Dr. Nicolai Lang
Institute for Theoretical Physics III, University of Stuttgart

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Problem 6.1: Time-reversal for spins and Kramers' theorem

[**Oral** | 7 pt(s)]

ID: ex_kramers_theorem:tqp25

Learning objective

In Problem 1.2 you derived Wigner's theorem which states that physical symmetries are represented by unitary or antiunitary operators on the Hilbert space. Kramers' theorem (Hans Kramers, 1930) applies to systems with an *antiunitary time-reversal symmetry*: It guarantees the degeneracy of eigenenergies for time-reversal invariant Hamiltonians of *half-integer total angular momentum*. This has consequences in many situations, e.g., for atomic physics where it explains the degeneracy of energy levels with half-integer total angular momentum in the absence of magnetic fields. In this exercise, you show how time-reversal acts on systems with arbitrary spin and subsequently prove Kramers' theorem.

In the lecture, you showed that time-reversal T is represented on the Hilbert space by an *antiunitary* operator $T_U = U\mathcal{K}$ that squares to plus *or* minus one. Here, $\mathcal{K}$ denotes complex conjugation (for some fixed basis) and U is a unitary operator that determines the representation on the Hilbert space.

Kramers' theorem ascertains that every energy level of a time-reversal invariant system (that is $[H, T_U] = 0$) with a time-reversal symmetry that squares to *minus* one ($T_U^2 = -\mathbb{1}$) possesses *even* degeneracy (i.e. is *at least* two-fold degenerate). This two-fold degeneracy is due to degenerate *Kramers' pairs* $\{|\Psi\rangle\,,\ T_U\,|\Psi\rangle\}$.

A physically reasonable time-reversal operation should *invert* the direction of angular momentum,

$$T_U \vec{J} T_U^{-1} = -\vec{J} \qquad \Leftrightarrow \qquad \{T_U, \vec{J}\} = 0\,, \tag{1}$$

that is, its representation T_U should *anticommute* with every component J_i for $i \in \{x, y, z\}$ of the angular momentum operator. In the following, we consider the angular momentum eigenbasis $|j, m\rangle$ defined by $J^2\,|j, m\rangle = j(j+1)\,|j, m\rangle$ and $J^z\,|j, m\rangle = m\,|j, m\rangle$ (we assume $\hbar = 1$).

In the first part of this exercise, you derive the representations U that satisfy Eq. (1), and in the second part you prove Kramers' theorem:

a) Show that condition (1) *uniquely* (up to a phase factor) defines **2**pt(s)

$$T_U = \sum_m (-1)^{j-m}\,|j, -m\rangle\,\langle j, m|\,\mathcal{K} \tag{2}$$

by explicitly calculating its matrix elements on the angular momentum Hilbert space. Here $\mathcal{K}$ denotes complex conjugation in the angular momentum eigenbasis $|j, m\rangle$.

Why is U unitary?

Hint: What is the action of J^2, J^z and the ladder operators $J^\pm \equiv J^x \pm iJ^y$ on $T_U\,|j, m\rangle$?

b) Show that $T_U = e^{i\pi J^y}\mathcal{K}$ satisfies condition (1). Here, $\mathcal{K}$ denotes complex conjugation in the angular momentum eigenbasis $|j, m\rangle$. **2**pt(s)

Why is $U = e^{i\pi J^y}$ unitary?

What do you obtain for the cases $j = 0$ and $j = \frac{1}{2}$? Compare this with T_U derived in subtask a).

Hint: Show that the ladder operator $J^{\pm} \equiv J^x \pm J^y$ are real matrices in the angular momentum eigenbasis.

c) Show that $T_U^2 = (-1)^{2j} \times \mathbb{1}$ for angular momentum $j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \ldots\}$. **1**pt(s)

What do you obtain for half-integer angular momenta?

Is this consistent with your physical intuition that applying time-reversal twice "does nothing?"

d) Finally: Prove Kramers' theorem. **2**pt(s)

What can you conclude for the degeneracy of electronic states in atoms with half-integer total angular momentum?

