↓ Lecture 9 [15.05.25]

5 | Action of TRS on Fock space:

Now we generalize these *single-particle* concepts to the *many-body* Hilbert space and Hamiltonian:

i | $\triangleleft$ Representation $\mathcal{T}_U$ of TRS on the fermionic Fock space $\hat{\mathcal{H}}$:

Definition: Time-reversal symmetry

Time-reversal $\mathcal{T}_U$ is antiunitary, $\mathcal{T}_U i \mathcal{T}_U^{-1} := -i$, and acts on fermion modes as

$$\mathcal{T}_U c_{i\alpha} \mathcal{T}_U^{-1} := \sum_\beta U^\dagger_{\alpha\beta} c_{i\beta} \quad \text{and} \quad \mathcal{T}_U c^\dagger_{i\alpha} \mathcal{T}_U^{-1} := \sum_\beta \underbrace{(U^\dagger_{\alpha\beta})^*}_{U_{\beta\alpha}} c^\dagger_{i\beta}\,. \tag{2.25}$$

Note that we assume that time-reversal only mixes *internal* degrees of freedom (α,β) but not *spatial* ones (i). This restriction complies with our everyday experience and simplifies the following discussion. Furthermore, we assume that TRS acts on every site in the same way (which is reasonable for translational invariant systems).

ii | Let us check that this definition of TRS on $\hat{\mathcal{H}}$ is consistent with our definition on $\mathcal{H}$ above:

$$\mathcal{T}_U \hat{H} \mathcal{T}_U^{-1} = \sum_{i\alpha',j\beta'} c^\dagger_{i\alpha'} \sum_{\alpha,\beta} \left[U_{\alpha'\alpha} H^*_{i\alpha,j\beta} U^\dagger_{\beta\beta'}\right] c_{j\beta'} \tag{2.26a}$$

$$\stackrel{!}{=} \sum_{i\alpha',j\beta'} c^\dagger_{i\alpha'} H_{i\alpha',j\beta'} c_{j\beta'} = \hat{H} \tag{2.26b}$$

$\stackrel{\circ}{\rightarrow}$ [use the form Eq. (2.17)]

$$\left[\hat{H},\mathcal{T}_U\right] = 0 \quad \Leftrightarrow \quad T_U H T_U^{-1} = H$$
$$\text{with} \quad T_U = \bar{U}\mathcal{K} \quad \text{where} \quad \bar{U} := \oplus_i U_i \quad \text{with} \quad U_i \equiv U \tag{2.27}$$

This is the form of TRS in the SP Hilbert space that we discussed earlier (where the role of U is now played by $\bar{U}$ since we have single-particle states on each site).

Note that $\bar{U}$ is a unitary $NM \times NM$-matrix whereas U is a unitary $M \times M$ matrix.

iii | We want to consider *translation invariant* systems →

$$\mathcal{T}_U c_{\boldsymbol{k}\alpha} \mathcal{T}_U^{-1} \stackrel{2.6}{=} \frac{1}{\sqrt{N}} \sum_i e^{-i\boldsymbol{x}_i\boldsymbol{k}} \sum_\beta U^\dagger_{\alpha\beta} c_{i\beta} = \sum_\beta U^\dagger_{\alpha\beta} c_{-\boldsymbol{k}\beta} \tag{2.28}$$

→ $\mathcal{T}_U$ inverts momenta & mixes internal DOFs

iv | For a time-reversal symmetric many-body Hamiltonian we find:

$$\mathcal{T}_U \hat{H} \mathcal{T}_U^{-1} \stackrel{2.5}{=} \sum_{\boldsymbol{k};\alpha',\beta'} c^\dagger_{-\boldsymbol{k}\alpha'} \sum_{\alpha,\beta} \left[U_{\alpha'\alpha} H^*_{\alpha\beta}(\boldsymbol{k}) U^\dagger_{\beta\beta'}\right] c_{-\boldsymbol{k}\beta'} \tag{2.29a}$$

$$\stackrel{!}{=} \sum_{\boldsymbol{k};\alpha',\beta'} c^\dagger_{-\boldsymbol{k}\alpha'} H_{\alpha'\beta'}(-\boldsymbol{k}) c_{-\boldsymbol{k}\beta'} = \hat{H} \tag{2.29b}$$

In the last equation we substituted $\boldsymbol{k} \to -\boldsymbol{k}$.

v | Thus we find a constraint on the Bloch Hamiltonians:

$$\left[\hat{H}, \mathcal{T}_U\right] = 0 \quad \Leftrightarrow \quad \tilde{T}_U H(\boldsymbol{k}) \tilde{T}_U^{-1} = H(-\boldsymbol{k}) \quad \text{with} \quad \tilde{T}_U = U\mathcal{K} \tag{2.30}$$

Note that $\tilde{T}_U$ maps between the mode spaces $\mathcal{H}(\boldsymbol{k})$ and $\mathcal{H}(-\boldsymbol{k})$ since TRS inverts momenta!

