Hunting for Hamiltonians

A computational approach to learning quantum models

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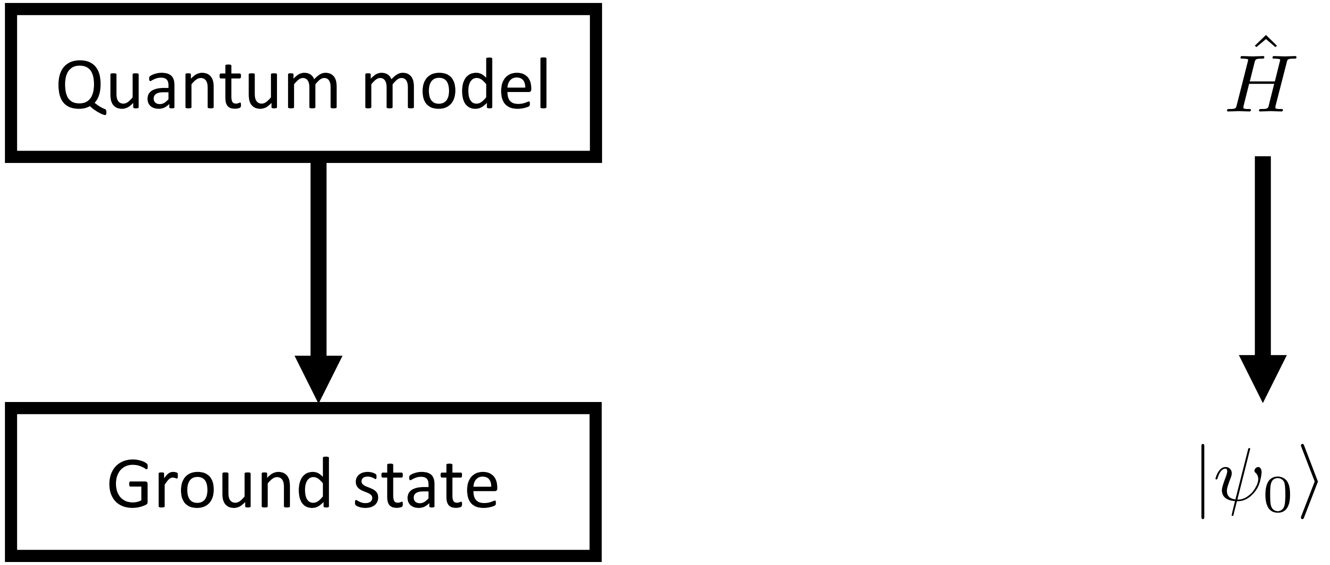
https://arxiv.org/abs/1802.01590