Problem 6.2: Edge modes from Dirac Hamiltonians

[**Written** | 5 pt(s)]

ID: ex_edge_modes_dirac_hamiltonians:tqp25

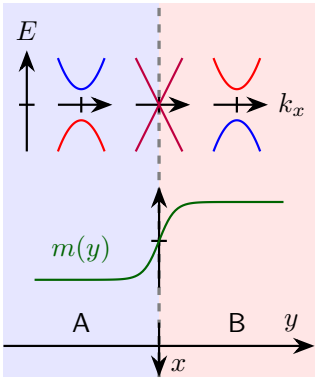
Learning objective

In the lecture, we argued that both the Chern insulator and the $\mathbb{Z}_2$ topological insulator feature gapless edge modes on boundaries of the system. The phenomenon that a topologically non-trivial bulk entails gapless modes on the surface is known as *bulk-boundary correspondence*. In this exercise, you show that the emergence of these gapless edge-localized modes already follows from the low-energy description in terms of Dirac Hamiltonians.

Consider an infinite 2D system that is effectively described by the *Dirac Hamiltonian* (in real space)

$$H_{\mathrm{D}} = -i\nabla \cdot \vec{\sigma} + m(y)\,\sigma^z = \begin{pmatrix} m(y) & -i\partial_x - \partial_y \\ -i\partial_x + \partial_y & -m(y) \end{pmatrix} \tag{3}$$

with a y-dependent Dirac mass term $m(y)$. Here $\vec{\sigma} \equiv (\sigma^x, \sigma^y)^T$ and σ^i for $i \in \{x, y, z\}$ are the Pauli matrices.
The mass term varies continuously and is negative (positive) in the left (right) half-plane. It vanishes on the x-axis which becomes the boundary that separates the two gapped systems A and B. This functional dependence $m(y)$ is depicted in the sketch on the right.



In Problem 5.3 you derived the expression

$$C = -\frac{\mathrm{sign}[m(y)]}{2} \tag{4}$$

to calculate the *change* in the Chern numbers for a Dirac Hamiltonian. Consequently, because of the sign change of the Dirac mass at the boundary, the Chern numbers of the two materials A and B must differ by $\Delta C = \pm 1$. One can think of material B as a *trivial insulator* with $C = 0$ and of material A as a *Chern insulator* with $C = 1$. Both insulators share an interface along the x-axis.

a) Use the *Hadamard transform* **4**pt(s)

$$H_{\mathrm{D}} \mapsto U_H H_{\mathrm{D}} U_H^\dagger \qquad \text{with} \qquad U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{5}$$

to solve the time-independent Schrödinger equation $H_{\mathrm{D}}\Psi(x,y) = E\Psi(x,y)$ with the two-component spinor $\Psi(x,y)$ and determine a solution which is normalizable in y-direction.

Where is this solution localized in y-direction?

Hint: Make a *product ansatz* to separate the PDEs after the Hadamard transform. You may set the separation constants to zero, as this excludes only solutions which are wave-like (i.e. not normalizable) in y-direction. Use the behavior of $m(y)$ sketched above to select a unique, non-diverging solution.

b) What is the spectrum $E(k_x)$ of the solution? **1**pt(s)

What is the group velocity along the boundary?

Problem 6.3: Edge modes of the Kane-Mele model (Numerics) [**Oral** | 5 (+6 bonus) pt(s)]

