Topological Insulators and Superconductors

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1 Topological Insulators

Quantum mechanics for a single particle in a region $\Omega \subseteq \mathbb{R}^3$ is described by a Hamiltonian of the form:

$$\widehat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

for some potential function V. Here we interpret $\widehat{H}$ as a symmetric operator on $L^2(\Omega)$ and one typically specifies a self-adjoint extension of $\widehat{H}$ (via choosing boundary conditions, for example) based on the physical situation one is trying to describe.

Let's consider the electrons in the interior of a metal (i.e. far away from the boundary). Due to the relative size of the electrons in the matal we can then make the idealization $\Omega = \mathbb{R}^3$. The nuclei of the atoms or molecules forming the metal are typically in the form of a crystal lattice and are many orders of magnitude more massive than the electrons. Thus we will initially begin our investigation by assuming that these nuclei are fixed and simply exert forces on our electrons through the potential V. If $\Lambda \subseteq \mathbb{R}^3$ is the collection of vectors which leave the lattice invariant then we assume that

$$V(x+v) = V(x) \text{ for all } x \in \mathbb{R}^3 \text{ and } v \in \Lambda.$$

Bloch's theorem then tells us that there exists a (generalized) basis of simultaneous eigenfunctions for $\widehat{H}$ and the translation operators T_v, $v \in V$. More precisely, if K is a fundamental domain for the dual lattice of Λ (this is called the **Brioullin zone**) then we have a direct integral decomposition

$$\widehat{H} = \int_K^{\oplus} \widehat{H}(k)dk, \quad L^2(\mathbb{R}^3)^\Gamma = \int_K^{\oplus} \mathcal{H}(k)dk$$

where $\mathcal{H}(k)$ is the Hilbert space of definite-momentum k-states, $\widehat{H}(k)$ is the action of $\widehat{H}$ on this Hilbert space and the above decompositions are equivariant with respect to T_v for $v \in \Lambda$. The key point is that:

$\widehat{H}(k)$ typically has discrete spectrum on $\mathcal{H}(k)$.

We write out its orthonormal eigenbasis as:

$$\widehat{H}(k)u_n(k) = E_n(k)u_n(k).$$

Before continuing, there are two important comments we should make:

1. In real life, there is more than one electron in a material like this. Also, electrons have spin and this should be taken into account in the Hamiltonian. Nevertheless, one still gets these decompositions of $\widehat{H}$ into $\widehat{H}(k)$ for these more general composite systems involving spin.

2. Instead of considering quantum states in the usual way (as wavefunctions) we will consider *statistical* quantum states. One can think of these as a probability distribution on the $\widehat{H}(k)$-eigenbasis for each k. Thus, when computing the expectation of a quantum observable with respect to a statistical state, one obtains a probability distribution as opposed to a number.

Often the state one is interested in is the one arising from the probability distribution $\rho(k)$ on $\mathbb{R}$ which maximizes the **Shanon entropy** of the distribution

$$\mathrm{Tr}(\rho(\widehat{H}(k))dE_{\widehat{H}(k)})$$

given certain constraints. Here $dE_{\widehat{H}(k)}$ is the spectral measure of $\widehat{H}(k)$. Since $\widehat{H}(k)$ has discrete spectrum, we view $\rho(k)$ as a sum of Dirac delta functions:

$$\rho(k) = \sum_{n=0}^{\infty} \rho_n(k)\delta_{E_n(k)}$$

and computing $\rho(k)$ becomes a standard constrained optimization problem. For example, if the total energy is fixed then we have two constraints (the second being that it is a probability measure) and the Lagrange multiplier $\beta = \beta(E)$ corresponding to the energy constraint is typically related to *temperature*. Often the resulting $\rho(k)$ is a Gibbs or Boltzmann distribution. A system which is in such a Shanon-entropy-maximizing state is said to be in **equilibrium**.

In general composite systems, k is refered to as the **crystal momentum** and is thought of as an external parameter for the statistical quantum mechanical system described by $\widehat{H}(k)$. The rate of change in total expected energy as a function of k decomposes as:

$$d\langle E(k)\rangle := d\,\mathrm{Tr}(\rho(\widehat{H})\widehat{H}(k)) = \frac{\partial\langle E(k)\rangle}{\partial\rho}d\rho + \frac{\partial\langle E(k)\rangle}{\partial\widehat{H}}d\widehat{H} =: \delta Q + \delta W$$

where δQ is the change in expected total energy due to the change in ρ since we assume we are in equilibrium for each k, and δW is the change in expected total energy due to the change in distribution of the eigenstates and eigenvalues of $\widehat{H}(k)$. δQ is refered to as the differential **heat** and δW as the differential **work**. These are all differential one forms on the space of parameters: $k \in K$, the Brioullin zone.