Summary:

Time-reversal invariance can be expressed equivalently as follows:

$$\left[\hat{H}, \mathcal{T}_U\right] = 0 \quad \Leftrightarrow \quad T_U H T_U^{-1} = H \tag{2.31a}$$

$$\Leftrightarrow \quad \bar{U} H^* \bar{U}^\dagger = H \tag{2.31b}$$

$$\Leftrightarrow \quad \tilde{T}_U H(\boldsymbol{k}) \tilde{T}_U^{-1} = H(-\boldsymbol{k}) \tag{2.31c}$$

$$\Leftrightarrow \quad U H^*(\boldsymbol{k}) U^\dagger = H(-\boldsymbol{k}) \tag{2.31d}$$

The last two lines are only defined if the system is translation invariant, the first two are generic.

- In words: A (non-interacting) many-body Hamiltonian $\hat{H}$ is time-reversal invariant if its single-particle Hamiltonian H is unitarily equivalent to its complex conjugate.
- Note that often the formal distinction between T_U and $\tilde{T}_U$ is not made in the literature (similarly for $\bar{U}$ and U) and one simply writes T_U (or even just T) for both.
- Conditions like $\bar{U} H^* \bar{U}^\dagger = H$ are sometimes referred to ↑ *reality conditions* on the Hamiltonian [92]. We will encounter another example when we discuss particle-hole symmetry later in this course.

Furthermore:

$$T_U^2 = +\mathbb{1} \quad \Leftrightarrow \quad \tilde{T}_U^2 = +\mathbb{1} \quad \Leftrightarrow \quad \mathcal{T}_U^2 \mathrel{\hat{=}} +\mathbb{1} \tag{2.32a}$$

$$T_U^2 = -\mathbb{1} \quad \Leftrightarrow \quad \tilde{T}_U^2 = -\mathbb{1} \quad \Leftrightarrow \quad \mathcal{T}_U^2 \mathrel{\hat{=}} (-\mathbb{1})^{\hat{N}} \tag{2.32b}$$

$\hat{N} := \sum_{i\alpha} c_{i\alpha}^\dagger c_{i\alpha}$: total fermion number operator

$\mathcal{P} := (-1)^{\hat{N}}$ is the fermion *parity operator*.

¡! Note that for $T_U^2 = -\mathbb{1}$ it is $\mathcal{T}_U^2 = (-\mathbb{1})^{\hat{N}}$ and *not* $\mathcal{T}_U^2 \mathrel{\not\hat{=}} -\mathbb{1}$, i.e., the representation depends on the *fermion parity sector*. This makes sense: If $T_U^2 = -\mathbb{1}$, the fermions have half-integer spins (← *above*). According the rules of ↓ *angular momentum addition*, an even (odd) number of such particles have integer (half-integer) *total* angular momentum, consistent with $\mathcal{T}_U^2 = +\mathbb{1}$ (N even) and $\mathcal{T}_U^2 = -\mathbb{1}$ (N odd).

6 | Consequence of TRS for the Spectrum:

$$H(\boldsymbol{k})|u_{n\boldsymbol{k}}\rangle = E_n(\boldsymbol{k})|u_{n\boldsymbol{k}}\rangle \tag{2.33a}$$

$$\overset{(2.31d)}{\Longrightarrow} \quad H(-\boldsymbol{k}) U |u_{n\boldsymbol{k}}\rangle^* = E_n(\boldsymbol{k}) U |u_{n\boldsymbol{k}}\rangle^* \tag{2.33b}$$

→ Eigenstate $U|u_{n\boldsymbol{k}}\rangle^*$ of $H(-\boldsymbol{k})$ has *same* energy $E_n(\boldsymbol{k})$ as eigenstate $|u_{n\boldsymbol{k}}\rangle$ of $H(\boldsymbol{k})$

→ Inversion-symmetric band structure

This means that for TRI systems, one half of the BZ is determined by the other half via $\tilde{T}_U$. This motivates the introduction of a so called → *effective Brillouin zone (EBZ)* (essentially "half" the original BZ) which has the topology of a cylinder [100].