ID: ex_edge_modes_kane_mele_model:tqp25

Learning objective

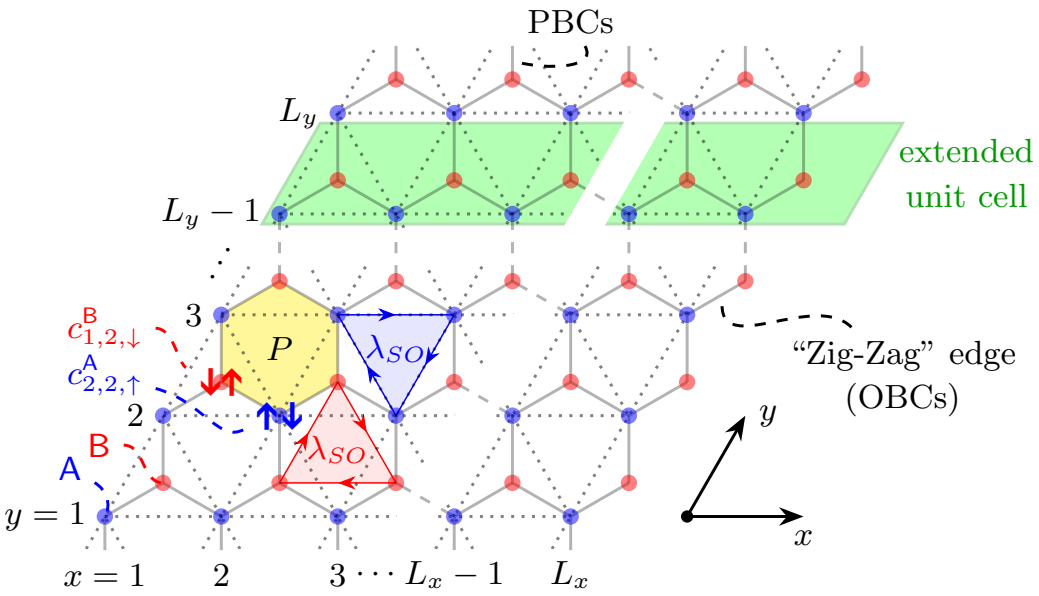
A characteristic feature of phases with topologically non-trivial bands is the emergence of gapless edge modes on boundaries of the system [see also Problem 6.2]. These modes make the system conducting on the boundaries whereas the bulk is a gapped insulator. Because it is a well-known fact that "one doesn't really understand what one cannot program," in this exercise you study the edge modes of the Kane-Mele topological insulator numerically.

In the lecture, we introduced the many-body Hamiltonian of the *Kane-Mele model* (here without Rashba spin-orbit coupling) as two time-inverted copies of the Haldane Chern insulator:

$$\hat{H}'_{\mathrm{KM}} = \sum_{\langle i,j\rangle,\alpha} c^\dagger_{i\alpha} c_{j\alpha} + m \sum_{i,\alpha} \epsilon_i c^\dagger_{i\alpha} c_{i\alpha} + \lambda_{\mathrm{SO}} \sum_{\langle\langle i,j\rangle\rangle,\alpha,\beta} i\eta_{ji}\, c^\dagger_{i\alpha} \mu^z_{\alpha\beta} c_{j\beta}\,. \tag{6}$$

Here, $i,j \in \mathcal{L}$ indexes the sites of the honeycomb lattice $\mathcal{L}$ and $\alpha \in \{\uparrow,\downarrow\}$ denotes the spin in the z-basis. The brackets $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote sums over nearest and next-nearest neighboring sites on the honeycomb lattice, respectively. The sign $\epsilon_i = \pm 1$ depends on the sublattice of the honeycomb grid and introduces a staggered potential which opens a mass gap of $2m$. The sign $\eta_{ji} = -\eta_{ij} = \pm 1$ of the complex phase in the Kane-Mele spin-orbit (SO) coupling term is chosen positive for an electron that moves *clockwise* (makes a right-turn) on a plaquette when hopping from j to i. μ^z denotes the Pauli z-matrix that acts on the spin degree of freedom and is responsible for inverting the hopping phase in the two spin sectors.

The goal of this exercise is to compute the band structure of Eq. (6) numerically for a strip geometry with periodic boundaries in y-direction and two boundaries of "zig-zag" shape in x-direction (see sketch below). We consider a strip with N_x (N_y) unit cells in x-direction (y-direction), so that the strip is of width $L_x = N_x a$ (length $L_y = N_y a$) with lattice constant a.