A path γ in K is called **adiabatic** if $\delta Q|_\gamma = 0$ (more precisely, δQ pulls back to zero along γ). One typically is only interested in the first few, say n, energy levels since with respect to these equilibrium distributions the remaining are incredibly unlikely to occur. Projecting down to this finite dimensional subspace we can unitarily diagonalize our Hamiltonian to get:

$$U^\dagger(k)\widehat{H}(k)U(k) = \begin{pmatrix} E_1(k) & & \\ & \ddots & \\ & & E_n(k) \end{pmatrix} \text{ for each } k \in K.$$

In this way we get a map

$$U : K \to \mathrm{U}(n).$$

The systems we will consider will have a *band gap* with Fermi energy E_F and at one fixed k we order the energy levels so that $E_1(k), \ldots, E_m(k) > E_F$ (these energy levels are considered to be *empty*) and $E_{m+1}(k), \ldots, E_n(k) < E_F$ (these energy levels are considered to be *occupied*). So the adiabatic deformations of the system we're allowed to consider are only those that preserve this band gap. As such, we can perform an adiabatic deformation

$$\gamma : [0, a] \to K$$

such that

$$U^\dagger(\gamma(a))\widehat{H}(\gamma(a))U(\gamma(a)) = \begin{pmatrix} 1_{m\times m} & 0 \\ 0 & -1_{(n-m)\times(n-m)} \end{pmatrix}.$$

The family of unitary matrices $U^\dagger(\gamma(s))$ at $\gamma(s) \in K$ describes how the eigenstates twist under this deformation since at each s they provide the diagonalization of the Hamiltonian $\widehat{H}(\gamma(s))$. Letting K° denote the interior of the Brioullin zone, we can combine these deformations together to get:

$$\gamma : [0, a] \times K^\circ \to K^\circ$$

with $\gamma(0, k) = k$ and $s \mapsto \gamma(s, k)$ our above adiabatic deformation for starting k. (TODO: do I want to look at maps from K° with certain conditions on ∂K or do I want to look at maps from ∂K?) (TODO: explain the $\mathrm{U}(m) \times \mathrm{U}(n-m)$ gauge redundancy)

As such, we obtain homotopy classes of maps (TODO: should I use ∂K below or a one point compactification of K°?):

$$\partial K \to \mathrm{U}(n)/\mathrm{U}(m) \times \mathrm{U}(n-m).$$

In dimension 3, ∂K is homeomorphic to S^2 meanwhile in dimension d, ∂K is homeomorphic to S^{d-1}.

Key Things to Learn:
The homotopy groups $\pi_d(\mathrm{U}(n)/\mathrm{U}(m) \times \mathrm{U}(n-m))$ classify certain statistical quantum mechanical states called **quantum Hall states** and are responsible for the experimentally observed **quantum Hall effect**. One goal here would be to:

1. Compute $\pi_d(\mathrm{U}(n)/\mathrm{U}(m) \times \mathrm{U}(n-m))$ for small values of d.
2. Consider the **Berry connections** $\langle u_n(k)|\partial_k|u_n(k)\rangle$ and show how their first Chern numbers correspond to the homotopy classes one obtains above.

3. Obtain realistic quantum Hall states for so-called **topological insulators** with non-zero Chern number by incorporating the spin of the electrons and the $\mathbb{Z}/2$-index of the spin structure.

2 Topological Superconductors

Here one has a similar setup to the previous section. Recall from page 2 the expression

$$d\langle E(k)\rangle = \delta Q + \delta W.$$

This definition of heat and work is often called the first law of thermodynamics and in a general thermodynamical system the left hand side is denoted by dU with the (classical) observable U called the **internal energy** of the system. Also, recall that δW is the differential one form one the space of external parameters of the system whose integrals over curves represents the work done by the system while remaining in equilibrium while traversing that curve. Similarly δQ is the differential 1-form governing *heat*, which is the change in total energy due to the change in equilibrium probability distribution given total energy.

Now, let's recall how this probability distribution ρ was obtained. For simplicitly, let's view ρ as a discrete probability distribution $\rho_1, \rho_2, \ldots$. Its Shanon entropy is then:

$$S = -\sum \rho_j \log \rho_j$$

and this is the function we are maximizing via the Lagrange multipliers method. One of our constraints was

$$\sum \rho_j E_j = E$$

and our other constraint is $\sum \rho_j = 1$. The Lagrange multipliers method gives us constants α, β and equations:

$$-(\log(\rho_j)) - 1 = \alpha - \beta E_j$$

so that

$$\rho_j = \exp(-1-\alpha)\exp(-\beta E_j)$$

and therefore our $\sum \rho_j = 1$ constraint yields:

$$\exp(1+\alpha) = \sum_j \exp(-\beta E_j).$$

So we're left with:

$$E = \left(\sum_j \exp(-\beta E_j)\right)^{-1} \sum_k E_k \exp(-\beta E_k)$$

We typically denote:

$$Z(\beta) := \sum_j \exp(-\beta E_j)$$

so that

$$E = -\frac{1}{Z} Z'(\beta) = -\frac{d}{d\beta} \log(Z).$$

We also have:

$$\begin{aligned} S &= -\frac{1}{Z}\sum_j \exp(-\beta E_j)\left(-\log(Z) - \beta E_j\right) \\ &= \log(Z) + \frac{\beta}{Z}\sum_j E_j \exp(-\beta E_j) \\ &= \log(Z) + \beta E. \end{aligned}$$

So we have:

$$E = \frac{1}{\beta}(S - \log(Z)).$$

This implies that $\log(Z)$ satisfies the differential equation:

$$\left(-\beta\frac{d}{d\beta} + 1\right)\log(Z) = S.$$

Hm. Perhaps the proper way to do this is as follows:

- Temperature is the canonically conjugate observable to entropy (and I'm pretty sure entropy is the same as Shanon entropy).
- We define the **Hemholtz energy** or **free energy** F to be the Legendre transform of the internal energy U. In U, entropy S is interpreted as an independent variable (so dS appears in expressions for dU) while in F temperature T is interpreted as an independent variable.