Hunting for Hamiltonians

A computational approach to learning quantum models

Eli Chertkov and Bryan K. Clark
University of Illinois at Urbana-Champaign

APS March Meeting 2018, Los Angeles, CA

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.

Quantum models

Target state

$\hat{H}_1, \hat{H}_2, \hat{H}_3, \ldots$

$|\psi_T\rangle$
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)

**Input**

State and a space of physical Hamiltonians

\[ |\psi_T\rangle \quad \text{and} \quad \{\hat{h}_a\}_{a=1}^{d_T} \]

**Output**

A space of eigenstate parent Hamiltonians

Some things you can do with EHC

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.
Quantum covariance matrix (QCM)

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

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

**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.

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

https://arxiv.org/abs/1802.01590
Example: Phase expansion of $XX$ chain ground state

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

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

and new parent Hamiltonians

null vectors or eigenstate parent Hamiltonians
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.
Example: Hamiltonian discovery for triplet dimer state

**Target state (input)**

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

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

**Space of physical Hamiltonians (input)**

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

\[ \hat{h}_1 = \]

\[ \hat{h}_2 = \]

\[ \hat{h}_3 = \]

\[ \hat{h}_4 = \]

\[ S_i^x S_j^x + S_i^y S_j^y \]

\[ S_i^z S_j^z \]
Spaces of triplet dimer state Hamiltonians

\[
\begin{align*}
|\psi_{TD}\rangle & \quad \text{EHC} \quad J_4 \\
\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4
\end{align*}
\]

(J_1 = -J_3/2)

Space of physical Hamiltonians

Eigenstate parent Hamiltonians

GS parent Hamiltonians
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 \( |\psi_T\rangle \)**