Reverse Engineering Hamiltonian from Spectrum

Hiroyuki Fujita, Institute for Solid State Physics

Collaborators

Yuya. O. Nakagawa
(PhD @ ISSP -> Fintech company)

S. Sugiura
(PD @ ISSP -> PD @ Harvard)

M. Oshikawa
(Prof. @ ISSP, now @ Wien)
I am going to talk about

something NOT deep

Deep to be interesting?
Image compression

Simple but not efficient $\rightarrow$ principal component analysis (PCA)

PCA is to find a subspace onto which the data are projected.

Optimization maximizing the data variance

e.g. (1) is better in the variance of the projected data
"Image compression" in cond. mat.?

Hubbard model

$$H = \sum_{i=1, \ldots, L, \sigma=\uparrow, \downarrow} t (c_{i+1, \sigma}^\dagger c_{i, \sigma} + c_{i, \sigma}^\dagger c_{i+1, \sigma}) + U n_i^\uparrow n_i^\downarrow$$

AFM Heisenberg model

$$H_{\text{spin}} = \frac{4t^2}{U} \sum_{i,j} \vec{S}_i \cdot \vec{S}_j + O \left( \frac{t^3}{U^3} \right)$$

half-filling, large $U$ → AFM Heisenberg model

Perturbation theory

$O \left( \frac{t^2}{U^2} \right)$

Low-energy model = “compressed image”

What is “PCA” for this problem?
Straightforward(?) approach

Totally unrealistic!

- e.g. $L = 10$ Hubbard chain

\[
4^{10} \times 4^{10} \quad \rightarrow \quad 2^{10} \times 2^{10}
\]

trillion pixel image  \quad million pixel image

We cannot simply use the (variant of) existing algorithms.
The “PCA” has to construct the effective model based on the low-energy properties of the Hubbard model

\[ A = \begin{pmatrix} \tilde{N} \times \tilde{N} \end{pmatrix} \]

= low-energy spectrum

Reconstruct the matrix \( A \)

\[ N \leq \tilde{N} \]

Can we solve the “inverse problem” of diagonalization?
Number counting

\[ A = \begin{pmatrix} \tilde{N} \times \tilde{N} \end{pmatrix} \]

Exact Diagonalization (ED)

\[ a_1, \ldots, a_N \]

Number of independent params of \( A \) is \( \tilde{N} \times \tilde{N} \)

Number of eigenvalues available is at most \( \tilde{N} \)

Parameters

- \# of params in \( A = O(\tilde{N} \times \tilde{N}) \)

Data

- \# of eigenvalues \( A = O(\tilde{N}) \) \( \tilde{N} \to \infty \)

Too many parameters……
Physicists point of view

“Being physical” is a powerful constraint on the Hamiltonian

Short-ranged interactions  Few-body interactions
Symmetries such as U(1), SU(2), ...

Dimension of Hilbert space is exponential in the system size

Parameters

\[ \# \text{ of params in } H = O(L^n) \]

\[ \lim_{L \to \infty} L \to 0 \]

Data

\[ \# \text{ of eigenvalues} = O(\tilde{N}) = O(e^L) \]

Solvable because it’s physics!
What can we do with (Exact Diagonalization)$^{-1}$

Original Hamiltonian \[\rightarrow\] \text{ED} \rightarrow \text{Low-energy spectrum} \[\rightarrow\] (ED)$^{-1}$ \rightarrow \text{Low-energy Hamiltonian}

\text{e.g. Hubbard model @ half-filling} \rightarrow \text{(ED)$^{-1}$} \rightarrow \text{Low-energy Hamiltonian} \text{e.g. AFM Heisenberg model}

Quantum state (w.f.) \[\rightarrow\] \text{ED} \rightarrow \text{entanglement spectrum} \[\rightarrow\] (ED)$^{-1}$ \rightarrow \text{Entanglement Hamiltonian}
Make the problem concrete

$H = \sum_{i=1,\ldots,L} \sum_{\sigma=\uparrow,\downarrow} t(c_{i+1,\sigma}^{\dagger} c_{i,\sigma} + c_{i,\sigma}^{\dagger} c_{i+1,\sigma}) + U_i n_i^{\uparrow} n_i^{\downarrow}$

Correlated electrons in 1D

$E_1, \ldots, E_N$ (Small number of eigenvalues)

