begin{aligned} \eta^{\text{Kubo}}(\delta f, \delta g) &\rightarrow \eta^{\text{Kubo}}(\delta f, \delta g) - \beta \lim_{s \rightarrow 0} \int_0^\infty dt e^{-st} \langle\langle \dot{A}(\delta f, t); J^N(\delta g) \rangle\rangle \\ &= \nu^{\text{Kubo}}(\delta f, \delta g) + \beta \langle\langle A(\delta f); J^N(\delta g) \rangle\rangle, \end{aligned} \quad (\text{C.24})$$

where we used properties of the Kubo pairing.

Before finding the variation of the magnetization term it is useful to rewrite it

slightly:

$$\begin{aligned}
& \mu^N(\delta f \cup \delta g) \\
&= \frac{1}{2} \sum_{p,q \in \Lambda} \left[ \frac{1}{3} \sum_{r \in \Lambda} \mu_{pqr}(g_p + g_q + g_r) - \frac{1}{2} \sum_{r \in \Lambda} \mu_{pqr}(g(p) + g(q)) \right] (f(q) - f(p)) \\
&= \frac{1}{2} \sum_{p,q \in \Lambda} \left[ \frac{1}{3} \sum_{r \in \Lambda} \mu_{pqr}(g_p + g_q + g_r) - \frac{1}{2} d\langle J_{pq}^N \rangle(g(p) + g(q)) \right] (f(q) - f(p)).
\end{aligned} \tag{C.25}$$

Note that one cannot expand the square brackets, since the two resulting sums over  $p, q$  will not converge separately.

Let us find the variation of  $\frac{1}{2} \langle J_{pq}^N \rangle(g(p) + g(q))$  under a Hamiltonian density redefinition. It reads

$$\begin{aligned}
\frac{1}{2} \langle J_{pq}^N \rangle(g(p) + g(q)) &\rightarrow \frac{1}{2} \langle J_{pq}^N \rangle(g(p) + g(q)) \\
&+ \frac{i}{2} \sum_{r \in \Lambda} \langle [A_{rq}, Q_p] - [A_{rp}, Q_q] \rangle(g(p) + g(q)).
\end{aligned} \tag{C.26}$$

The last term can be rewritten as follows:

$$\begin{aligned}
& \frac{i}{2} \sum_{r \in \Lambda} \langle [A_{rq}, Q_p] - [A_{rp}, Q_q] \rangle(g(p) + g(q)) \\
&= \frac{\beta}{2} \sum_{r \in \Lambda} \langle \langle g(p) \dot{Q}_p; A_{rq} \rangle \rangle + \frac{\beta}{2} \sum_{r \in \Lambda} \langle \langle \dot{Q}_p; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q),
\end{aligned} \tag{C.27}$$

where we used the properties of the Kubo pairing. The first term in this expression can be rewritten as

$$\begin{aligned}
& \sum_{r \in \Lambda} \langle \langle g(p) \dot{Q}_p; A_{rq} \rangle \rangle - (p \leftrightarrow q) = -\frac{1}{2} \sum_{s,r \in \Lambda} \langle \langle J_{sp}(g(s) + g(p)); A_{rq} \rangle \rangle - (p \leftrightarrow q) \\
&= -\frac{1}{2} \sum_{s,r \in \Lambda} \langle \langle J_{sp}^N(g(s) + g(p)) + J_{ps}^N(g(s) - g(p)); A_{rq} \rangle \rangle - (p \leftrightarrow q) = \langle \langle J^N(\delta g); A_{qp} \rangle \rangle \\
& \quad - \frac{1}{2} \sum_{r,s \in \Lambda} \left[ \langle \langle J_{rp}^N(g(r) + g(p)); A_{sq} \rangle \rangle + \langle \langle J_{ps}^N(g(s) - g(p)); A_{rq} \rangle \rangle + 2 \text{ perms} \right],
\end{aligned} \tag{C.28}$$

where "2 perms" means the two cyclic permutations in  $p, q, r$ . Note that the term in square brackets is skew-symmetric in  $p, q, r$ . The second term can be rewritten as

$$\begin{aligned}
& \sum_{r \in \Lambda} \langle \langle \dot{Q}_p; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q) = - \sum_{s, r \in \Lambda} \langle \langle J_{sp}^N; g(q) A_{rq} \rangle \rangle - (p \leftrightarrow q) \\
& = -\frac{1}{2} \sum_{s, r \in \Lambda} \langle \langle J_{sp}^N; A_{rq}(g(q) + g(r)) + A_{qr}(g(r) - g(q)) \rangle \rangle - (p \leftrightarrow q) = \langle \langle J_{pq}^N; A(\delta g) \rangle \rangle \\
& \quad - \frac{1}{2} \sum_{s, r \in \Lambda} \left[ \langle \langle J_{sp}^N; A_{rq}(g(q) + g(r)) \rangle \rangle + \langle \langle J_{rp}^N; A_{qr}(g(r) - g(q)) \rangle \rangle + 2 \text{ perms} \right].
\end{aligned} \tag{C.29}$$

Note that term in square brackets is skew-symmetric in  $p, q, r$

By combining equations (C.25-C.29) we find that the magnetization contribution changes under a redefinition of the Hamiltonian density as follows:

$$\begin{aligned}
\mu^N(\delta f \cup \delta g) \rightarrow \mu^N(\delta f \cup \delta g) - \frac{\beta}{2} d \langle \langle J^N(\delta f); A(\delta g) \rangle \rangle + \frac{\beta}{2} d \langle \langle J^N(\delta g); A(\delta f) \rangle \rangle \\
+ \frac{1}{2} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p)),
\end{aligned} \tag{C.30}$$

where  $C_{pqr}$  is a skew-symmetric function of  $p, q, r$  which is combination of skew-symmetric parts (and their derivatives) in the right-hand sides of Eqs. (C.25-C.29).

Due to its skew-symmetry we find that

$$\begin{aligned}
& \frac{1}{2} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p)) \\
& = \frac{1}{6} \sum_{p, q, r \in \Lambda} C_{pqr}(f(q) - f(p) + f(p) - f(s) + f(s) - f(q)) = 0.
\end{aligned} \tag{C.31}$$

We see that the variation of the magnetization exactly compensates the variation of the Kubo parts. Thus the skew-symmetric parts of the thermoelectric tensors are invariant under a redefinition of the Hamiltonian density.

Now let us consider the symmetric parts

$$v_{xy}^S = \frac{1}{2} \left( v^{\text{Kubo}}(\delta f, \delta g) + v^{\text{Kubo}}(\delta g, \delta f) \right) + \beta U(\delta f, \delta g), \tag{C.32}$$

$$\eta_{xy}^S = \frac{1}{2} \left( \eta^{\text{Kubo}}(\delta f, \delta g) + \eta^{\text{Kubo}}(\delta g, \delta f) \right) - U(\delta f, \delta g). \tag{C.33}$$

The variation of Kubo parts were already determined before, so we focus on the transformation of  $U$ . Under (C.5) it transforms as follows:

$$U(\delta f, \delta g) \rightarrow U(\delta f, \delta g) + \frac{i}{4} \sum_{p,q \in \Lambda} \langle [\partial A_q, Q_p] + [\partial A_p, Q_q] \rangle (f(q) - f(p))(g(q) - g(p)). \quad (\text{C.34})$$

We can rewrite this equation by noticing that

$$\frac{i}{2} \langle [\partial A_q, Q_p] + [\partial A_p, Q_q] \rangle (g(q) - g(p)) = -\frac{\beta}{2} \langle \langle g(p) \dot{Q}_p; \partial A_q \rangle \rangle + \frac{\beta}{2} \langle \langle \dot{Q}_p; \partial g(q) A_q \rangle \rangle - (p \leftrightarrow q). \quad (\text{C.35})$$

Then using eqs. (C.28, C.29) we find

$$U(\delta f, \delta g) \rightarrow U(\delta f, \delta g) + \frac{\beta}{2} \langle \langle J^N(\delta f); A(\delta g) \rangle \rangle + \frac{\beta}{2} \langle \langle J^N(\delta g); A(\delta f) \rangle \rangle \quad (\text{C.36})$$

We see that the variation of this term cancels the variations of the Kubo parts.

One can do the same checks for the thermal Hall conductivity and verify that the microscopic formula for it is invariant under a redefinition of the Hamiltonian density. To linear order in  $A_{pq}$  all the manipulations are almost the same except for the replacement  $Q_p \rightarrow H_p$  and  $J^N \rightarrow J^E$ .