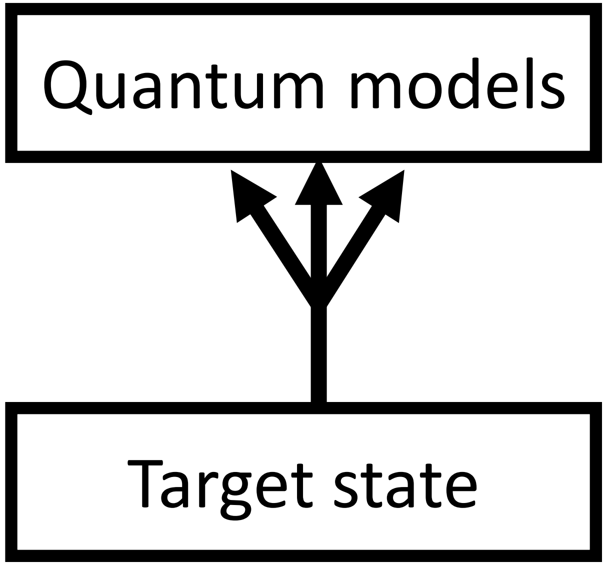
The quantum forward problem

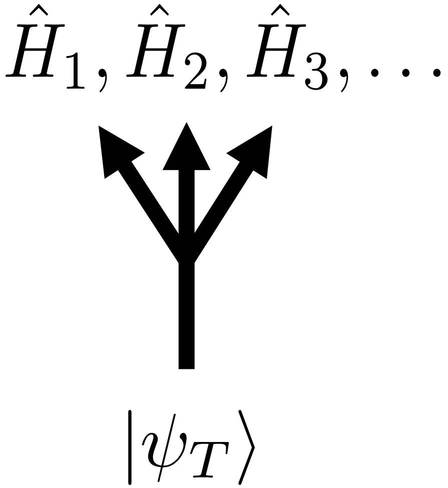


Limitations

- *Generically, very difficult to solve analytically or numerically.*
- *Restricts our attention to only a few model Hamiltonians.*
- *Difficult to target specific ground state properties.*

The quantum inverse problem





Addresses limitations of forward method

- *Allows us to study many models that might contain interesting physics not seen in current models.*
- *Allows us to target specific physical properties in our models.*
- *For target eigenstates, can be solved efficiently.*

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Vector spaces of Hamiltonians

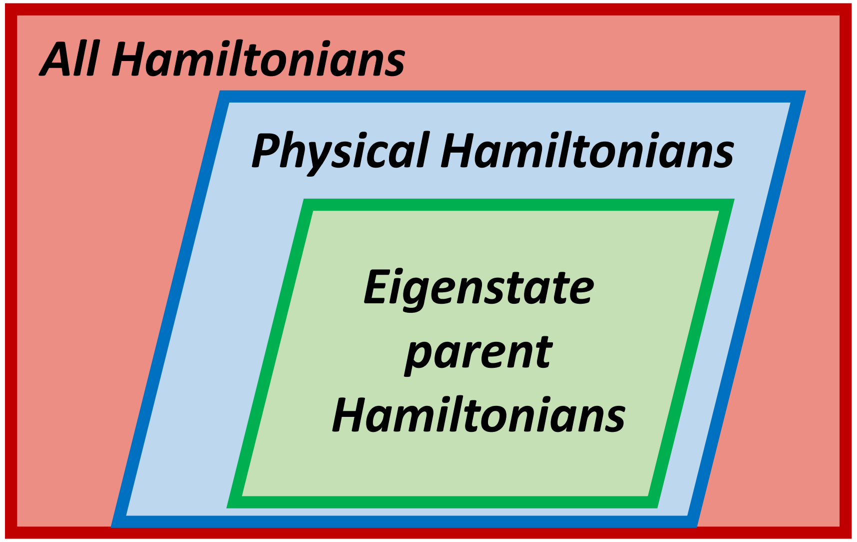
The set of ***all Hamiltonians*** forms a vector space.

We consider a space of ***physical Hamiltonians*** of the form

$$\hat{H} = \sum_{a=1}^{d_T} J_a \hat{h}_a$$

Examples:

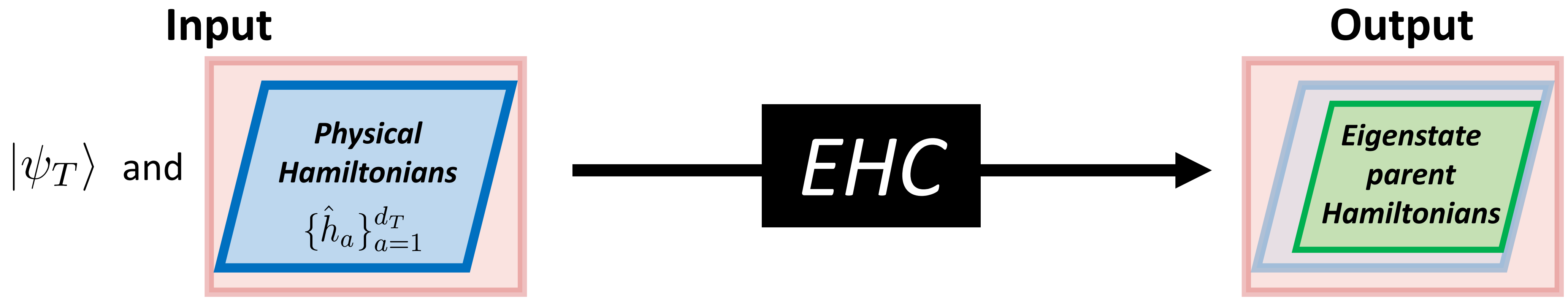
- *Local Hamiltonians*
- *Those possible in AMO experiments*



