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July 8th, 2025
SS 2025

Problem 11.1: The AKLT model and DMRG - Numerical exploration [**Oral** | 8 (+2 bonus) pt(s)]

ID: ex_aklt_numerics:tqp25

Learning objective

In Problem 10.1 and Problem 10.2 you examined the exact ground state of the Affleck–Kennedy–Lieb–Tasaki (AKLT) model *analytically*. In this exercise, you complement this analysis with numerical methods based on matrix product states (MPS).

You employ the *density matrix renormalization group* (DMRG) algorithm to study the topological ground state manifold of the AKLT model. You first verify prior analytical results, and then explore regimes that are no longer accessible by exact methods. This implies the famous *Haldane conjecture* and the connection between the AKLT- and the Haldane model (antiferromagnetic spin-1 Heisenberg chain). To this end, you make use of the `TeNPy` library [a] [b] which implements optimized DMRG algorithms.

[a] https://scipost.org/10.21468/SciPostPhysLectNotes.5
[b] https://tenpy.readthedocs.io/en/latest/literature.html

To get started with the `TeNPy` library, you can download a `Jupyter` notebook that contains the template code for this exercise here:

https://itp3.info/akltipynb

If you prefer to run native `Python` instead, you can download the same code as a `Python` script here:

https://itp3.info/akltpy

Before you start, make sure that you have all required libraries installed:

```
pip install physics-tenpy numpy matplotlib ipykernel
```

You should now be able to run the preliminary check in the `Jupyter` notebook or the `Python` script.

We start by verifying some analytical results you derived previously in Problem 10.1 and Problem 10.2:

a) Implement the AKLT-like Hamiltonian **1**pt(s)

$$H = \sum_{i=1}^{L-1} \left[J\, \boldsymbol{S}_i \boldsymbol{S}_{i+1} + \beta\, \left(\boldsymbol{S}_i \boldsymbol{S}_{i+1} \right)^2 \right] \,, \tag{1}$$

for an *open* chain of length $L = 20$ with parameters $J = 1$ and $\beta = \frac{1}{3}$ (up to a constant, this is the AKLT point). Here, $\boldsymbol{S}_i$ denote spin-1 operators for $i = 1, \ldots, L$.

Run the DMRG algorithm to find a ground state of this Hamiltonian.

What ground state energy and entanglement entropy do you expect?

Compare your expectations with the numerical results.

b) Use the ground state $|\Psi\rangle$ obtained in subtask a) to calculate the expectation value of the ferromagnetic order parameter $\langle\psi| S_i^z S_j^z |\psi\rangle$ for $i = 4$ and $j \in \{4, 5, \ldots, L\}$. **1pt(s)**

Then calculate the string order parameter $\langle\psi| S_i^z \left(\prod_{i<k<j} R_k^z\right) S_j^z |\psi\rangle$ where $R_k^z = \exp(i\pi S_i^z)$.

Plot both order parameters as a function of $|i - j|$.

Compare your results with the analytical results from Problem 10.1 and Problem 10.2.

For the AKLT model with *open boundary conditions*, we expect a *four-fold* degenerate ground state manifold, where each ground state can be distinguished by its fractional (spin-$\frac{1}{2}$) edge degrees of freedom. Let us verify this hallmark of one-dimensional SPTs numerically:

c) Plot the local onsite magnetization $\langle\psi| S_i^z |\psi\rangle$ for $i \in \{1, 2, \ldots, L\}$ of the ground state obtained in subtask a) to visualize the spin-$\frac{1}{2}$ boundary degrees of freedom. **1pt(s)**

Does this result meet your expectations? Which "trick" in the code is responsible for this result?

d) The DMRG algorithm implemented by `TeNPy` can also find low-lying excited states. **2pt(s)**

Use this to find the next *four* excited states (and eigenenergies) of the Hamiltonian (1).

Do you find the expected four-fold ground state degeneracy?

How do the boundary spin-$\frac{1}{2}$ of the four ground states differ from each other?

Note: One way to get excited states via DMRG is to add a large energy penalty to the Hamiltonian for the projector onto all previously found low-lying eigenstates. `TeNPy` uses a related approach, where the state during the DMRG sweep is always projected onto the orthogonal complement of the previously found states.