### C.3 Thermoelectric coefficients for free fermions

In this appendix we use the same Hamiltonian and relevant definitions as in B.6.

#### Magnetization term

The magnetization differential for an arbitrary deformation  $dh$  of the 1-particle Hamiltonian is given by

$$\mu^N(\delta f \cup \delta g) = \frac{1}{4\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \left( G_+ dh G_+ \left\{ [h, f] G_+ [h, g] - [h, g] G_+ [h, f] \right\} \right) - (G_+ \rightarrow G_-). \quad (\text{C.37})$$

For temperature variations this expression can be simplified to

$$\begin{aligned} \tau^N(\delta f \cup \delta g) = & \frac{1}{4\pi} \int_{-\infty}^{\infty} dz \text{Tr} \left( \mathfrak{f}(z) (G_+ - G_-) [h^2, f] G_-^2 [h, g] \right. \\ & - \mathfrak{f}(z) (G_+ - G_-) [h^2, g] G_+^2 [h, f] + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_+ [h, f] \\ & \left. + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_- [h, f] \right) - (f \leftrightarrow g). \quad (\text{C.38}) \end{aligned}$$

These expressions are needed only for the evaluation of skew-symmetric parts of the thermoelectric coefficients.

### ***U*-term**

Let us study the term (6.8) for free fermionic system. In this case the relevant many-body operators become

$$([Q_p, H_q] + [Q_q, H_p]) = a^\dagger [h, \delta_p \delta_q] a, \quad (\text{C.39})$$

where  $\delta_p$  is a Kronecker delta function equal 1 on site  $p$  and 0 on all other sites. A product of two delta functions enforces  $q = p$  in the summation over  $p$  and  $q$ . Since  $U$  also involves a factor of  $(g(p) - g(q))(f(p) - f(q))$ ,  $U(\delta f, \delta g)$  vanishes for systems of free fermions.

More generally, one can a system of fermions with only density-dependent interactions. Namely, suppose we allow the following interaction term in the Hamiltonian (B.34):

$$H^{\text{int}} = \sum_{p_1, \dots, p_n \in \Lambda} V(p_1, \dots, p_n) Q_{p_1} \dots Q_{p_n}, \quad (\text{C.40})$$

where  $V(p_1, \dots, p_n)$  is a function of  $n$  sites which describes the potential energy of many-body interaction and decays rapidly when the points  $p_1, \dots, p_n$  are far from each other. One can see that this term will leave eq. (C.39) unaffected since  $Q_p$  commute with each other. We conclude that for fermionic system with only density-dependent interactions there is no correction originating from  $U$  to the symmetric thermoelectric coefficients provided  $H_p$  is chosen in the manner explained above.

### **Skew-symmetric part**

Consider the variation of the Kubo parts (C.21,C.22) of the skew-symmetric thermoelectric coefficients under a rescaling of the Hamiltonian:  $dh = h d\lambda_0$ . We get

$$\begin{aligned} dv_{\text{Kubo}}^A &= \beta d\eta_{\text{Kubo}}^A (\delta f \cup \delta g) = \frac{d\lambda_0}{4\pi} \int_{-\infty}^{\infty} dz \text{Tr} \left( \mathfrak{f}(z) (G_+ - G_-) [h^2, f] G_-^2 [h, g] \right. \\ &\quad - \mathfrak{f}(z) (G_+ - G_-) [h^2, g] G_+^2 [h, f] + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_+ [h, f] \\ &\quad + \mathfrak{f}'(z) (G_+ - G_-) h [h, g] G_- [h, f] - 2\mathfrak{f}'(z) h^2 (G_+ - G_-) [h, f] G_+^2 [h, g] \\ &\quad \left. + 2\mathfrak{f}'(z) h^2 (G_+ - G_-) [h, g] G_-^2 [h, f] \right) - (f \leftrightarrow g). \quad (\text{C.41}) \end{aligned}$$

Summing up this contributions with the magnetization contribution gives

$$\begin{aligned} \frac{dv^A}{dT} &= \frac{d}{dT} \left( \frac{\eta^A}{T} \right) = \frac{1}{2\pi T^2} \int_{-\infty}^{\infty} dz \mathfrak{f}'(z) z^2 \text{Tr} \left( (G_+ - G_-) [h, f] G_+^2 [h, g] \right. \\ &\quad \left. - (G_+ - G_-) [h, g] G_-^2 [h, f] - (f \leftrightarrow g) \right). \quad (\text{C.42}) \end{aligned}$$

Integrating over the temperature and using the formula

$$\int_T^\infty \frac{dT}{T^2} \mathfrak{f}'(z) = \frac{c_1(\mathfrak{f}(z)) - \log 2}{z^2}, \quad (\text{C.43})$$

where

$$c_1(x) = \int_0^x dt \log\left(\frac{1-t}{t}\right) = -x \log x - (1-x) \log(1-x), \quad (\text{C.44})$$

gives

$$\begin{aligned} \nu^A = \frac{\eta^A}{T} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz c_1(\mathfrak{f}(z)) \text{Tr} \left( (G_+ - G_-)[h, f] G_+^2[h, g] \right. \\ \left. - (G_+ - G_-)[h, g] G_-^2[h, f] \right) - (f \leftrightarrow g). \end{aligned} \quad (\text{C.45})$$

Here we normalized the thermoelectric coefficients to be 0 in the infinite-temperature state. Note that since in the limit  $T \rightarrow 0$  the Fermi-Dirac distribution  $\mathfrak{f}(z)$  becomes a step-function, and since  $c_1(0) = c_1(1) = 0$ , both  $\nu^A(T)$  and  $\eta^A(T)/T$  vanish at  $T = 0$  regardless of the choice of the Hamiltonian  $h$ .

### Symmetric part

Symmetric parts of transverse thermoelectric coefficients are

$$\begin{aligned} \nu_{xy}^S &= -\frac{\beta}{8\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \{ [h, f] G_+^2[h^2, g] (G_+ - G_-) \\ &\quad - [h, f] (G_+ - G_-)[h^2, g] G_-^2 \} + (f \leftrightarrow g), \\ \eta_{xy}^S &= -\frac{1}{8\pi} \int_{-\infty}^{\infty} dz \mathfrak{f}(z) \text{Tr} \{ [h^2, f] G_+^2[h, g] (G_+ - G_-) \\ &\quad - [h^2, f] (G_+ - G_-)[h, g] G_-^2 \} + (f \leftrightarrow g). \end{aligned}$$

As explained in the body of the thesis, longitudinal parts are given by the same formulas with a more general choice of the functions  $f, g$ .



*Appendix D*

APPENDICES TO CHAPTER VII

**D.1 Středa formulas**

In this appendix we recall the derivation of Středa formulas for the Hall and Nernst coefficients. The argument is essentially the same as the one presented in [51].

Consider a finite size homogeneous system coupled to two reservoirs with temperatures  $T_1, T_2$  and electrochemical potentials  $\mu_1, \mu_2$  respectively. The system will relax to a non-equilibrium steady state with a linearly changing temperature  $T(\mathbf{r})$  and electrochemical potential  $\mu(\mathbf{r})$ . In the bulk of the sample away from the edges and reservoirs, the electric current can be decomposed as

$$\begin{aligned} j_i(\mathbf{r}) &= j_i^{\text{tr}}(\mathbf{r}) + j_i^{\text{mag}}(\mathbf{r}) = -\sigma_{ik}\partial_k\mu - \nu_{ik}\partial_kT + \varepsilon_{ikl}\partial_kM_l(\mathbf{r}) \\ &= -\sigma_{ik}\partial_k\mu - \nu_{ik}\partial_kT + \varepsilon_{ikl}\partial_k\mu(\mathbf{r})\frac{\partial M_l(\mathbf{r})}{\partial\mu} + \varepsilon_{ikl}\partial_kT(\mathbf{r})\frac{\partial M_l(\mathbf{r})}{\partial T}, \end{aligned} \quad (\text{D.1})$$

where  $\mathbf{j}^{\text{mag}}(\mathbf{r}) = \nabla \times \mathbf{M}(\mathbf{r})$  is circulating currents which don't contribute to the net current across any section, and  $j_i^{\text{tr}}(\mathbf{r}) = -\sigma_{ik}\partial_k\mu - \nu_{ik}\partial_kT$  is the transport current. In the gapped phase at low temperature all bulk current across any macroscopic section should be exponentially suppressed for any values of  $\partial_k\mu$  and  $\partial_kT$ . Therefore we find

$$\sigma_{ik} = \varepsilon_{ikl}\frac{\partial M_l}{\partial\mu}, \quad (\text{D.2})$$

$$\nu_{ik} = \varepsilon_{ikl}\frac{\partial M_l}{\partial T}. \quad (\text{D.3})$$

One can see from the derivation that these formulas are only correct up to exponentially suppressed terms in the temperature arising from bulk currents. On the other hand, it can be shown that Středa formulas provide exact expressions for “static” Hall and Nernst coefficients which describe the equilibrium response of a system to an electric field and a temperature gradient [4].