7 | Consequence of TRS for the Chern number: [Remember: $H(\boldsymbol{k}) = \varepsilon(\boldsymbol{k})\,\mathbb{1} + \vec{d}(\boldsymbol{k})\cdot\vec{\sigma}$]

- ⊲ Two bands from pseudo-spin-$\frac{1}{2}$: $\tilde{T}_0 = \mathcal{K}$

  "Pseudo-spin-$\frac{1}{2}$" refers to degrees of freedom that are not related to angular momentum and therefore remain invariant under time reversal (e.g. sublattice degrees of freedom).

$$H^*(\boldsymbol{k}) = H(-\boldsymbol{k}) \quad \overset{(2.8)}{\Leftrightarrow} \quad \begin{cases} d_{x,z}(\boldsymbol{k}) = d_{x,z}(-\boldsymbol{k}) \\ d_y(\boldsymbol{k}) = -d_y(-\boldsymbol{k}) \end{cases} \tag{2.34}$$

  Note that Eq. (2.34) implies $|\vec{d}(\boldsymbol{k})| = |\vec{d}(-\boldsymbol{k})|$ such that $\hat{d}_{x,z}(\boldsymbol{k}) = \hat{d}_{x,z}(-\boldsymbol{k})$ and $\hat{d}_y(\boldsymbol{k}) = -\hat{d}_y(-\boldsymbol{k})$ follows also for the *normalized* Bloch vector.

- ⊲ Two bands from real spin-$\frac{1}{2}$: $\tilde{T}_{\frac{1}{2}} = \sigma^y\mathcal{K}$

$$\sigma^y H^*(\boldsymbol{k})\sigma^y = H(-\boldsymbol{k}) \quad \overset{(2.8)}{\Leftrightarrow} \quad \vec{d}(\boldsymbol{k}) = -\vec{d}(-\boldsymbol{k}) \tag{2.35}$$

  Again it follows also for the *normalized* Bloch vector $\hat{d}(\boldsymbol{k}) = -\hat{d}(-\boldsymbol{k})$.

Both cases →

$$C \overset{2.13}{=} -\frac{1}{4\pi}\int_{-\pi}^{\pi} \mathrm{d}k_x \int_{-\pi}^{\pi} \mathrm{d}k_y \epsilon_{ijk}\hat{d}_i(\boldsymbol{k})\tilde{\partial}_x\hat{d}_j(\boldsymbol{k})\tilde{\partial}_y\hat{d}_k(\boldsymbol{k}) \overset{\circ}{=} 0 \tag{2.36}$$

This follows since $\hat{d}_i(\boldsymbol{k})\tilde{\partial}_x\hat{d}_j(\boldsymbol{k})\tilde{\partial}_y\hat{d}_k(\boldsymbol{k})$ is *antisymmetric* for both representations if i, j, k are pairwise distinct (which is enforced by ϵ_{ijk}). →

> **¡! Important**
>
> Systems with Chern bands must *break* time-reversal symmetry.

This is true in general, i.e., even for models with more than two bands.

- Note that this is completely consistent with the IQHE (or the Hofstadter model) where we found Chern bands and the *magnetic field* breaks TRS.
- This also makes sense from another perspective: Conductivity transforms as $\sigma \mapsto -\sigma$ under time-reversal since $\vec{J} = \sigma\vec{E}$ and $\vec{J} \mapsto -\vec{J}$ but $\vec{E} \mapsto \vec{E}$ (↓ *Maxwell equations*). Thus in a *time-reversal invariant* system it must be $\sigma = \sigma_a + \sigma_s = 0$. Note that $\sigma_a \neq 0$ indeed requires a magnetic field (which breaks time-reversal symmetry) and $\sigma_s \neq 0$ requires dissipation (recall the ← *Drude model*) and breaks time-reversal symmetry because of entropy production.
- This is a restriction (and a hint) for the construction of a Chern insulator.

