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### Problem 8.1: The Bogoliubov-de Gennes Hamiltonian and particle-hole "symmetry" [Oral | 4 pt(s)]

ID: ex_bogoliubov_de_gennes_hamiltonian_particle_hole_symmetry:tqp25

> **Learning objective**
>
> For the topological classification of the Majorana chain, we used the "intrinsic" particle-hole symmetry of the Bogoliubov-de Gennes (BdG) Hamiltonian. In the lecture, it was claimed that this is not a real symmetry (in the sense that some operator commutes with the Hamiltonian) but rather a tautological constraint on the BdG Hamiltonian that arises from the algebra of fermion operators. Here you study this claim in detail.

We are interested in the most generic quadratic fermion Hamiltonian

$$\hat{H} = \sum_{i,j=1}^{L} \left[ H_{ij}\, c_i^\dagger c_j + \frac{1}{2} \left( \Delta_{ij}\, c_i^\dagger c_j^\dagger + \Delta_{ij}^*\, c_j c_i \right) \right] \tag{1}$$

with mean-field pairing terms parametrized by $\Delta_{ij} \in \mathbb{C}$ and Hermitian hopping Hamiltonian $H_{ij} \in \mathbb{C}$. In the following, we write $H \equiv (H_{ij})_{ij}$ and $\Delta \equiv (\Delta_{ij})_{ij}$ for the corresponding $L \times L$-matrices.

a) Show that for a Hermitian Hamiltonian $\hat{H}$, it follows that $H^\dagger = H$ and w.l.o.g. $\Delta^T = -\Delta$. **1** pt(s)

b) Now introduce the $2L$-component *Nambu spinor* **1** pt(s)

$$\boldsymbol{\Psi} \equiv \left( c_1, \ldots, c_L, c_1^\dagger, \ldots, c_L^\dagger \right)^T \tag{2}$$

and show that the Hamiltonian can be written in the form

$$\hat{H} = \frac{1}{2} \boldsymbol{\Psi}^\dagger\, H_{\text{BdG}}\, \boldsymbol{\Psi} + \text{const.} \tag{3}$$

with the *Bogoliubov-de Gennes* Hamiltonian

$$H_{\text{BdG}} = \begin{pmatrix} H & \Delta \\ -\Delta^* & -H^* \end{pmatrix} . \tag{4}$$

c) Show that $H_{\text{BdG}}$ features a particle-hole "symmetry" as defined in the lecture and required for the tenfold way classification. **1** pt(s)

**Note:** Convince yourself that this reality constraint on $H_{\text{BdG}}$ does not impose any constraints on $\hat{H}$, but follows simply from the algebraic properties of the fermion operators; it is, in this sense, "intrinsic" or "tautological."

d) At no point did we use that superconductivity is really *present* ($\Delta \neq 0$). This suggests that the above construction also works for particle-number conserving models. So did we miss some topological phases when discussing such models by ignoring this "symmetry?" Why not? **1** pt(s)

**Hint:** Have a look at Eq. (4).

## Problem 8.2: From the Majorana chain to the transverse-field Ising model [**Written** | 7 pt(s)]

ID: ex_majorana_chain_transverse_field_ising_model:tqp25

**Learning objective**

As discussed at the beginning of this course, the transverse-field Ising model is a one-dimensional spin-$\frac{1}{2}$ model of interacting spins with a quantum phase transition that exemplifies the notion of spontaneous symmetry breaking. By contrast, the Majorana chain is a quadratic fermion model that can be solved exactly and features a topological phase transition without symmetry breaking. Remarkably, there is a mathematically exact mapping between fermionic and spin-$\frac{1}{2}$ systems known as *Jordan-Wigner transformation* that relates these two models. The point of this task is then (1) to solve the transverse-field Ising model exactly by mapping it to the Majorana chain, and (2) to understand how the *topological* phase transition of the Majorana chain translates to the *spontaneous symmetry breaking* phase transition of the transverse-field Ising model.

In the lecture, we introduced the mean-field Hamiltonian of a one-dimensional $p$-wave superconductor (with open boundary conditions)

$$\hat{H}_{\text{MC}} = -\frac{\mu}{2}\sum_{i=1}^{L}(i\gamma_{2i-1}\gamma_{2i}) + w\sum_{i=1}^{L-1}(i\gamma_{2i}\gamma_{2i+1}) \qquad \text{(OBC)}\,, \tag{5}$$

commonly referred to as *Majorana chain*. Here, $w = \Delta$ denotes the hopping amplitude/superconducting gap parameter and $\mu$ the chemical potential; the $\gamma_n$ are $2L$ Majorana operators which satisfy $\{\gamma_n, \gamma_m\} = 2\delta_{nm}$ and $\gamma_n^\dagger = \gamma_n$. Since the Hamiltonian is quadratic in fermion operators, we had no trouble computing the spectrum in the Bogoliubov-de Gennes representation.