Since the strip is only periodic in y-direction, it is convenient to treat the system as a "1D chain" in y-direction with a very large unit cell (green box) that encompasses all $2L_x$ sites along a strip in x-direction:

*a) Fourier transform the Hamiltonian (6) in y-direction and show that it takes the form +3pt(s)

$$\hat{H}_{\mathrm{KM}} = \sum_{k_y \in \mathrm{BZ}} \mathbf{\Psi}^\dagger_{k_y} H(k_y) \mathbf{\Psi}_{k_y} \tag{7}$$

with *Bloch Hamiltonian*

$$H(k_y) = \begin{pmatrix} H_\uparrow(k_y) & 0 \\ 0 & H_\downarrow(k_y) \end{pmatrix} \tag{8}$$

that depends on the y-momentum $k_y \in [0, 2\pi/a) \equiv \mathrm{BZ}$ in the Brillouin zone.
$H(k_y)$ is a $4L_x \times 4L_x$-matrix with two $2L_x \times 2L_x$-block tridiagonal submatrices of the form

$$H_\alpha(k_y) = \begin{pmatrix} G_\alpha(k_y) & D^\dagger_\alpha(k_y) & 0 & 0 & \dots \\ D_\alpha(k_y) & G_\alpha(k_y) & D^\dagger_\alpha(k_y) & 0 & \ddots \\ 0 & D_\alpha(k_y) & G_\alpha(k_y) & D^\dagger_\alpha(k_y) & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{9}$$

In $H_\alpha(k_y)$, each block is a 2×2-matrix and repeated for $\sim L_x$ times along the (off-)diagonals. The blocks on the main diagonal are of the form

$$G_\alpha(k_y) = \begin{pmatrix} m - 2\lambda^\alpha_{\mathrm{SO}} \sin(k_y a) & 1 + e^{-ik_y a} \\ 1 + e^{ik_y a} & -m + 2\lambda^\alpha_{\mathrm{SO}} \sin(k_y a) \end{pmatrix}, \tag{10}$$

and the blocks on the lower off-diagonal are given by

$$D_\alpha(k_y) = \begin{pmatrix} i\lambda^\alpha_{\mathrm{SO}}(1 - e^{ik_y a}) & 1 \\ 0 & -i\lambda^\alpha_{\mathrm{SO}}(1 - e^{ik_y a}) \end{pmatrix}. \tag{11}$$

Here we define $\lambda_{\text{SO}}^{\uparrow} = +\lambda_{\text{SO}}$ and $\lambda_{\text{SO}}^{\downarrow} = -\lambda_{\text{SO}}$ for $\alpha \in \{\uparrow, \downarrow\}$.

The fermion modes in the Hamiltonian (7) are given by $4L_x$-component spinors of the form

$$\boldsymbol{\Psi}_{k_y} = \left(\tilde{c}^A_{1,k_y,\uparrow},\ \tilde{c}^B_{1,k_y,\uparrow},\ \ldots,\ \tilde{c}^A_{L_x,k_y,\uparrow},\ \tilde{c}^B_{L_x,k_y,\uparrow},\ \tilde{c}^A_{1,k_y,\downarrow},\ \tilde{c}^B_{1,k_y,\downarrow},\ \ldots,\ \tilde{c}^A_{L_x,k_y,\downarrow},\ \tilde{c}^B_{L_x,k_y,\downarrow}\right)^T$$

with fermion modes $\tilde{c}^{\beta}_{x,k_y,\alpha}$ with y-momentum k_y, for different x-positions $x \in \{1, \ldots, N_x\}$ and spins $\alpha \in \{\uparrow, \downarrow\}$ on the different sublattices $\beta \in \{A, B\}$.

Hint: The generic site index $i \leftrightarrow (x, y, \beta) \in \mathcal{L}$ in the fermion modes $c_{i\alpha} \leftrightarrow c^{\beta}_{x,y,\alpha}$ of the Hamiltonian (6) must be carefully translated into a triple of positions $x \in \{1, \ldots, N_x\}$ and $y \in \{1, \ldots, N_y\}$ and sublattice $\beta \in \{A, B\}$, taking into account the *connectivity* of the honeycomb lattice (see sketch above). Then a discrete Fourier transform in y-direction yields the modes $\tilde{c}^{\beta}_{x,k_y,\alpha}$.

The Bloch Hamiltonian $H(k_y)$ can be interpreted as the single particle Hamiltonian of a periodic 1D-chain with $2 \times 2 \times L_x = 4L_x$ orbitals (fermion modes) per unit cell. We should therefore expect a 1D band structure with $4L_x$ bands.

Henceforth, we set $a = 1$ and assume $L_y \to \infty$ so that we can choose $k_y \in \text{BZ}$ continuously.