2.1.3. Dirac fermions

As last preliminary step, we introduce a class of free fermion Hamiltonians *in the continuum* that is very useful to understand topological bands; we will use it as a starting point to construct our first Chern insulator *on the lattice*:

1 | ⊲ ↓ *Dirac equation* in 2D: ($\hbar = 1$)

$$H_D\Psi = \left(\beta m + \sum_{n=1}^{2} \alpha_n p_n\right)\Psi = i\partial_t\Psi \tag{2.37}$$

For a motivation/derivation in 3D see my script on ↑ *Quantum Field Theory* [101, Section 3.1].

with

- $\alpha_1, \alpha_2, \beta$: Hermitian matrices
- $\alpha_1^2 = \alpha_2^2 = \beta^2 = \mathbb{1}$
- $\{\alpha_1, \alpha_2\} = \{\beta, \alpha_1\} = \{\beta, \alpha_2\} = 0$

→ Solution: $\alpha_1 = \sigma^x, \alpha_2 = \sigma^y, \beta = \sigma^z$ with 2-dimensional spinor $\Psi = \Psi(t, \boldsymbol{x})$

In 3D there is a *third* α-matrix and the algebra can only be solved by 4×4-matrices (↓ *γ-matrices*).

2 | Fourier transform of H_D ($\boldsymbol{k} \in \mathbb{R}^2$):

Note that the spinor $\Psi(t, \boldsymbol{x})$ lives on continuous space $\boldsymbol{x} \in \mathbb{R}^2$, not on a lattice!

$$H_D(\boldsymbol{k}) = k_x\sigma^x + k_y\sigma^y + m\sigma^z = \vec{d}(\boldsymbol{k})\cdot\vec{\sigma} \quad \text{with} \quad \vec{d}(\boldsymbol{k}) = \begin{pmatrix} k_x \\ k_y \\ m \end{pmatrix} \tag{2.38}$$

Here we used that in Fourier space the momentum operator $p_n = -i\partial_n$ is simply k_n.

Fermions in condensed matter physics that are (approximately) described by a 2-band *Bloch Hamiltonian* of the form Eq. (2.38) are therefore known as ⁂ *Dirac fermions* (this also refers to more general Hamiltonians linear in $\boldsymbol{k}$, → *below*).

→ Spectrum:

$$E_\pm(\boldsymbol{k}) \overset{2.9}{=} \pm|\vec{d}(\boldsymbol{k})| = \pm\sqrt{\boldsymbol{k}^2 + m^2} \tag{2.39}$$

→ Gapped if $m \neq 0$

This is where the name "mass gap" comes from.

3 | Time-reversal symmetry:

- $\tilde{T}_0 = \mathcal{K} \to d_x(\boldsymbol{k}) \overset{!}{=} d_x(-\boldsymbol{k}) \to H_D$ not TRI!
- $\tilde{T}_{\frac{1}{2}} = \sigma^y\mathcal{K} \to d_z(\boldsymbol{k}) \overset{!}{=} -d_z(-\boldsymbol{k}) \to H_D$ not TRI for $m \neq 0$!

→ H_D is only TRI for $m = 0$, but there the gap closes anyway!

→ Non-zero Chern number *possible* ...

4 | Berry curvature: (of the lower band)

$$\mathcal{F}_{xy}(\boldsymbol{k}) \overset{\circ}{=} \frac{m}{2(\boldsymbol{k}^2 + m^2)^{3/2}} \tag{2.40}$$

Proof: ➲ Problemset 5

Use the form Eq. (2.13) to show this and remember that here momentum space is not a torus (Brillouin zone) but $\mathbb{R}^2$ (→ *next*).

5 | "Chern number": (➲ Problemset 5)

$$C \overset{2.13}{=} -\frac{1}{2\pi}\int_{\mathbb{R}^2} \mathcal{F}_{xy}(\boldsymbol{k})\,\mathrm{d}^2k = -\int_0^\infty \frac{mk}{2(k^2+m^2)^{3/2}}\mathrm{d}k \triangleq -\frac{\operatorname{sign}(m)}{2} \tag{2.41}$$

Why $C \notin \mathbb{Z}$?

The quantization of C is based on Stokes theorem (← Section 1.3.1) which is only valid for integrations over *compact* manifolds (sphere, torus). Here, however, we integrate over the non-compact $\mathbb{R}^2$ instead, so we cannot expect C to be quantized.