**D.2 Proving Eqs. (7.49), (7.50)**

We now prove Eqs. (7.49), (7.50). To this end, we need to introduce some notation. First, we let  $\mathcal{V}_a$  denote the subspace spanned by all edge states  $|i, j, a\rangle$  within a fixed topological sector  $a$ . As in the main text we will drop the “a” index from now on,

since it always be fixed. Thus we will use the notation  $\mathcal{V}_a \rightarrow \mathcal{V}$  and  $|i, j, a\rangle \rightarrow |i, j\rangle$  in what follows.

Next, we let “ $|\Omega, \Omega\rangle$ ” denote the state  $|i, j\rangle$  in  $\mathcal{V}$  with the minimum value of the “energy”

$$(E_i^b - \mu_b N_i^b) + (E_j^t - \mu_t N_j^t). \quad (\text{D.4})$$

We will assume for simplicity that

$$E_\Omega^b - \mu_b N_\Omega^b = 0, \quad E_\Omega^t - \mu_t N_\Omega^t = 0, \quad (\text{D.5})$$

so that  $|\Omega, \Omega\rangle$  has an “energy” of exactly 0.

A final piece of notation: for each  $\delta > 0$ , we define  $\mathcal{V}_\delta$  to be subspace of  $\mathcal{V}$  spanned by states of the form  $|i, j\rangle$  with

$$E_i^b - \mu_b N_i^b \leq \delta, \quad E_j^t - \mu_t N_j^t \leq \delta. \quad (\text{D.6})$$

Roughly speaking,  $\mathcal{V}_\delta$  contains all states with “energies” of at most  $\delta$  on both edges.

Our proof relies on three assumptions about the  $|i, j\rangle$  edge states:

- **Assumption 1: (Existence of local operators)** For each  $i, i'$ , there exists an operator  $O_{i'i}^b$  supported near the bottom edge such that  $O_{i'i}^b|i, j\rangle = |i', j\rangle$  for all  $j$ . Likewise, for each  $j, j'$  there exists an operator  $O_{j'j}^t$  supported near the top edge such that  $O_{j'j}^t|i, j\rangle = |i, j'\rangle$  for all  $i$ .
- **Assumption 2: (Short range correlations)** For each  $i, j$ , the state  $|i, j\rangle$  has short-range correlations between the top and bottom edge: that is, for any operators  $O^b, O^t$  supported near the bottom and top edges respectively,

$$\langle i, j|O^b O^t|i, j\rangle = \langle i, j|O^b|i, j\rangle\langle i, j|O^t|i, j\rangle. \quad (\text{D.7})$$

- **Assumption 3: ( $U$  does not create bulk excitations)** There exists a  $\delta > 0$  such that  $U \cdot \mathcal{V}_\delta \subset \mathcal{V}$ . We will also assume that  $T_b, T_t \ll \delta$  so that  $\rho_0$  is a mixture of states  $|i, j\rangle$  belonging to  $\mathcal{V}_\delta$ .

We will now use these assumptions to prove the claims. Our argument proceeds in three steps.

**Step 1: Showing that  $U|\Omega, \Omega\rangle$  is factorizable**

In the first step, we will show that there exists operators  $S_b, S_t$  support near the bottom and top edges respectively, such that

$$U|\Omega, \Omega\rangle = S^b S^t |\Omega, \Omega\rangle \quad (\text{D.8})$$

To prove this, we note that Assumption 3 implies that  $U|\Omega, \Omega\rangle \in \mathcal{V}$ . Hence,

$$U|\Omega, \Omega\rangle = \sum_{ij} X_{ij} |i, j\rangle \quad (\text{D.9})$$

for some complex coefficients  $X_{ij}$ . Multiplying this equation by its adjoint, we conclude that

$$U|\Omega, \Omega\rangle\langle\Omega, \Omega|U^\dagger = \sum_{ii'jj'} X_{ij} X_{i'j'}^* |i, j\rangle\langle i', j'| \quad (\text{D.10})$$

or equivalently

$$U\rho_\Omega U^\dagger = \sum_{ii'jj'} X_{ij} X_{i'j'}^* |i, j\rangle\langle i', j'| \quad (\text{D.11})$$

where  $\rho_\Omega \equiv |\Omega, \Omega\rangle\langle\Omega, \Omega|$ . Using Assumption 1, we deduce that

$$\text{Tr}(O_{i'i}^b O_{j'j}^t U\rho_\Omega U^\dagger) = X_{ij} X_{i'j'}^* \quad (\text{D.12})$$

We can rewrite this relation as

$$\text{Tr}(\tilde{O}_{i'i}^b \tilde{O}_{j'j}^t \rho_\Omega) = X_{ij} X_{i'j'}^* \quad (\text{D.13})$$

where

$$\tilde{O}_{i'i}^b = U^\dagger O_{i'i}^b U, \quad \tilde{O}_{j'j}^t = U^\dagger O_{j'j}^t U \quad (\text{D.14})$$

Now, since  $U$  is a local unitary transformation of the form (7.44), we know that  $\tilde{O}_{i'i}^b$  and  $\tilde{O}_{j'j}^t$  are supported near the bottom and top edges respectively (this follows from Lieb-Robinson bounds [26]). Therefore, by Assumption 2, we can factor the left hand side of (D.13) to obtain

$$\text{Tr}(\tilde{O}_{i'i}^b \rho_\Omega) \cdot \text{Tr}(\tilde{O}_{j'j}^t \rho_\Omega) = X_{ij} X_{i'j'}^*. \quad (\text{D.15})$$

Equivalently, we can write this relation as

$$\tau_{i'i}^b \tau_{j'j}^t = X_{ij} X_{i'j'}^*, \quad (\text{D.16})$$

where

$$\tau_{i'i}^b = \text{Tr}(\tilde{O}_{i'i}^b \rho_\Omega), \quad \tau_{j'j}^t = \text{Tr}(\tilde{O}_{j'j}^t \rho_\Omega). \quad (\text{D.17})$$

An immediate mathematical consequence of (D.16) is that  $X_{ij}$  can be factored as

$$X_{ij} = \alpha_i \beta_j \quad (\text{D.18})$$

for some complex coefficients  $\alpha_i, \beta_j$ . One way to see this is to note that the right hand side of (D.16) looks like the density matrix for a pure state with wave function  $X_{ij}$ . From this point of view, Eq. (D.16) implies that the density matrix corresponding to  $X_{ij}$  can be written as the tensor product of two density matrices for  $i$  and  $j$  separately. Hence  $X_{ij}$  has no entanglement between  $i$  and  $j$ , which implies that  $X_{ij}$  can be written in the form (D.18).

We now substitute (D.18) into (D.9) to derive

$$U|\Omega, \Omega\rangle = \sum_{ij} \alpha_i \beta_j |i, j\rangle. \quad (\text{D.19})$$

We can now construct the required operators  $S^b, S^t$ :

$$S^b = \sum_i \alpha_i O_{i\Omega}^b, \quad S^t = \sum_j \beta_j O_{j\Omega}^t. \quad (\text{D.20})$$

By construction,  $S^b, S^t$  obey equation (D.8). This proves the claim.

### Step 2: Showing $\langle i, j|U|i', j'\rangle$ is factorizable

In the second step, we show that  $\langle i, j|U|i', j'\rangle$  is factorizable, i.e.

$$\langle i, j|U|i', j'\rangle = Y_{i'i'}^b Y_{j'j}^t \quad (\text{D.21})$$

for some complex coefficients  $Y_{i'i'}^b, Y_{j'j}^t$ .

To show this, we note that by Assumption 1, we can write  $\langle i, j|U|i', j'\rangle$  as

$$\langle i, j|U|i', j'\rangle = \langle \Omega, \Omega|(O_{j\Omega}^t)^\dagger (O_{i\Omega}^b)^\dagger U O_{i'\Omega}^b O_{j'\Omega}^t |\Omega, \Omega\rangle. \quad (\text{D.22})$$

Equivalently, we can write this as

$$\langle i, j|U|i', j'\rangle = \langle \Omega, \Omega|(O_{j\Omega}^t)^\dagger (O_{i\Omega}^b)^\dagger \bar{O}_{i'\Omega}^b \bar{O}_{j'\Omega}^t U |\Omega, \Omega\rangle, \quad (\text{D.23})$$

where  $\bar{O}_{i'i}^b = U O_{i'i}^b U^\dagger$ , and  $\bar{O}_{j'j}^t = U O_{j'j}^t U^\dagger$ .