Our goal is to find ***eigenstate parent Hamiltonians*** in this space that have a target wave function as an energy eigenstate

$$\hat{H}|\psi_T\rangle = E_T|\psi_T\rangle \iff \langle\psi_T|\hat{H}^2|\psi_T\rangle - (\langle\psi_T|\hat{H}|\psi_T\rangle)^2 = 0$$

Eigenstate-to-Hamiltonian Construction (EHC)



State** and a space of **physical Hamiltonians

*A space of **eigenstate parent Hamiltonians***

Some things you can do with EHC

Will give an example

Hamiltonian discovery

To find new Hamiltonians with new eigenstates.

State collision

To find Hamiltonians with specific degenerate eigenstates.

Phase expansion

To expand the ground state phase diagram of known models.

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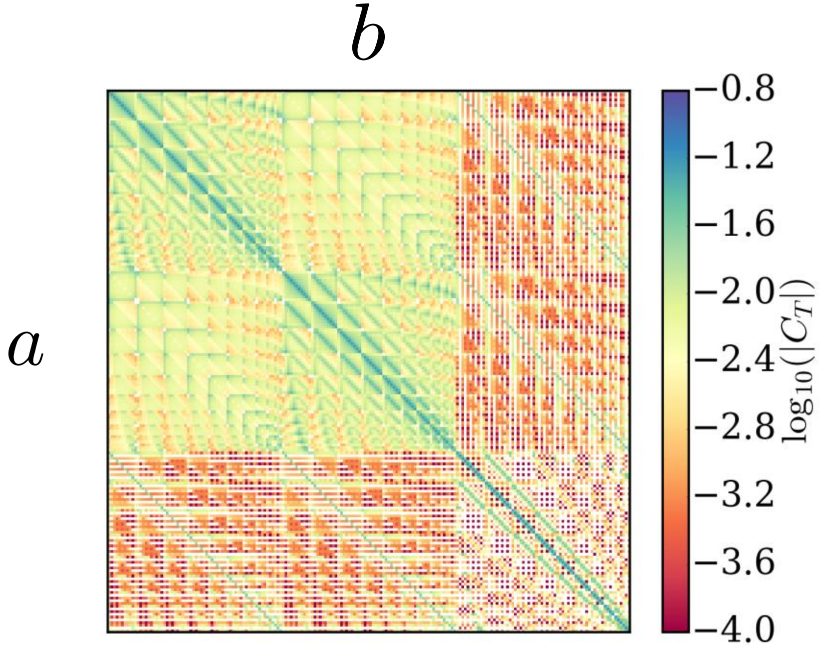
Quantum covariance matrix (QCM)

The main tool of the EHC method is the **quantum covariance matrix (QCM)**

See also: Xiao-Liang Qi and Daniel Ranard, arxiv:1712.01850

$$(C_T)_{ab} = \langle\psi_T|\hat{h}_a\hat{h}_b|\psi_T\rangle - \langle\psi_T|\hat{h}_a|\psi_T\rangle\langle\psi_T|\hat{h}_b|\psi_T\rangle \qquad (a, b = 1, \ldots, d_T)$$



Properties of the QCM:

- The eigenvectors of the QCM correspond to Hamiltonians with variance given by the eigenvalue.
- Zero eigenvalue eigenvectors (***null vectors***) correspond to ***eigenstate parent Hamiltonians***.