The goal is to show that this Hamiltonian can be mapped exactly onto the *transverse-field Ising model* (TIM), given by the spin-$\frac{1}{2}$ Hamiltonian

$$H_{\text{TIM}} = -J\sum_{i=1}^{L-1}\sigma_i^x\sigma_{i+1}^x + h\sum_{i=1}^{L}\sigma_i^z \qquad \text{(OBC)} \tag{6}$$

which we introduced in the first lecture of this course as an example of spontaneous symmetry breaking. Here, $J > 0$ denotes the ferromagnetic coupling strength and $h \in \mathbb{R}$ the transverse magnetic field.

a) Consider the Hilbert space $\mathcal{H}_{\text{Spin}} = (\mathbb{C}^2)^{\otimes L}$ of a spin-$\frac{1}{2}$ system with $L$ spins and Pauli matrices $\sigma_i^\alpha$ for $\alpha = x, y, z$ and $i = 1, \dots, L$. **1**pt(s)

Show that the operators

$$\gamma_{2i-1} := \left[\prod_{j<i}\sigma_j^z\right]\sigma_i^x \quad \text{and} \quad \gamma_{2i} := \left[\prod_{j<i}\sigma_j^z\right]\sigma_i^y \tag{7}$$

satisfy the algebraic relations of Majorana fermions, i.e., $\gamma_n^\dagger = \gamma_n$ and $\{\gamma_n, \gamma_m\} = 2\delta_{nm}$.

Hence, these operators define a Fock space representation $\mathcal{H}_{\text{Fock}} \simeq \mathcal{H}_{\text{Spin}}$ via $c_i = \frac{1}{2}(\gamma_{2i-1} + i\gamma_{2i})$. This transformation is known as *Jordan-Wigner transformation*.

**Note:** The transformation Eq. (7) is highly non-local! The non-local product of $\sigma^z$-operators is sometimes referred to as *Jordan-Wigner string* which can be troublesome for the simulation of fermionic systems on quantum computers (because qubits = spin-$\frac{1}{2}$).

b) Apply the Jordan-Wigner transformation (7) to the Majorana chain (5) and show that it results in the transverse-field Ising model (6). How do the parameters of the two models relate? 3pt(s)

Conclude from this where the gap of the transverse-field Ising model closes and the symmetry-breaking phase transition occurs.

Do you see why we consider open boundary conditions? What would happen for periodic boundary conditions?

**Note:** Your results in a) and b) demonstrate that a Jordan-Wigner transformation can be applied to *any* fermionic system in order to translate it into an equivalent spin system – irrespective of dimensionality and spatial connectivity! However, only in *one* spatial dimension (and with open boundary conditions) the non-local Jordan-Wigner strings have a chance to cancel, such that a *local* fermion model maps to a *local* spin model (and vice versa).

c) Demonstrate how the ground state(s) of the Majorana chain at the fixed points (trivial: $w = 0$ and $\mu > 0$; topological: $w > 0$ and $\mu = 0$) map to the ground state(s) of the transverse-field Ising model. 3pt(s)

What happens to the long-range correlations $\lim_{|i-j|\to\infty}\langle\sigma_i^x\sigma_j^x\rangle$ of the transverse-field Ising model (in the symmetry-broken phase) under Jordan-Wigner transformation?

What is the fermionic counterpart of the global spin-flip symmetry

$$Z = \prod_i \sigma_i^z \quad \text{with} \quad [Z, H_{\text{TIM}}] = 0 \tag{8}$$

of the transverse-field Ising model?

*Fun fact:* Here you showed how the *transverse-field Ising model* in one dimension can be exactly solved by first mapping it to a non-interacting fermion model (the *Majorana chain*), and then solving the latter with the usual tricks (a unitary Bogoliubov transformation in Fock space).

It is remarkable (and quite surprising) that the *quantum* transverse-field Ising model in *one* spatial dimension, in turn, can be mapped to the *classical* Ising model in *two* spatial dimensions at *finite temperature* (and without magnetic field)[1]! This mapping therefore translates the quantum phase transition of the Majorana chain, via the quantum phase transition of the transverse-field Ising model, to the *thermal* phase transition of the two-dimensional classical Ising model. The latter is described by the famous *Onsager solution*[2] (who didn't use this mapping trick).