Next, using (D.8), we can rewrite this as

$$\langle i, j|U|i', j'\rangle = \langle \Omega, \Omega|(O_{j\Omega}^t)^\dagger (O_{i\Omega}^b)^\dagger \bar{O}_{i'\Omega}^b \bar{O}_{j'\Omega}^t S^b S^t|\Omega, \Omega\rangle. \quad (\text{D.24})$$

Now using Assumption 2, we can factor the right hand side into two parts:

$$\langle i, j|U|i', j'\rangle = Y_{ii'}^b Y_{jj'}^t,$$

where

$$\begin{aligned} Y_{ii'}^b &= \langle \Omega, \Omega|(O_{i\Omega}^b)^\dagger \bar{O}_{i'\Omega}^b S^b|\Omega, \Omega\rangle, \\ Y_{jj'}^t &= \langle \Omega, \Omega|(O_{j\Omega}^t)^\dagger \bar{O}_{j'\Omega}^t S^t|\Omega, \Omega\rangle. \end{aligned} \quad (\text{D.25})$$

This establishes the factorization (D.21).

### Finishing the proof

We are now ready to finish the proof: we will prove Eqs. (7.49), (7.50). The first step is to note that the matrices  $Y^b$  and  $Y^t$  that appear in (D.21) are guaranteed to obey a unitarity property. To be precise,  $Y^b$  and  $Y^t$  obey

$$[(Y^b)^\dagger Y^b]_{i'i} = \delta_{i'i}, \quad [(Y^t)^\dagger Y^t]_{j'j} = \delta_{j'j} \quad (\text{D.26})$$

for any  $i, i', j, j'$  such that  $|i, j\rangle, |i', j'\rangle \in \mathcal{V}_\delta$  where  $\mathcal{V}_\delta$  is defined as in Assumption 3 above. Indeed, the above property follows from the fact that  $U$  is unitary and that  $U|i, j\rangle, U|i', j'\rangle \in V$  (according to Assumption 3).<sup>1</sup>

To prove (7.49), we note that the initial density matrix  $\rho_0$  can be factorized as

$$\langle i, j|\rho_0|i', j'\rangle = \rho_{ii'}^b \rho_{jj'}^t. \quad (\text{D.27})$$

Therefore, by (D.21), we have

$$\langle i, j|U\rho_0U^\dagger|i', j'\rangle = \sigma_{ii'}^b \sigma_{jj'}^t, \quad (\text{D.28})$$

where

$$\sigma^b = Y^b \rho^b (Y^b)^\dagger, \quad \sigma^t = Y^t \rho^t (Y^t)^\dagger. \quad (\text{D.29})$$

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<sup>1</sup>More precisely, the fact that  $U$  is unitary implies that  $Y^b, Y^t$  can always be rescaled by a scalar factor  $Y^b \rightarrow Y^b \cdot \lambda, Y^t \rightarrow Y^t \cdot \lambda^{-1}$  so that they obey the unitarity property (D.26). We will assume this rescaling in what follows.

Furthermore, it is clear from the above expressions that  $\sigma^b$  and  $\sigma^t$  are Hermitian. This completes our proof of (7.49).

As for (7.50), the unitarity property (D.26) implies that

$$\begin{aligned}\mathrm{Tr}[(\sigma^b)^n] &= \mathrm{Tr}[(\rho^b)^n], \\ \mathrm{Tr}[(\sigma^t)^n] &= \mathrm{Tr}[(\rho^t)^n]\end{aligned}\tag{D.30}$$

for any positive integer  $n$  and hence

$$\begin{aligned}\mathrm{Spec}(\sigma^b) &= \mathrm{Spec}(\rho^b) \\ \mathrm{Spec}(\sigma^t) &= \mathrm{Spec}(\rho^t).\end{aligned}\tag{D.31}$$

This completes our proof of (7.50).

## APPENDICES TO CHAPTER VIII

**E.1 Quantization of higher Berry curvatures**

Consider a family of gapped systems in spatial dimension  $D$ . In the body of the thesis we showed how to define a closed form  $\Omega^{(D+2)}$  on the parameter space  $M$ . It depends on some additional data ( $D$  functions on  $\Lambda$ ), but the cohomology class was shown to be independent of these data. Thus periods of  $\Omega^{(D+2)}$  are also independent of these additional data. In this appendix we argue that if all systems in the family are Short-Range Entangled (SRE), and if  $h$  is a spherical cycle in  $M$  (i.e. a map  $h : S^{D+2} \rightarrow M$ ), then the integral of  $\Omega^{(D+2)}$  over such a cycle is "quantized":

$$\frac{1}{2\pi} \int_{S^{D+2}} h^*(\Omega^{(D+2)}) \in \mathbb{Z}. \quad (\text{E.1})$$

We begin with the 1d case, where there is no topological order, and thus all gapped systems without spontaneous symmetry breaking are SRE. Thus all systems in the family belong to the same SRE phase. In the bosonic case, this means that they can all be deformed to a trivial system whose Hamiltonian is a sum of one-site operators and the ground state is a product state. In the fermionic case, there is a unique non-trivial SRE phase corresponding to Kitaev's Majorana chain. So there are two options: either all systems in the family are in the trivial phase, or they can all be deformed to the Majorana chain. In the latter case we can stack the whole family with the "constant" Majorana chain and get a family of fermionic systems in the trivial phase. Since  $\Omega^3(f)$  is unchanged under stacking the family with a system independent of parameters, this reduces the problem to studying a family of systems in the trivial phase.

Let  $f(p) = \theta(p)$  (a step-function on  $\Lambda \subset \mathbb{R}$ ). Recall that we denote the space of all gapped 1d system by  $\mathfrak{M}_1$ . (Our argument will be the same for bosonic and fermionic systems, so we do not need to distinguish the two possibilities). This is an infinite-dimensional space which can be thought of as a union of an infinite number of finite-dimensional manifolds. The parameter space  $M$  is a submanifold in this infinite-dimensional space, and the 3-form  $\Omega^{(3)}$  on  $M$  is a restriction of the 3-form on  $\mathfrak{M}_1$  defined in exactly the same way. Let us fix a particular trivial system  $\mathbf{m}_0 \in \mathfrak{M}_1$ . Each point in  $M$  can be connected to  $\mathbf{m}_0$  by a continuous path in  $\mathfrak{M}_1$ .

This applies to all points in the image of the spherical cycle  $h$ . If this could be done continuously over the whole  $S^3$ , it would mean that the cycle is contractible to a point  $\mathbf{m}_0$  in  $\mathfrak{M}_1$ , and the corresponding integral  $\int_{S^3} h^*(\Omega^{(3)}(f))$  would be zero. While in general it is not possible to contract the whole spherical cycle, it is always possible to contract  $S^3$  with a point removed. In particular, it is possible to contract  $S^3$  without either north or south pole. Let  $S_S^3$  and  $S_N^3$  be  $S^3$  with the north and south poles removed, respectively. Let us denote the contractions in the space of the gapped Hamiltonians by  $\mathcal{P}_S$  and  $\mathcal{P}_N$ . These are continuous maps from  $[0, 1] \times S_S^3$  to  $\mathfrak{M}_1$  and from  $[0, 1] \times S_N^3$  to  $\mathfrak{M}_1$ , respectively. Let us parameterize  $[0, 1]$  by  $t$ . For  $t = 0$  they are just restrictions of  $h$  to  $S_S^3$  and  $S_N^3$ . For  $t = 1$  they are constant maps to  $\mathbf{m}_0$ .