Note: Computing the QCM only requires a quadratic number of expectation values. This can be done with matrix product states and variational Monte Carlo.

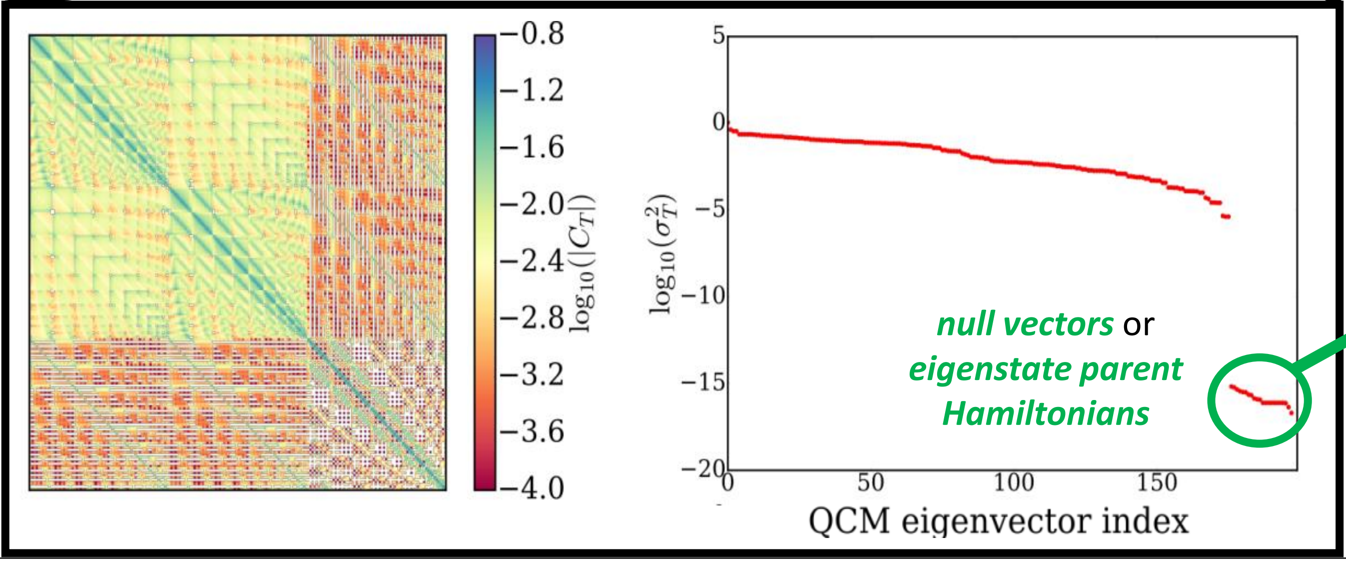
Example: Phase expansion of *XX* chain ground state

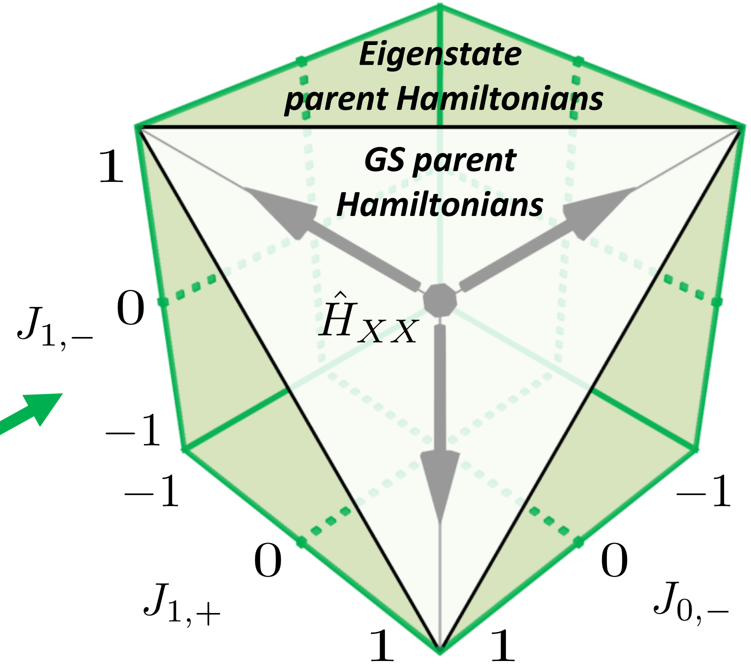
$$\hat{H}_{XX} = \sum_{i=1}^{N} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) \longrightarrow |\psi_{XX}\rangle$$ ***ground state***