Remember the geometric interpretation of the Chern number for two-band models as the number of times the sphere S^2 is covered by the Bloch vector when sweeping over momentum space (← Section 2.1.1). When you are on a *non-compact* space like $\mathbb{R}^2$, you can start at one point where the Bloch vector points, say, at the north pole of S^2. Then you let the vector continuously move towards the equator of S^2 for $|\boldsymbol{k}| \to \infty$ where the direction on S^2 is determined by the direction of $\boldsymbol{k}$ in $\mathbb{R}^2$. This produces a *continuous* function $\hat{d}(\boldsymbol{k})$ that wraps S^2 only "half." Convince yourself that this construction necessarily fails on a *compact* momentum space like S^2 or T^2.

Eq. (2.41) → Change from $m < 0$ to $m > 0 \Rightarrow$ Change of Chern number $\Delta C = -1$

6 | ∢ 2-Band lattice model $H_\Gamma(\boldsymbol{k}) = \varepsilon_\Gamma(\boldsymbol{k})\mathbb{1} + \vec{d}_\Gamma(\boldsymbol{k})\cdot\vec{\sigma}$

Γ: parameters of the model

We say that $\boldsymbol{K} \in T^2$ is a ⁂ *Dirac point* if

$$H_\Gamma(\boldsymbol{K}+\boldsymbol{k}) = v_F\left[k_x\sigma^x + k_y\sigma^y + v_F m_\Gamma\,\sigma^z\right] + \mathcal{O}(k^2) \tag{2.42}$$

$m_\Gamma = 0 \to$ Band structure at $\boldsymbol{K}$: $E_\pm(\boldsymbol{K}+\boldsymbol{k}) = \pm v_F|\boldsymbol{k}| \to$ ⁂ *Dirac cone*

v_F: Fermi velocity (corresponds to the speed of light c in the Dirac equation)

In the following we set always $|v_F| = 1$.

Dirac points are interesting because they harbour "half a (anti-)skyrmion" (depending on the sign of m_Γ). When the sign of m_Γ changes at a gap closing (by varying Γ), this can change the (quantized) Chern number of the bands by ± 1 (as discussed ← *above*).

2.2. The Qi-Wu-Zhang Model

Historically, the Haldane model (see → *below*) was the first Chern insulator. However, it is not the *simplest* one (at least its momentum space representation is rather complex due to the honeycomb lattice). Later, QI, WU and ZHANG introduced a simpler model on the square lattice [102] which we will discuss first. "Simpler" refers here to its representation in momentum space – the real-space representation of the QWZ model is rather unintuitive.

1 | Idea: "Regularize" Dirac Hamiltonian on a lattice →

$\triangleleft\ H_{\text{QWZ}}(\boldsymbol{k}) = \vec{d}(\boldsymbol{k}) \cdot \vec{\sigma}$ with

$$d_x := \sin(k_x) \qquad = k_x + \mathcal{O}(k^2) \tag{2.43a}$$

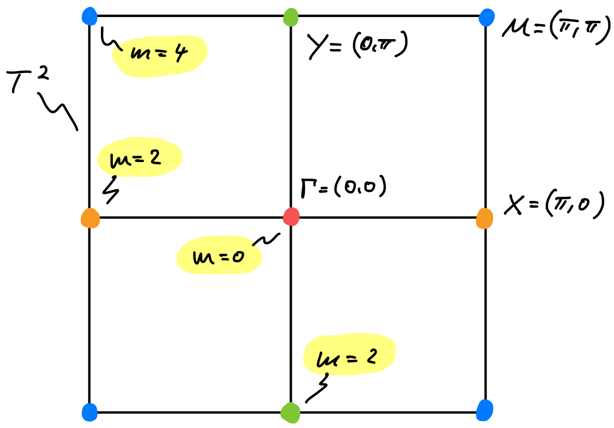
$$d_y := \sin(k_y) \qquad = k_y + \mathcal{O}(k^2) \tag{2.43b}$$

$$d_z := -m + 2 - \cos(k_x) - \cos(k_y) = -m + \mathcal{O}(k^2) \tag{2.43c}$$

$m \in \mathbb{R}$: only parameter of the theory

- The inverted sign of m is convention and motivated by the results (→ *below*).
- The two bands are interpreted as spin-$\frac{1}{2}$ degrees of freedom of fermions hopping on a square lattice (→ *below*).

2 | Spectrum: $E_\pm(\boldsymbol{k}) = \pm|\vec{d}(\boldsymbol{k})| \neq 0$ for all $\boldsymbol{k} \in T^2 \setminus \{\boldsymbol{\Gamma}, \boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{M}\}$ with



In the sketch we indicate for which parameter m the gap *closes* at which point in the BZ. This follows directly by inspection of d_z in Eq. (2.43c).