By the way, the mapping between $D$-dimensional *quantum* systems (at zero temperature) and $D+1$-dimensional *classical* systems (at finite temperature) is generic[3] and not a special feature of the TIM.

[1] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Two-Dimensional Ising Model as a Soluble Problem of Many Fermions, Reviews of Modern Physics, Vol. 36, No. 3 (1964)

[2] L. Onsager, Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition, Physical Review, Vol. 65, No. 3–4 (1944)

[3] M. Suzuki, Generalized Trotter's formula and systematic approximants of exponential operators and inner derivations with applications to many-body problems, Communications in Mathematical Physics, Vol. 51, No. 2 (1976)

## Problem 8.3: Effects of interactions on the topological classification of free fermion systems (Numerics)

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

ID: ex_effects_of_interactions_on_topological_classification:tqp25

**Learning objective**

In the lecture, we discussed that interactions can change the topological classification of free fermion systems. In this exercise, you study an example of this explicitly using numerics: You consider stacks of *interacting* Majorana chains with time-reversal symmetry (symmetry class **BDI**) and show that for *eight* chains the topological phase can be connected to the trivial phase *without closing the gap* while *preserving time-reversal symmetry*. This demonstrates the breakdown of the $\mathbb{Z}$ topological index of **BDI** to a $\mathbb{Z}_8$ index in the presence of interactions. This particular example was introduced and studied by Fidkowski and Kitaev in 2010 [a].

[a] L. Fidkowski and A. Kitaev, Effects of interactions on the topological classification of free fermion systems, PRB **81**, 134509 (2010)

In the lecture, Majorana fermions were introduced as self-adjoint operators

$$\gamma_{2i-1} = c_i + c_i^\dagger \quad \text{and} \quad \gamma_{2i} = i(c_i^\dagger - c_i) \tag{9}$$

for fermionic annihilation and creation operators $c_i$ and $c_i^\dagger$.

Furthermore, in Problem 8.2 you showed that Majorana fermions can be represented as spin-$\frac{1}{2}$ operators

$$\gamma_{2i-1} = \left[\prod_{j<i} \sigma_j^z\right] \sigma_i^x \quad \text{and} \quad \gamma_{2i} = \left[\prod_{j<i} \sigma_j^z\right] \sigma_i^y \tag{10}$$

via a *Jordan-Wigner transformation*.

In the lecture, you learned that the non-interacting Majorana chain can be thought of as a model in symmetry class **BDI** in one dimension with a topological $\mathbb{Z}$-index. **BDI** is protected by time-reversal symmetry (TRS $\mathcal{T}$ with $\mathcal{T}^2 = +\mathbb{1}$) and particle-hole symmetry (PHS $\mathcal{C}$ with $\mathcal{C}^2 = +\mathbb{1}$). While the latter is intrinsic to superconductors and cannot be broken [recall Problem 8.1], time-reversal symmetry is a true symmetry of the many-body Hamiltonian and restricts allowed perturbations.

a) To construct interactions that respect time-reversal symmetry, specify the representation of time-reversal $\mathcal{T} = U\mathcal{K}$ for the Majorana chain and show that **1**pt(s)

$$\mathcal{T}\gamma_{2i-1}\mathcal{T}^{-1} = +\gamma_{2i-1} \quad \text{and} \quad \mathcal{T}\gamma_{2i}\mathcal{T}^{-1} = -\gamma_{2i}\,. \tag{11}$$

How is this realized in the Jordan-Wigner representation (10)?

How does Eq. (11) restrict allowed interactions of the form $\gamma_n\gamma_m\gamma_l\ldots$?

We now consider 8 stacked Majorana chains with the non-interacting Hamiltonian $H_{\text{tot}} = \sum_{\alpha=1}^{8} H_{\text{MC}}^\alpha$, where each chain is described by the usual Majorana chain Hamiltonian

$$H_{\text{MC}}^\alpha = -\frac{\mu}{2}\sum_{i=1}^{L} i\gamma_{2i-1}^\alpha\gamma_{2i}^\alpha + w\sum_{i=1}^{L-1} i\gamma_{2i}^\alpha\gamma_{2i+1}^\alpha \tag{12}$$

where $\gamma_n^\alpha$ denotes the $n$th Majorana mode on chain $\alpha = 1, \ldots, 8$. Note that all 8 chains are parametrized by the same couplings $\mu$ and $w$. We define TRS to act like Eq. (11) for all $\alpha$.