$|\psi_{XX}\rangle$

$\hat{h}_a = S_i^x S_j^x, S_i^y S_j^y, S_i^z S_j^z$

$\}$ — **EHC** → $\hat{H}_{XX}$ ***and new parent Hamiltonians***





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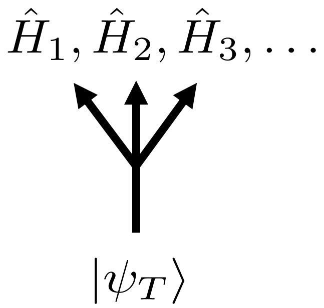
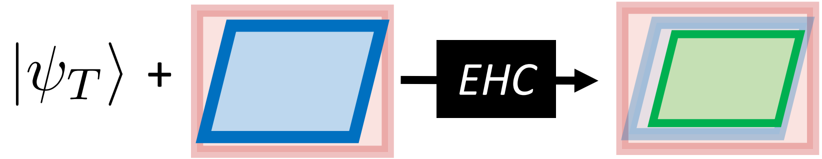
Summary

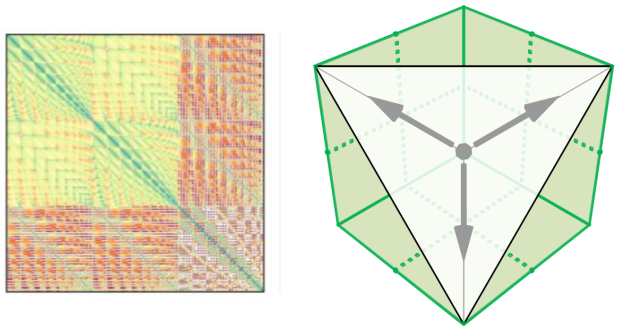
Quantum inverse problem



Eigenstate-to-Hamiltonian Construction



Example application



Other examples

We illustrated our EHC method with many different examples.

In each case, we found many Hamiltonians with the given target state as an eigenstate.