Let the Hamiltonian corresponding to a point  $\mathbf{m} \in \mathfrak{M}_1$  be  $H(\mathbf{m}) = \sum_p H_p(\mathbf{m})$ . The family of Hamiltonians corresponding to the spherical cycle  $h$  is  $H[\mathbf{s}] = \sum_p H_p(h(\mathbf{s}))$ , where  $\mathbf{s} \in S^3$ . For  $\mathbf{s} \in S_N^3$  we define another Hamiltonian  $H^+[\mathbf{s}]$  which is the same as  $H[\mathbf{s}]$  except that on the far right part of the lattice  $p \gg 0$  it adiabatically interpolates to  $H(\mathbf{m}_0)$ . More precisely,  $H^+[\mathbf{s}] = \sum_{p \in \Lambda} H_p^+[\mathbf{s}]$  is sum of on-site Hamiltonians  $H_p^+[\mathbf{s}] = H_p(\mathbf{m}(\mathbf{s}, p))$  where we let the parameters of the Hamiltonian depend slowly on  $p$  as  $\mathbf{m}(\mathbf{s}, p) = \mathcal{P}_N(t_N(p), \mathbf{s})$ . The function  $t_N : \mathbb{R} \rightarrow \mathbb{R}$  is equal to 1 for  $p \in [2L, +\infty)$ , smoothly interpolates from 1 to 0 in the region  $p \in [L, 2L]$ , and is 0 for  $p \in (-\infty, L]$ . Similarly, we define a local Hamiltonian  $H^-[\mathbf{s}]$  for all  $\mathbf{s} \in S_S^3$  via  $H^-[\mathbf{s}] = \sum_{p \in \Lambda} H_p(P_S(t_S(p), \mathbf{s}))$ , where the function  $t_S : \mathbb{R} \rightarrow \mathbb{R}$  is 1 for  $p \in (-\infty, -2L]$ , smoothly interpolates from 1 to 0 in the region  $p \in [-2L, -L]$ , and is 0 for  $p \in [-L, +\infty)$ . Lastly, we define  $H_p^{+-}[\mathbf{s}]$  for all  $\mathbf{s} \in S_N^3 \cap S_S^3$  as a Hamiltonian which coincides with  $H_p[\mathbf{s}]$  in the region  $p \in [-L, L]$ , coincides with  $H_p(\mathbf{m}_0)$  for  $p \notin [-2L, 2L]$ , and smoothly interpolates between these regions using the paths  $\mathcal{P}_S$  and  $\mathcal{P}_N$ . Our main assumption is that all these families of Hamiltonians are gapped for sufficiently large  $L$ . This seems reasonable since for a fixed  $t$  and  $\mathbf{s}$  all Hamiltonians  $H(\mathcal{P}_N(t, \mathbf{s}))$  and  $H(\mathcal{P}_S(t, \mathbf{s}))$  are gapped and there should be an upper bound on the correlation length. However, a proof of this would be very desirable. We denote by  $\Omega_+^{(3)}(f)$ ,  $\Omega_-^{(3)}(f)$ , and  $\Omega_{+-}^{(3)}(f)$  the 3-forms corresponding to the families  $H^+$ ,  $H^-$  and  $H^{+-}$ . They are defined on  $S_N^3$ ,  $S_S^3$ , and  $S_N^3 \cap S_S^3$ , respectively.

We write an integral over  $S^3$  as a sum of integrals over its lower and upper hemi-



spheres which we call  $B_-$  and  $B_+$ :

$$\begin{aligned} \int_{S^3} h^*(\Omega^{(3)}(f)) &= \int_{B_+} h^*(\Omega^{(3)}(f)) + \int_{B_-} h^*(\Omega^{(3)}(f)) \\ &= \int_{B_+} \Omega_+^{(3)}(f) + \int_{B_-} \Omega_-^{(3)}(f) + O(L^{-\infty}). \end{aligned}$$

In the last step we replaced  $h^*(\Omega^{(3)})$  with  $\Omega_{\pm}^{(3)}$  on  $B_{\pm}$ . Since by our assumption  $H[\mathbf{s}]$ ,  $H^+[\mathbf{s}]$ , and  $H^-[\mathbf{s}]$  are all gapped, the 3-form  $h^*(\Omega^{(3)})$  is only sensitive to the Hamiltonian of the system in the neighborhood of the point  $p = 0$  where the function  $f(p) = \theta(p)$  has a discontinuity. Since all these Hamiltonians coincide near the point  $p = 0$ , for large  $L$  the error introduced by this replacement is of order  $L^{-\infty}$ .

Let us now define  $f_+(p) = \theta(p - 3L)$  and  $f_-(p) = \theta(p + 3L)$  and write

$$\begin{aligned} \int_{B_+} \Omega_+^{(3)}(f) + \int_{B_-} \Omega_-^{(3)}(f) &= \int_{B_+} \Omega_+^{(3)}(f_+) + \int_{B_-} \Omega_-^{(3)}(f_-) \\ &\quad + \int_{B_+} \Omega_+^{(3)}(f - f_+) + \int_{B_-} \Omega_-^{(3)}(f - f_-). \end{aligned} \quad (\text{E.2})$$

The on-site Hamiltonian  $H_p^+[\mathbf{s}]$  coincides with the constant Hamiltonian  $H_p(\mathbf{m}_0)$  near  $p = 3L$ . Therefore the form  $\Omega_+^{(3)}(f_+)$  is of order  $L^{-\infty}$ , and so is its integral over  $B_+$ . Similarly,  $\int_{B_-} \Omega_-^{(3)}(f_-) = O(L^{-\infty})$ . The remaining terms in the above equation contain functions  $f_{\pm} - f$  which have compact support. For any such function  $g : \Lambda \rightarrow \mathbb{R}$  we can write  $\Omega_{\pm}^{(3)}(g) = F_{\pm}^{(3)}(\delta g) = dF_{\pm}^{(2)}(g)$ . Therefore we get

$$\int_{B_+} \Omega_+^{(3)}(f - f_+) + \int_{B_-} \Omega_-^{(3)}(f - f_-) = \int_{S^2} F_+^{(2)}(f - f_+) - \int_{S^2} F_-^{(2)}(f - f_-), \quad (\text{E.3})$$

where  $S^2$  is the equator of  $S^3$  and the common boundary of  $B_-$  and  $B_+$ . The minus sign arises because the orientation on  $S^2$  induced by  $B_-$  is opposite to the one induced by  $B_+$ . We can now replace  $F_+^{(2)}$  and  $F_-^{(2)}$  with  $F_{+-}^{(2)}$  in both integrals, since the integrands are only sensitive to the Hamiltonian of the system in the region where  $H_p^+[\mathbf{s}] = H_p^{+-}[\mathbf{s}]$  and  $H_p^-[\mathbf{s}] = H_p^{+-}[\mathbf{s}]$ . Such a replacement introduces an error of order  $L^{-\infty}$ . Therefore the above expression becomes

$$\begin{aligned} \int_{S^2} F_+^{(2)}(f - f_+) - \int_{S^2} F_-^{(2)}(f - f_-) &= \int_{S^2} F_{+-}^{(2)}(f - f_+) \\ &\quad - \int_{S^2} F_{+-}^{(2)}(f - f_-) + O(L^{-\infty}) = - \int_{S^2} F_{+-}^{(2)}(f_+ - f_-) + O(L^{-\infty}). \end{aligned} \quad (\text{E.4})$$

By construction  $H_p^{+-}[\mathbf{s}] = H_p[\mathbf{s}]$  for  $p \in [-L, L]$ , while  $H_p^{+-}[\mathbf{s}] = H(\mathbf{m}_0)$  for  $p \notin [-2L, 2L]$ . Since outside  $[-2L, 2L]$  the Hamiltonian is constant, that part of

the system does not contribute to  $F^{(2)}$  and can be discarded. What remains is a system with a finite-dimensional Hilbert space. Since  $f_+ - f_- = \theta(p-3L) - \theta(p+3L)$  and thus is equal  $-1$  in the region  $[-2L, 2L]$ , we have

$$-F_{+-}^{(2)}(f_+ - f_-) = \sum_{p \in [-2L, 2L]} F_{+-p}^{(2)} + O(L^{-\infty}). \quad (\text{E.5})$$

This is simply the Berry curvature of this finite-dimensional system. Therefore its integral over  $S^2$  is an integer multiple of  $2\pi$ . We conclude that

$$\int_{S^3} h^*(\Omega^{(3)}(f)) = 2\pi n + O(L^{-\infty}), \quad n \in \mathbb{Z}. \quad (\text{E.6})$$

Taking the limit  $L \rightarrow \infty$  we get the desired result.