In the lecture you learned about the *Haldane conjecture*, which states that for *integer* spin, the antiferromagnetic Heisenberg model has a gap, whereas for *half-integer* spin the model is gapless. Since these models cannot be solved exactly in general, let us again use DMRG to verify this claim numerically:

e) Demonstrate the validity of the Haldane conjecture explicitly for chains with spin $S \in \{\frac{1}{2}, 1\}$. Do so by calculating and plotting the eigenenergies of the five lowest eigenstates of the antiferromagnetic Heisenberg model for different system sizes $L \in \{20, 30, 40, 50, 100\}$. **2pt(s)**

Interpret your results.

Hint: The antiferromagnetic Heisenberg model is obtained from the Hamiltonian (1) for $\beta = 0$.

Note: Of course you can also show this for higher spins (e.g. $S \in \{\frac{3}{2}, 2\}$). However, due to the larger Hilbert space dimension, these simulations take longer to run (try it ...).

The AKLT model was introduced because, first, its ground state can be computed analytically, and second, it is believed to be in the same symmetry-protected topological phase as the antiferromagnetic spin-1 Heisenberg model (which cannot be solved exactly). This SPT phase is know as the *Haldane phase*.

Let us use the magic of DMRG to validate this (still unproven) claim numerically:

f) Demonstrate that the antiferromagnetic spin-1 Heisenberg model can be adiabatically (= without closing the gap) connected to the AKLT model by tuning the parameter β in the Hamiltonian (1) from $\beta = 0$ to $\beta = \frac{1}{3}$. **1pt(s)**

Note: To validate that this gap is not a finite size effect, you should compute it for different system sizes.

By tuning the parameter β, you essentially added a symmetry preserving *perturbation* to the Hamiltonian. Your results demonstrate that the four-fold ground state degeneracy of the AKLT model (or the Haldane chain) is *robust* against such perturbations in the thermodynamic limit ($L \to \infty$).

Conversely, by adding a *symmetry-breaking* perturbation to the Hamiltonian, this degeneracy should be lifted. You can verify this numerically:

*g) Which symmetries protect the Haldane phase, and why does a magnetic field $H_{\text{pert}} = h_z \sum_i S_i^z$ break these symmetries? **+2pt(s)**

What do you expect happens to the four-fold ground state degeneracy of the AKLT model when you add such a magnetic field to the Hamiltonian (1)?

Verify your expectation numerically.

Problem 11.2: Twisted group cohomology

[**Oral** | 6 (+1 bonus) pt(s)]

ID: ex_twisted_group_cohomology:tqp25

Learning objective

In the lecture, we studied *unitary* symmetries and how their (second) cohomology groups classify symmetry-protected topological phases. By contrast, in our prior study of quadratic fermion theories, *anti*unitary symmetries played an important role (think of time-reversal symmetry). In this exercise, you retrace and generalize the cohomology classification for symmetry groups where some elements are represented as antiunitary operators. This leads to the concept of "twisted" group cohomology. You show for the simple group $G = \mathbb{Z}_2$ that these "twists" directly affect the possibility to protect non-trivial topological phases.

On Problem 1.2 you proved *Wigner's theorem*. It states that, in quantum mechanics, every symmetry operation can be represented by either a unitary or an antiunitary operator that acts on the Hilbert space.

Let us consider a symmetry group $(G, \bullet)$ and a representation ρ acting on the Hilbert space of some quantum system. Then the operator $\rho(g)$ for each group element $g \in G$ is either unitary or antiunitary. We can encode this property by a map

$$\sigma : G \to \mathbb{Z}_2 \quad \text{with} \quad g \mapsto \sigma(g) = \begin{cases} +1 & \text{if } \rho(g) \text{ is unitary,} \\ -1 & \text{if } \rho(g) \text{ is antiunitary.} \end{cases} \tag{2}$$

a) Show that σ must be a group homomorphism, i.e., show that $\sigma(g_1 \bullet g_2) = \sigma(g_1) \cdot \sigma(g_2)$. **1pt(s)**

What are the possible choices of σ for $G = \mathbb{Z}_2$ and $G = \mathbb{Z}_3$?