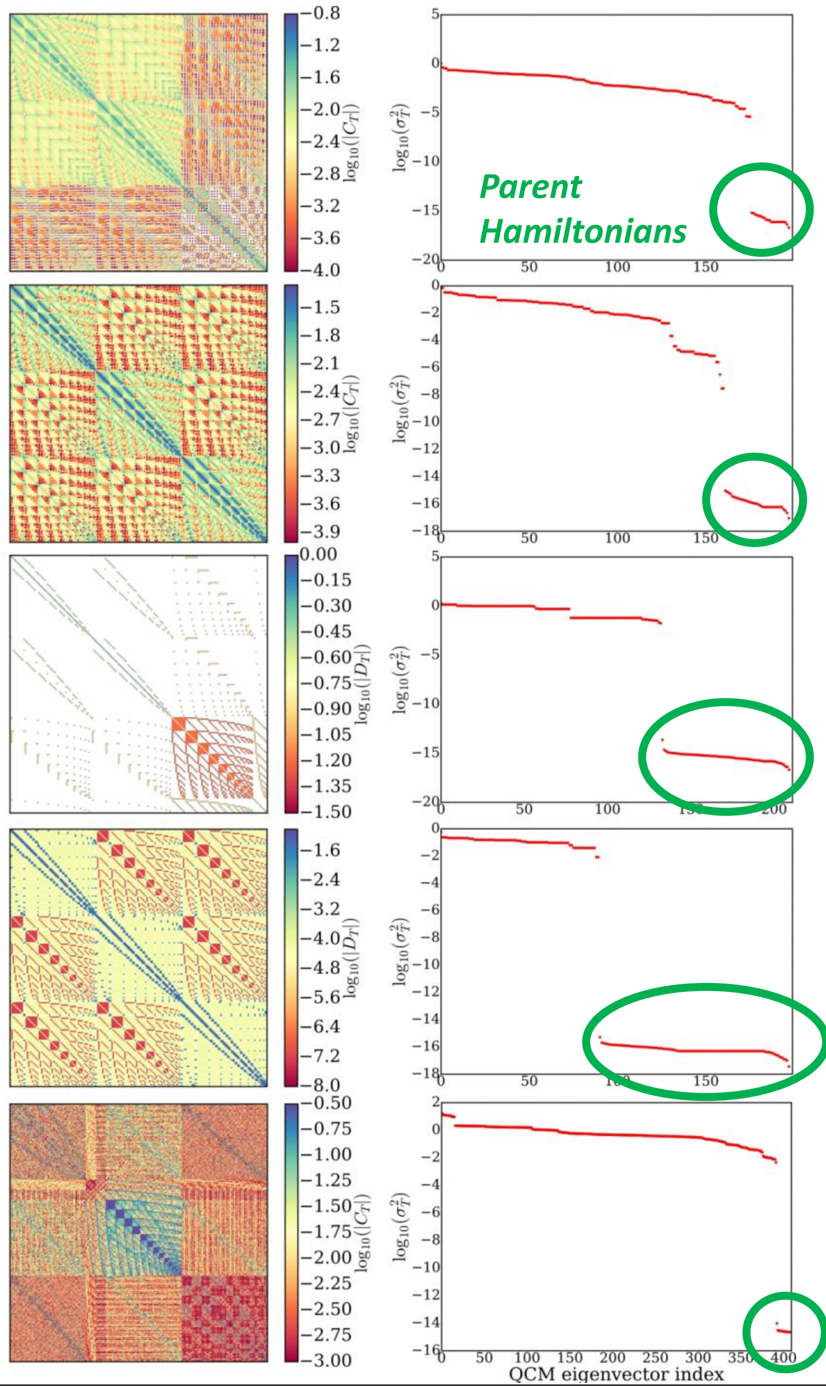
XX chain ground state $|\psi_{XX}\rangle$

Heisenberg chain GS $|\psi_{H}\rangle$

Kitaev chain GSs $|\psi^{\pm}_{KC}\rangle$

Majumdar-Ghosh model GSs $|\psi^{\pm}_{SD}\rangle$

2D BdG model GS $|\psi_{BCS}\rangle$

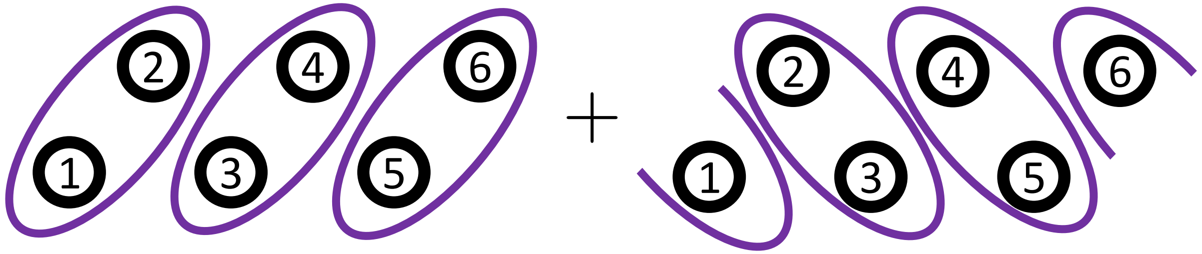


Example: Hamiltonian discovery for triplet dimer state

Target state (input)

$$|\psi_{TD}\rangle = \frac{1}{\sqrt{2}}\left(|\phi_{1,2}\cdots\phi_{N-1,N}\rangle + |\phi_{2,3}\cdots\phi_{N,1}\rangle\right)$$