This stack of 8 non-interacting Majorana chains is in a topological phase for $2|w| > |\mu|$, and in the trivial phase for $2|w| < |\mu|$. The topological phase realizes the topological index $\nu = 8$ from the $\mathbb{Z}$-classification of symmetry class **BDI**. For only quadratic couplings between the chains (i.e. $\gamma_n^\alpha \gamma_m^\beta$), phases with different topological index $\nu$ cannot be connected to each other without closing the gap (do you see why?).

Our goal is now to connect the topological $\nu = 8$ phase with the trivial phase (by using quartic interactions between the chains) *without* closing the gap and *without* violating time-reversal symmetry (11). This can only be possible if one invalidates one of the assumptions for the classification of topological phases of free fermions. The claim is that once *interactions* (non-quadratic terms of Majorana operators) are allowed, such an adiabatic connection of the two phases becomes possible!

To this end, Fidkowski and Kitaev suggested the following quartic interaction

$$W_{\text{tot}} = \lambda \sum_{i=1}^{L} \left(W_{2i-1} + W_{2i}\right) \,, \tag{13}$$

where each term $W_n$ only couples the eight Majorana modes $\gamma_n^\alpha$ with the same site index $n$ but different chain indices $\alpha$ as follows:

$$\begin{aligned} W = \quad & \gamma^1\gamma^2\gamma^3\gamma^4 + \gamma^5\gamma^6\gamma^7\gamma^8 + \gamma^1\gamma^2\gamma^5\gamma^6 + \gamma^3\gamma^4\gamma^7\gamma^8 - \gamma^2\gamma^3\gamma^6\gamma^7 - \gamma^1\gamma^4\gamma^5\gamma^8 + \gamma^1\gamma^3\gamma^5\gamma^7 \\ & + \gamma^3\gamma^4\gamma^5\gamma^6 + \gamma^1\gamma^2\gamma^7\gamma^8 - \gamma^2\gamma^3\gamma^5\gamma^8 - \gamma^1\gamma^4\gamma^6\gamma^7 + \gamma^2\gamma^4\gamma^6\gamma^8 - \gamma^1\gamma^3\gamma^6\gamma^8 - \gamma^2\gamma^4\gamma^5\gamma^7 \,. \end{aligned} \tag{14}$$

Here we omit the site subscripts for simplicity (the $W$s are translation invariant).

**Note:** Fidkowski and Kitaev used rather involved arguments from representation theory to construct this particular interaction. Here we simply take it as given and study its properties.

b) Show that this interaction term is time-reversal symmetric. **1**pt(s)

c) Consider a point in the topological phase with $\mu = 0$ and $w, \lambda > 0$. **1**pt(s)

   Why is it sufficient to only consider a block of 16 Majorana fermions $\gamma_0^\alpha$ and $\gamma_1^\alpha$ for $\alpha = 1, \ldots, 8$?

   Map the 16 Majorana fermions to 8 spin-$\frac{1}{2}$ (which are labeled by $\alpha = 1, \ldots, 8$) by using the Jordan-Wigner transformation (10).

   Why is the spin-$\frac{1}{2}$ representation more convenient for numerical calculations than the fermionic representation (9)?

d) Finally, using the spin-$\frac{1}{2}$ representation from subtask c), implement the Hamiltonian **2**pt(s)

$$H = w \sum_{\alpha=1}^{8} i\gamma_0^\alpha \gamma_1^\alpha + \lambda \left[W_0 + W_1\right] \tag{15}$$

   as a $256 \times 256$ matrix using a computer algebra system or programming language of your choice.

   Then show numerically that for the parametrization $w = t$ and $\lambda = 1 - t$ the Hamiltonian remains gapped along the path $t \in [0, 1]$.

   Use this result to argue that one can adiabatically connect the topological phase ($\mu = \lambda = 0$, $w > 0$) and the trivial phase ($\mu > 0$, $w = \lambda = 0$) of Eq. (12) via a continuous path using the interaction term $W$ *without closing the bulk gap.*

What does this imply for the $\mathbb{Z}$-index of **BDI** if interactions are allowed?

**Hint:** Construct the $\gamma$ operators in terms of spin-$\frac{1}{2}$ operators as tensor products of the individual Pauli matrices (and identity matrices). Then use these individual $(256 \times 256)$ matrices to construct the full Hamiltonian (15).