In general we proceed by induction in  $D$ . For  $D > 1$  the restriction to SRE systems is a nontrivial constraint on the kind of families we allow. Other than that, we can proceed in the same way as for  $D = 1$ . First we tensor with a suitable constant SRE system to reduce to the case of a family of systems in a trivial phase. Then we remove the north and south pole from  $S^{D+2}$  and define three families of gapped Hamiltonians  $H^+[\mathbf{s}]$ ,  $H^-[\mathbf{s}]$ , and  $H^{+-}[\mathbf{s}]$  which are defined on  $S_N^{D+2}$ ,  $S_S^{D+2}$  and  $S_N^{D+2} \cap S_S^{D+2}$ , respectively. They approach  $H(\mathbf{m}_0)$  on the far right, far left, and both far right and far left, respectively. By far right we mean the region  $x^D(p) \gg 0$ , while far left is the region  $x^D(p) \ll 0$ . The same manipulations as before reduce the integral of  $\Omega^{(D+2)}$  over  $S^{D+2}$  to an integral of  $\Omega^{(D+1)}$  over the equatorial  $S^{D+1}$  up to terms of order  $L^{-\infty}$ . This completes the inductive step.

An interpolation between  $H(\mathbf{m})$  and  $H(\mathbf{m}_0)$  can also be viewed as a gapped boundary condition for  $H(\mathbf{m})$ . Given a smooth family of gapped boundary conditions for  $H[\mathbf{s}]$  defined on some open subset  $U \subset S^3$  (not necessarily arising from a smooth interpolation as above), one can write  $\Omega^{(D+2)}(f_1, \dots, f_D)|_U$  as an exact form. This is done in exactly the same way as above. Therefore if the cohomology class of  $\Omega^{(D+2)}$  is non-trivial, it is impossible to find a family of gapped boundary conditions for  $H[\mathbf{s}]$  which is defined on the whole  $S^3$  and varies smoothly with  $\mathbf{s}$ . For  $D = 0$  the analogous statement is that the cohomology class of the Berry curvature is an obstruction to finding a family of ground states on the whole parameter space which depends continuously on the parameters.

## E.2 Higher Berry curvature for 1d insulators of class A

In this appendix we compute the higher Berry curvature 3-form in the case of gapped systems of free fermions in 1d with conserved charge (that is, insulators of class

A). Then we specialize to the case of translationally-invariant systems and compare with forms constructed out of the Bloch-Berry connection.

We start with the many-body expression for the 3-form  $F_{pq}^{(3)}$  divided by  $2\pi$ :

$$\begin{aligned} \frac{F_{pq}^{(3)}}{2\pi} = & -\frac{i}{12\pi} \oint_{z=E_0} \frac{dz}{2\pi i} \text{Tr}(2GdHG^2dH_pGdH_q \\ & + GdHGdH_pG^2dH_q) - (p \leftrightarrow q). \end{aligned} \quad (\text{E.7})$$

We will consider the following many-body Hamiltonian:

$$H_p = \frac{1}{2} \sum_{m \in \Lambda} \left( a_p^\dagger h(p, m) a_m + a_m^\dagger h(m, p) a_p \right). \quad (\text{E.8})$$

Here  $h(p, q)$  is an Hermitian matrix  $h(p, q)^* = h(q, p)$ . The fermionic creation-annihilation operators  $a_p^\dagger, a_p$  satisfy canonical anti-commutation relations

$$\begin{aligned} \{a_p^\dagger, a_q\} &= \delta_{pq}, \\ \{a_p, a_q\} &= \{a_p^\dagger, a_q^\dagger\} = 0, \end{aligned} \quad (\text{E.9})$$

where  $\delta_{pq}$  is the Kronecker delta.

Since all relevant operators are sums of single particle operators, matrix elements  $\langle m|A|n\rangle$  vanish unless many-body states  $n$  and  $m$  differ by exactly one single-particle excitation. The above expression can be written in terms of one-particle quantities as follows:

$$\frac{F_{pq}^{(3)}}{2\pi} = -\frac{i}{12\pi} \oint \frac{dz}{2\pi i} \text{tr}(2gdhg^2dh_pgdh_q + gdhgdh_pg^2dh_q) - (p \leftrightarrow q). \quad (\text{E.10})$$

Here the contour of integration encloses all states below Fermi level and all lower case letters denote the corresponding single-particle operators acting on the single-particle Hilbert space  $\ell^2(\Lambda)$ . Naively, this integral contains additional contributions compared to (E.7) where a fermion jumps from an empty state or jumps into a filled state. But these contributions cancel each other and the result coincides with (E.7).

Hamiltonian density at a point  $p$  can be written as  $h_p = \frac{1}{2}(\delta_p h + h\delta_p)$ , where  $\delta_p$  is Kronecker's delta (equal 1 on  $p$  and 0 on other sites) and functions are understood as operators on the one-particle Hilbert space acting by multiplication. Contracting  $F_{pq}^{(3)}$  with the cochain  $f(q) - f(p)$  we find

$$\begin{aligned} \frac{1}{2\pi} \langle F^{(3)}, \delta f \rangle = & -\frac{i}{24\pi} \oint \frac{dz}{2\pi i} \text{tr} \left( [dh, f](gdhgdhg^2 - g^2dhgdhg) \right. \\ & \left. - 2[h, f](gdhg^2dhgdhg - gdhgdhg^2dhg) \right). \end{aligned} \quad (\text{E.11})$$

Note that multiplication by  $f$  is not a trace class operator, since it acts on infinitely many sites. Therefore traces containing them are not guaranteed to exist. On the other hand, commutators like  $[dh, f]$  are supported only on a finite number of sites, and therefore traces containing them are well-defined.

On the other hand, given a gapped 1d system of free fermions with translational symmetry which depends on three parameters  $\lambda_1, \lambda_2, \lambda_3$ , one may consider the Bloch bundle of filled states over the product of the Brillouin zone  $S^1$  and the parameter space  $\Sigma$ . It carries the non-Abelian Bloch-Berry connection, and one can consider various Chern-Weil forms on  $S^1 \times \Sigma$  constructed out of this connection. In particular, one can consider the degree-4 component of the Chern character of the Berry-Bloch connection and its integral over  $S^1 \times \Sigma$ :

$$\int_{S^1 \times \Sigma} \text{Ch}(\mathcal{F}) = -\frac{1}{8\pi^2} \int_{S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}). \quad (\text{E.12})$$

Here  $\mathcal{F}$  is the non-Abelian curvature 2-form of the Bloch-Berry connection and trace is taken over filled bands. It can be shown (see Sec. IIIA in [46]) that this quantity can be expressed in terms of the one-particle Green's function as follows:

$$\begin{aligned} -\frac{1}{8\pi^2} \int_{S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}) &= \frac{\pi^2}{15} \epsilon^{\mu\nu\rho\sigma\tau} \oint \frac{dz}{2\pi i} \int_{S^1} \frac{dk}{2\pi} \int_{\Sigma} \frac{d^3\lambda}{(2\pi)^3} \\ &\times \text{tr}' \left[ \left( g \frac{\partial g^{-1}}{\partial q^\mu} \right) \left( g \frac{\partial g^{-1}}{\partial q^\nu} \right) \left( g \frac{\partial g^{-1}}{\partial q^\rho} \right) \left( g \frac{\partial g^{-1}}{\partial q^\sigma} \right) \left( g \frac{\partial g^{-1}}{\partial q^\tau} \right) \right], \end{aligned} \quad (\text{E.13})$$

where  $q^\mu = (z, k, \lambda_1, \lambda_2, \lambda_3)$ . The first integral encloses filled levels, the second integral is over the Brillouin zone, and the last integral is over the parameter space  $\Sigma$ . The trace  $\text{tr}'$  is taken over subspace with fixed momentum  $k$ . In translationally invariant system we can interpret  $\int_{S^1} \frac{dk}{2\pi}$  as part of the trace  $\text{tr}$  over the whole one-particle Hilbert space and substitute  $\frac{\partial g^{-1}}{\partial k} = -\frac{\partial h}{\partial k} = -i[h, f]$ . Expanding the derivatives  $\partial/\partial q^\mu$  and combining parameter derivatives into forms,  $\sum_i \frac{\partial h}{\partial \lambda^i} d\lambda^i = dh$ , we find

$$\begin{aligned} -\frac{1}{8\pi^2} \int_{S^1 \times \Sigma} \text{Tr}(\mathcal{F} \wedge \mathcal{F}) &= \frac{i}{24\pi} \oint \frac{dz}{2\pi i} \int_{\Sigma} \text{tr} \left( g^2 [h, f] g dh g dh g dh \right. \\ &\left. - g^2 dh g [h, f] g dh g dh + g^2 dh g dh g [h, f] g dh - g^2 dh g dh g dh g [h, f] \right). \end{aligned} \quad (\text{E.14})$$

One can see that the integrand of this expression differs from (E.11) by a total derivative proportional to

$$d \left( \oint \frac{dz}{2\pi i} \text{tr} \left( [h, f] (g dh g dh g^2 - g^2 dh g dh g) \right) \right). \quad (\text{E.15})$$

Since  $\Sigma$  was an arbitrary three-dimensional submanifold of the parameter space, we have shown that the first higher Berry 3-form divided by  $2\pi$  is in the same cohomology class as  $\int_{S^1 \times \Sigma} \text{Ch}(\mathcal{F})$ . We conjecture that more generally for class A insulators in  $D$  dimensions the form  $\Omega^{(D+2)}$  is in the same cohomology class as the integral of the degree  $2D + 2$  component of the Chern character of the Bloch-Berry connection over the Brillouin zone.