Use your preferred programming language to *construct* and *diagonalize* the Bloch Hamiltonian $H(k_y)$ as a function of k_y for given parameters L_x, m and λ_{SO}. You should have access to both the *eigenvalues* and the corresponding *eigenvectors*.

Hint: In the following, it is useful to diagonalize the two spin sectors $H_\alpha(k_y)$ separately, and plot their spectra with different colors in the same plots to distinguish and compare the spin-polarized bands.

b) Let us start with graphene. Set $L_x = 50$ and $m = \lambda_{\text{SO}} = 0$ and plot the full spectrum of $H(k_y)$ over the Brillouin zone. **1**pt(s)

You should see (projections of) the two *Dirac cones* that make graphene a semimetal. Note that the tips of the cones are connected by two *flat bands*. This is a peculiar feature of the zig-zag edges, as already mentioned in the first paper by Kane & Mele in 2005[1].

c) Now add a small staggered potential with $m \approx 0.2$. **1**pt(s)

Both Dirac cones should obtain a gap. What is the size of the mass gap?

In this case, there are no gapless edge modes since the spin-polarized bands have no Chern number (you already know this from the Haldane model discussed in the lecture).

d) Switch off the staggered potential by setting $m = 0$ and instead open a gap using a small Kane-Mele spin-orbit coupling $\lambda_{\text{SO}} \approx 0.03$. **1**pt(s)

Compare your spectrum to Kane & Mele's plot in their original paper (Figure 1 in Ref. [1]).

How many bands cross the gap?

e) Start now with $\lambda_{\text{SO}} = 0.06$ and $m = 0$ and ramp up the staggered potential m to observe how the two spin-manifolds separate. **2**pt(s)

Plot the spectrum in the topological phase for $m = 0.1$, at the critical point for $m = 3\sqrt{3}\,\lambda_{\text{SO}}$, and in the trivial phase for $m = 0.4$.

Compare your spectra to Kane & Mele's plot in their follow-up paper (Figure 1 in Ref. [2]).

Can you explain the differences in the region where the gapless bands connect to the bulk?

[1] C. L. Kane and E. J. Mele, Quantum Spin Hall Effect in Graphene, PRL **95**, 226801 (2005)
[2] C. L. Kane and E. J. Mele, Z_2 Topological Order and the Quantum Spin Hall Effect, PRL **95**, 146802 (2005)

In the topological phase, you should see *four* separate gapless bands which cross at four distinct points. As you will verify in subtask g) below, the states of the crossing gapless bands are *helical edge states* which make the strip conducting on the edges. But first, we focus on the four crossings of these bands:

*f) Consider a system with $m = 0.25$ and $\lambda_{\mathrm{SO}} = 0.06$ in the topological phase *close to the phase transition*. Compare the spectra for a wide strip of width $L_x = 50$ and for a narrow strip of width $L_x = 10$. **+1**pt(s)

Which edge modes gap out for small systems and which do not? Can you explain this phenomenon?

Hint: Remind yourself of Kramers' theorem that you studied in Problem 6.1.

Finally, we want to identify the states of the gapless bands as *helical edge states*:

*g) Consider the topological phase for $\lambda_{\mathrm{SO}} = 0.06$ and $m = 0.1$ and select one *eigenvector* of the Bloch Hamiltonian with eigenenergy close to zero for each of the four bands that cross zero energy (= Fermi energy). **+2**pt(s)

Plot the absolute value of the $2L_x$ components in each spin sector as a function of the x-position across the width of the strip. Use this to correlate ...

i. where the states on the four crossing bands are located in x-direction,

ii. their spin polarization, and

iii. their group velocity in y-direction.

To demonstrate that the localization of these states is special, plot a few states picked from the gapped bulk spectrum for comparison.

It is the *exponential localization* on the edges of the strip, combined with their *gapless* nature, that marks them as *gapless edge states/modes*. Since spin and group velocity are locked, these are *helical edge modes*. Physically, the strip has scattering-free conducting channels on its edges, where group velocity and spin-polarization are correlated, while being a gapped insulator in the bulk. These edge modes cannot be localized (via backscattering) unless time-reversal symmetry is broken!