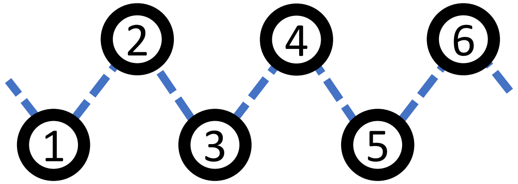
$$\left(|\phi_{i,j}\rangle \equiv \frac{1}{\sqrt{2}}\left(|\uparrow_i\downarrow_j\rangle + |\downarrow_i\uparrow_j\rangle\right)\right)$$



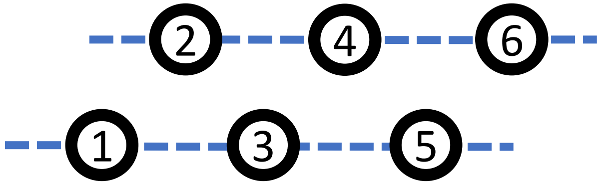
Space of physical Hamiltonians (input)

$$\hat{H} = J_1\hat{h}_1 + J_2\hat{h}_2 + J_3\hat{h}_3 + J_4\hat{h}_4$$

$\hat{h}_1 =$

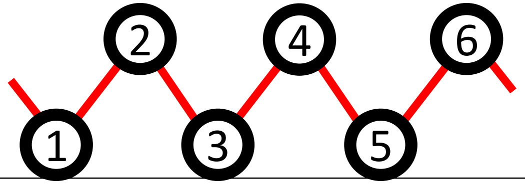


$\hat{h}_3 =$

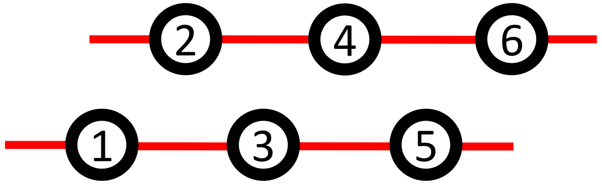


$S_i^x S_j^x + S_i^y S_j^y$

$\hat{h}_2 =$



$\hat{h}_4 =$



$S_i^z S_j^z$

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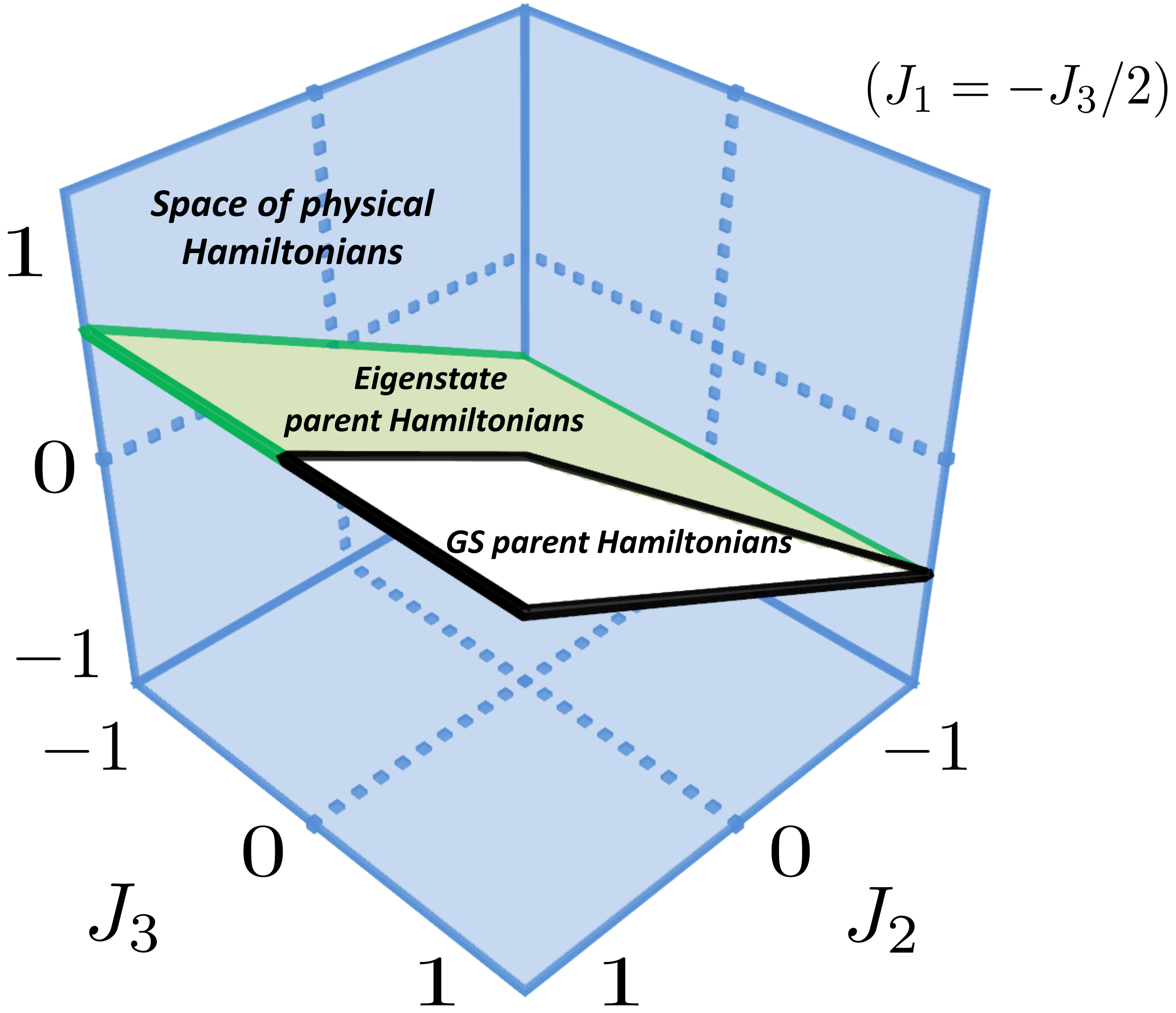
Spaces of triplet dimer state Hamiltonians

$|\psi_{TD}\rangle$

$\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4$

EHC → J_4



Details about quantum covariance matrix (QCM)

Eigenstates have zero energy variance: $\sigma_T^2 = \langle \psi_T | \hat{H}^2 | \psi_T \rangle - (\langle \psi_T | \hat{H} | \psi_T \rangle)^2 = 0$

For Hamiltonians in the target space, the variance can be written as

$$\sigma_T^2 = \sum_{a=1}^{d_T} \sum_{b=1}^{d_T} J_a (C_T)_{ab} J_b$$

where

$$(C_T)_{ab} = \langle \psi_T | \hat{h}_a \hat{h}_b | \psi_T \rangle - \langle \psi_T | \hat{h}_a | \psi_T \rangle \langle \psi_T | \hat{h}_b | \psi_T \rangle$$

is the **quantum covariance matrix (QCM)**. It is of size $d_T \times d_T$ and depends on the target space and target state.

$|\psi_T\rangle$ is an eigenstate of the Hamiltonian $\tilde{H} = \sum_a \tilde{J}_a \hat{h}_a$ when $\tilde{J}_a$ is a zero eigenvalue eigenvector of C_T

In summary, the null vectors of the QCM correspond to Hamiltonians in the eigenstate space of $|\psi_T\rangle$