An example of a free 1d fermion system with a non-trivial integral  $\int_{S^1 \times \Sigma} \text{Ch}(\mathcal{F})$  can be constructed using the 4d Chern insulator (see sec. IIIB of [46]). The Hamiltonian is

$$H = \sum_{k_x} \psi_{k_x}^\dagger d_a(k_x, \vec{\lambda}) \Gamma^a \psi_{k_x}, \quad (\text{E.16})$$

where  $\Gamma^a$  are five Dirac matrices generating a Clifford algebra, and

$$d_a(k_x, \vec{\lambda}) = \left[ (m + c + \cos k_x + c \sum_{i=1}^3 \cos \lambda_i), \sin k_x, \sin \lambda_1, \sin \lambda_2, \sin \lambda_3 \right]. \quad (\text{E.17})$$

It was shown in Ref. [46] that if we chose  $\Sigma$  to be 3-torus  $S^1 \times S^1 \times S^1$  defined by identification  $\lambda_i \sim \lambda_i + 2\pi$  this model has a non-zero integer value of the integral  $\int_{S^1 \times S^1 \times S^1 \times S^1} \text{Ch}(\mathcal{F})$  for a particular choice of  $m$  and  $c$ . One can think about this family of 1d models as a "dimensional reduction" of the 4d Chern insulator where we treat three out of four components of momentum as parameters.

Note that the Atiyah-Singer index theorem [3] implies that the integral of the Chern character of a vector bundle over a four-torus is an integer. Therefore the integral of  $\Omega^{(3)}$  over the parameter space  $T^3$  is  $2\pi$  times an integer, despite the fact that the parameter space is a torus rather than a sphere.

## APPENDICES TO CHAPTER IX

**F.1 Quantization of the Thouless charge pump and its descendants**

The proof of quantization for the Thouless pump essentially repeats the one for Higher Berry curvature presented in Appendix E.1, but for clearness we will repeat it in details.

Consider a family of gapped  $U(1)$ -invariant systems in  $D$  dimensions parameterized by a  $D$ -dimensional sphere. Suppose also that all systems in the family are in a Short-Range Entangled (SRE) phase. In this appendix we argue that for such a family the descendant Thouless charge pump invariant is an integer.

We start with the ordinary Thouless charge pump  $Q^{(1)}(f)$  for gapped 1d systems. As far as we know, its integrality for interacting systems was shown only recently [5]. We will provide an alternative argument for it. Let us first sketch the rough idea. Due to a finite correlation length of gapped systems the 1-form  $Q^{(1)}(f)$  depends only on the static linear response in the neighborhood of the region where the function  $f$  is non-constant. For the specific choice  $f(p) = \theta(p - a)$  one can see from (9.25) that only points which are a few correlation lengths away from  $a$  contribute significantly to  $Q^{(1)}(f)$ . Naively, one could expect that if we terminate the system away from point  $a$  by replacing the rest of the Hamiltonian with a trivial one it would not change the value of  $Q^{(1)}(f)$ . The flaw of this procedure is that the modified Hamiltonian is not guaranteed to be gapped for all values of the parameters. If for some values of parameters the gap closes, the correlation length might diverge and this might lead to additional contributions to  $Q^{(1)}(f)$  which depend on the behavior of the system far from the point  $a$ . Moreover, if a termination without gapless edge modes were possible everywhere in the parameter space, it would prove that the 1-form  $Q^{(1)}(f)$  is exact via (9.30), and its integral over any cycle would be zero. Thus a nonzero value for periods of  $Q^{(1)}(f)$  is an obstruction for finding a gapped termination which varies continuously with parameters.

Despite this, we will argue below that if we focus on a particular loop in the parameter space and cover it with two semi-circles, it is possible to find a family of gapped terminations for each of the two semi-circles separately. A termination is constructed via a choice of a path in the parameter space and an adiabatic deformation (i.e. a

slow spatial variation) of the original Hamiltonian on a half-line. Since the loop is assumed to be non-contractible, one cannot choose the path in the parameter space so that it depends continuously on the starting point and is defined everywhere on the loop. But it can be chosen continuously for any contractible part of the loop, such as the two semi-circles. We define via this procedure two families of gapped boundary conditions: one on the far right of the lattice (using the first semi-circle) and another one on the far left of the lattice (using the second semi-circle). The modifications made to the family would not affect the value of  $Q^{(1)}(f)$  and one can show that result of integration reduces to the charge of the finite system on the equator of the cycle (i.e. two points separating the semi-circles) which is integrally quantized.

After this rough exposition, let us describe the argument in more detail. Consider a loop  $\phi : S^1 \rightarrow M$  in the parameter space  $M$ . Let  $f(p) = \theta(p)$ . We will show that

$$\int_{S^1} \phi^*(Q^{(1)}(f)) \in \mathbb{Z}. \quad (\text{F.1})$$

There is no topological order for 1d systems and thus all gapped systems of the family are in the same SRE phase. For gapped 1d systems with  $U(1)$  symmetry, there is only one SRE phase: the trivial one. Therefore all systems in the family are in the trivial phase.

Let  $\mathbf{m}_0 \in M$  be some specific system in the trivial phase. That is,  $\mathbf{m}_0$  is some particular gapped Hamiltonian  $H = \sum_p H_p$  where each  $H_p$  acts only on site  $p$ , is  $U(1)$ -invariant, and has a unique ground state. Each point in the image of  $\phi$  can be connected to  $\mathbf{m}_0$  by a continuous path in  $M$ . But since the loop  $\phi$  is assumed to be non-contractible, one cannot choose these paths for all points on  $S^1$  in a continuous fashion. Let us delete the north (resp. south) pole of  $S^1$  and call the resulting subset  $S^1_S$  (resp.  $S^1_N$ ). Since they are contractible, their images can be continuously deformed to  $\mathbf{m}_0$ , and we denote the corresponding homotopies by  $\mathcal{P}_S$  and  $\mathcal{P}_N$ . These are continuous maps from  $[0, 1] \times S^1_S$  to  $M$  and from  $[0, 1] \times S^1_N$  to  $M$ , respectively. They satisfy  $\mathcal{P}_S(0, \lambda) = \phi(\lambda)$  and  $\mathcal{P}_N(0, \lambda) = \phi(\lambda)$  and  $\mathcal{P}_S(1, \lambda) = \mathbf{m}_0$  and  $\mathcal{P}_N(1, \lambda) = \mathbf{m}_0$ . The parameter  $\lambda$  takes values in  $S^1$ .

Denote the Hamiltonian corresponding to a point  $\mathbf{m} \in M$  by  $H(\mathbf{m}) = \sum_p H_p(\mathbf{m})$ . The Hamiltonian corresponding to  $\lambda \in S^1$  is  $H[\lambda] = \sum_p H_p(\phi(\lambda))$ . For a point  $\lambda \in S^1_N$  of the circle we define a new Hamiltonian  $H_p^+[\lambda] = H_p(\mathbf{m}(\lambda, p))$  where we let the parameters of the Hamiltonian to depend adiabatically on the site  $p$  as  $\mathbf{m}(\lambda, p) = \mathcal{P}_N(t_N(p), \lambda)$ . The function  $t_N : \mathbb{R} \rightarrow [0, 1]$  is equal to 1 for

$p \in [2L, +\infty)$ , smoothly interpolates from 1 to 0 in the region  $p \in [L, 2L]$ , and is 0 for  $p \in (-\infty, L]$ . Similarly, we define another local Hamiltonian  $H^-[\lambda]$  for all points  $\lambda \in S_S^1$  as  $H^-[\lambda] = \sum_{p \in \Lambda} H_p(P_S(t_S(p), \lambda))$  where the function  $t_S : \mathbb{R} \rightarrow [0, 1]$  is equal to 1 for  $p \in (-\infty, -2L]$ , smoothly interpolates between 1 to 0 for  $p \in [-2L, -L]$ , and is 0 for  $p \in [-L, +\infty)$ . The last Hamiltonian we define is  $H_p^+[\lambda]$  for all point  $\lambda$  in the intersection  $\in S_N^1 \cap S_S^1$  which coincides with  $H_p[\lambda]$  for  $p \in [-L, L]$ , coincides with  $H_p^+[\lambda]$  for  $p \in [L, +\infty)$ , and coincides with  $H_p^-[\lambda]$  for  $p \in (-\infty, -L]$ .