As shown in the lecture (using the matrix product state formalism), to characterize symmetry-protected topological phases of one-dimensional spin systems, we must study the *projective* representations of the protecting symmetry group. Such representations satisfy the multiplication rule of conventional linear representations "up to a phase,"

$$\rho(g) \cdot \rho(h) = \chi(g, h)\, \rho(g \bullet h) \quad \text{for all } g, h \in G\,, \tag{3}$$

where $\chi : G \times G \to U(1)$ is called *(2-)cocycle* and characterizes the projective representation.

Your goal is now to trace the modifications required (compared to the lecture) if some $\rho(g)$ are *antiunitary* (as encoded by some given homomorphism σ):

b) Show that χ must satisfy the σ-twisted cocycle condition **1pt(s)**

$$\chi(g_1, g_2)\chi(g_1 g_2, g_3) = \chi^{\sigma(g_1)}(g_2, g_3)\chi(g_1, g_2 g_3) \tag{4}$$

where $\chi^{-1} = \chi^*$ denotes complex conjugation.

Hint: Use the associativity of G and note that we omit the group multiplication $\bullet$ for simplicity.

Note: For the trivial homomorphism $\sigma \equiv 1$ this reduces to the "untwisted" cocycle condition derived in the lecture.

The set of σ-twisted cocycles is denoted

$$Z^2_\sigma(G, U(1)) := \{\ \chi : G \times G \to U(1) \mid \chi \text{ satisfies Eq. (4) } \} \tag{5}$$

and forms a group under pointwise multiplication (why?).

As motivated in the lecture, two projective representations $\tilde{\rho}(g) = f(g)\rho(g)$ related by an element-dependent phase factor $f(g) \in U(1)$ are equivalent.

c) Show that two representations ρ and $\tilde{\rho}$ are equivalent if and only if their cocycles fulfill **1pt(s)**

$$\tilde{\chi}(g, h) = \frac{f(g) f^{\sigma(g)}(h)}{f(gh)} \chi(g, h)\,, \tag{6}$$

for some function $f : G \to U(1)$.

We denote the equivalence relation (6) by R_σ and write $\chi \overset{R_\sigma}{\sim} \tilde{\chi}$ for two equivalent cocycles.

The *σ-twisted (second) cohomology group* of G in $U(1)$ is then defined as the group of 2-cocycles modulo this equivalence relation:

$$H^2_\sigma(G, U(1)) := Z^2_\sigma(G, U(1)) \,/\, R_\sigma. \tag{7}$$

It classifies the inequivalent projective representations of G, where group elements are represented antiunitarily according to σ.

In the remainder of this exercise we study the group $G = \mathbb{Z}_2$. We denote the trivial homomorphism by σ_0 and the (only) nontrivial homomorphism by σ_1 [recall subtask a)].

d) Show that the untwisted cohomology group $H^2_{\sigma_0}(\mathbb{Z}_2, U(1)) \cong \mathbb{Z}_1$ is trivial. **1pt(s)**

Are there SPT phases protected by a unitary $\mathbb{Z}_2$ symmetry?

e) Now show that the twisted cohomology group $H^2_{\sigma_1}(\mathbb{Z}_2, U(1)) \cong \mathbb{Z}_2$ is non-trivial. **2pt(s)**

Are there SPT phases protected by an *anti*unitary $\mathbb{Z}_2$ symmetry?

In the lecture you showed that $H^2_{\sigma_0}(D_2, U(1)) \cong \mathbb{Z}_2$ for the dihedral group $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$.

*f) Compare your results from subtasks d) and e) and the result from the lecture with the findings reported in Chen *et al.*: **+1pt(s)**

Symmetry protected topological orders and the group cohomology of their symmetry group
Physical Review B 87, 155114 (2013)

Hint: To simplify notation one usually writes $H^2(G, U(1)) \equiv H^2_{\sigma_0}(G, U(1))$ for a general symmetry group G. Chen *et al.* use furthermore the shorthand notation $H^2(Z_2^T, U(1)) \equiv H^2_{\sigma_1}(\mathbb{Z}_2, U(1))$.