In order for our argument to work, we need to assume that all these Hamiltonians are gapped for sufficiently large  $L$ . Since the correlation lengths of the Hamiltonians  $H[\lambda]$  are bounded from above and  $L$  can be taken much larger than this bound, this assumption seems very plausible. Let  $Q_+^{(1)}(f)$ ,  $Q_-^{(1)}(f)$  and  $Q_{+-}^{(1)}(f)$  be the 1-forms corresponding to the families  $H^+$ ,  $H^-$  and  $H^{+-}$ , respectively. They are defined on  $S_N^1$ ,  $S_S^1$  and  $S_N^1 \cap S_S^1$ , respectively. We separate the integral over  $S^1$  into a sum of integrals over the north and south semi-circles  $B_+$  and  $B_-$ :

$$\begin{aligned} \int_{S^1} \phi^*(Q^{(1)}(f)) &= \int_{B_+} \phi^*(Q^{(1)}(f)) + \int_{B_-} \phi^*(Q^{(1)}(f)) \\ &= \int_{B_+} Q_+^{(1)}(f) + \int_{B_-} Q_-^{(1)}(f) + O(L^{-\infty}), \end{aligned}$$

where in the last step we replaced  $\phi^*(Q^{(1)}(f))$  with  $Q_{\pm}^{(1)}(f)$ . By our assumption, all three Hamiltonians  $H[\lambda]$ ,  $H^+[\lambda]$ , and  $H^-[\lambda]$  are gapped, and the 1-form  $\phi^*(Q^{(1)}(f))$  is sensitive only to the behavior of the system in a neighborhood of the point  $p = 0$  where the function  $f(p) = \theta(p)$  is non-constant. These three families differ from each other only outside of the interval  $p \in [-L, L]$ , and for large  $L$  the difference between these 1-form is of order  $L^{-\infty}$ .

Next we define  $f_+(p) = \theta(p - 3L)$  and  $f_-(p) = \theta(p + 3L)$  and write

$$\begin{aligned} &\int_{B_+} Q_+^{(1)}(f) + \int_{B_-} Q_-^{(1)}(f) \\ &= \int_{B_+} Q_+^{(1)}(f_+) + \int_{B_-} Q_-^{(1)}(f_-) + \int_{B_+} Q_+^{(1)}(f - f_+) + \int_{B_-} Q_-^{(1)}(f - f_-). \end{aligned} \tag{F.2}$$

Near the point  $p = 3L$  the Hamiltonian  $H^+[\lambda]$  coincides with the constant Hamiltonian  $H(\mathbf{m}_0)$  and therefore the form  $Q_+^{(1)}(f_+)$  as well as its integral over  $B_+$  is of order  $L^{-\infty}$ . Similarly, the integral  $\int_{B_-} Q_-^{(1)}(f_-) = O(L^{-\infty})$ . The remaining two terms contain compactly supported functions  $f_{\pm} - f$ . For any function  $g$  with compact support one can use the equation (9.30) which gives  $Q_{\pm}^{(1)}(g) = T_{\pm}^{(1)}(\delta g) = dT_{\pm}^{(0)}(g)$ . Here



$T_{\pm}^{(0)}$  is the 0-chain with components  $\langle Q_p \rangle$ . It depends on the Hamiltonian through the ground state. Therefore we find

$$\begin{aligned} & \int_{B_+} Q_+^{(1)}(f - f_+) + \int_{B_-} Q_-^{(1)}(f - f_-) \\ &= T_+^{(0)}(\lambda_e; f - f_+) - T_+^{(0)}(\lambda_w; f - f_+) - T_-^{(0)}(\lambda_e; f - f_-) - T_-^{(0)}(\lambda_w; f - f_-), \end{aligned} \quad (\text{F.3})$$

where  $\lambda_e, \lambda_w$  are the two points constituting the common boundary of  $B_+$  and  $B_-$ , and  $T_{\pm}^{(0)}(\lambda)$  are computed for the corresponding Hamiltonians at these points. The signs in this formula are defined by the orientations of the boundaries. Now we can replace  $T_+^{(0)}$  and  $T_-^{(0)}$  with  $T_{+-}^{(0)}$  in both sums. Such a replacement introduces an error of order  $L^{-\infty}$ , because the summands are only sensitive to the the Hamiltonian of the systems in the region where  $H_p^+[\lambda] = H_p^{+-}[\lambda]$  and  $H_p^-[\lambda] = H_p^{+-}[\lambda]$ . This gives

$$\begin{aligned} & T_+^{(0)}(\lambda_e; f - f_+) - T_+^{(0)}(\lambda_w; f - f_+) - T_-^{(0)}(\lambda_e; f - f_-) - T_-^{(0)}(\lambda_w; f - f_-) \\ &= T_{+-}^{(0)}(\lambda_e; f - f_+) - T_{+-}^{(0)}(\lambda_w; f - f_+) - T_{+-}^{(0)}(\lambda_e; f - f_-) - T_{+-}^{(0)}(\lambda_w; f - f_-) \\ &+ O(L^{-\infty}) = -T_{+-}^{(0)}(\lambda_e; f_+ - f_-) - T_{+-}^{(0)}(\lambda_w; f_+ - f_-) + O(L^{-\infty}). \end{aligned} \quad (\text{F.4})$$

Recall that by construction when  $p \notin [-2L, 2L]$  the Hamiltonian  $H_p^{+-}[\lambda] = H_p(\mathbf{m}_0)$  is a collection of decoupled  $U(1)$ -invariant Hamiltonians. In this region  $\langle Q_p \rangle$  is integral and independent of  $\lambda$ , so the contributions of  $\lambda_e$  and  $\lambda_w$  to eq. (F.4) cancel for each  $p$  separately. Thus the sum over  $p$  implicit in eq. (F.4) can be restricted to  $p \in [-2L, 2L]$ . Since the region  $p \in [-2L, 2L]$  is decoupled from the rest of the system, we are dealing with a finite size system of length  $4L$  (or more precisely, two such systems corresponding to points  $\lambda_e$  and  $\lambda_w$ ). Further, the function  $f_+(p) - f_-(p) = \theta(p - 3L) - \theta(p + 3L)$  is equal to  $-1$  in this region, so the evaluation of the chain on a cochain in (F.4) is the difference of ground-state charges of two finite systems corresponding to parameters  $\lambda_w$  and  $\lambda_e$ . This difference is obviously integral. Thus we showed that

$$\int_{S^1} \phi^*(Q^{(1)}(f)) = n + O(L^{-\infty}), \quad n \in \mathbb{Z}. \quad (\text{F.5})$$

Taking the limit  $L \rightarrow \infty$  we conclude that the Thouless charge pump invariant for a gapped 1d system with a unique ground state is integral.

To extend this argument to higher dimensions, we use induction in  $D$ . We need to assume that all systems in the family are in a Short-Range Entangled phase.

This is to be expected, since in the presence of topological order one expects topological invariants to become fractional. Other than that, the inductive step proceeds exactly as for  $D = 1$ . First we reduce to the case of systems in a trivial phase by stacking the family under consideration with a fixed Short-Range Entangled system. Then we cover the parameter space  $S^D$  with two contractible charts,  $S_S^D$  and  $S_N^D$ , and on each of these charts construct a  $D$ -parameter family of Hamiltonians with adiabatically varying parameters which reduces to the trivial Hamiltonian for  $x^D(p) \ll 0$  and  $x^D(p) \gg 0$ , respectively. We also construct a third family  $H_{+-}$  which is defined on  $S_N^D \cap S_S^D$  and interpolates to the trivial Hamiltonian both for  $x^D(p) \gg 0$  and  $x^D(p) \ll 0$ . The same manipulations as for  $D = 1$  show that the invariant  $Q^{(D)}(f_1, \dots, f_D)$  is equal, up to terms of order  $L^{-\infty}$ , to the invariant  $Q^{(D-1)}(f_1, \dots, f_{D-1})$  of a certain family of gapped  $(D - 1)$ -dimensional systems occupying the region  $x^D(p) \in [-2L, 2L]$  in  $\mathbb{R}^D$  and parameterized by the equatorial  $S^{D-1}$ . This concludes the inductive step.