$H = \sum_{i=1,\ldots,M} c_i H_i$

Spin model with parameters to be optimized

Heisenberg, four-spins interactions, …

What we have to do is to

1. find a proper form of the ansatz

2. find the proper parameters for the fixed ansatz
Formulate as a supervised learning problem

\[ E_1, \ldots, E_N \quad H = \sum_{i=1,\ldots,M} c_i H_i \quad \text{ED} \quad E'_1, \ldots, E'_N \]

= data \((x_i = i, y_i = E_i)\) = model \(f(x)\)

Gradient descent algorithm

1. Define cost function
   
   \[ \text{Cost}(E, E'(\{c_j\})) = \frac{1}{2N} \sum_{i=1}^{N} (E'_i - E_i)^2 \]

2. Calculate the gradient in terms of the parameters

3. Update the parameters as
   
   \[ c_j = c_j - \alpha \frac{\partial}{\partial c_j} \text{Cost}(E, E'(\{c_j\})) \]

\[ E_1, \ldots, E_n \quad \text{cost evaluation} \]

\[ E'_1, \ldots, E'_n \quad \text{gradient descent} \]

\[ H = \sum_{i=1,\ldots,M} c_i H_i \quad \text{diagonalization} \]

\[ \text{Cost} \quad C_j \]
"Quantum computation" of the gradient

\[
\frac{\partial}{\partial c_j} \text{Cost}(E, E'(\{c_j\})) = \left( \frac{\partial}{\partial c_j} E' \right) = \frac{\partial}{\partial E'} \text{Cost}(E, E'(\{c_j\})) \quad \text{trivial}
\]

How?

Luckily, we know the perturbation theory of quantum mechanics:

\[ H \rightarrow \sum_{i=1,\ldots,M} c_i H_i + \delta c_j H_j \rightarrow E_i \rightarrow E_i + \delta c_j \langle \Psi_i | H_j | \Psi_i \rangle \]

\[ H = \sum_{i=1,\ldots,M} c_i H_i \rightarrow E'_1, \ldots, E'_N \]

.: For a given ansatz, we can optimize its parameters

What we have to do is to

1. find a proper form of the ansatz
2. find the proper parameters for the fixed ansatz
Model selection by regularization

\[ \text{Cost}(E, E') \rightarrow \text{Cost}(E, E') + \lambda \sum_{j=1,\ldots,M} |c_j| \]

L1 norm regularization
Prefer small parameters

"Sparse" nature of the estimation $\rightarrow$ Model selection
Demonstration: Hubbard chain at half-filling

Effective model of

\[ H = \sum_{i=1, \ldots, L} \sum_{\sigma = \uparrow, \downarrow} t(c_{i+1, \sigma}^\dagger c_{i, \sigma} + c_{i, \sigma}^\dagger c_{i+1, \sigma}) + U_i n_i^\uparrow n_i^\downarrow \]

Spin model ansatz

\[ H - F_0 = \sum_{i=1}^L \sum_{i', \omega} J_{i, \omega} S_i \cdot S_{i+\omega} \cdot \sum_{i=1}^L \sum_{\omega, \gamma} \frac{K_{\omega, \gamma}}{2} (S_i \cdot S_{i+\omega})(S_{i+\omega} \cdot S_{i+\gamma}) \]

Model selection based on the **insensitivity** to the regularization \( \lambda \)

<table>
<thead>
<tr>
<th>( A(\lambda) / A(0) )</th>
<th>optimized A w/o regul.</th>
<th>w/o regul. trapped by local minima</th>
</tr>
</thead>
<tbody>
<tr>
<td>optimized A with regul.</td>
<td>“Important” terms should survive under strong ( \lambda )</td>
<td></td>
</tr>
</tbody>
</table>
Hierarchical structure

insensitivity to the regul.

\[ J_1 \gg J_2 \gg J_3, K_2, K_3 \gg \text{others} \]

Hierarchical structure

\sim \text{order of importance?}

Simplified model

→ Estimate parameters again \textbf{WITHOUT} regul.
Comparison with perturbation theory

**Perturbation theory**


\[
\frac{J^p}{l} = \frac{4t}{U} - \frac{16t^3}{U^3} + \frac{116t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
\]


\[
\frac{J_3^p}{l} = \frac{4t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
\]

\[
\frac{K^p}{t} = -\frac{16t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
\]

\[
\frac{J_3^p}{t} = \frac{4t^3}{U^3} - \frac{120t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
\]

\[
\frac{K_3^p}{t} = -\frac{16t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
\]

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\frac{J^p}{l} = \frac{4t}{U} - \frac{16t^3}{U^3} + \frac{116t^5}{U^5} + O\left(\frac{t^7}{U^7}\right)
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\]

Difference betw. ML & Macdonald et. al.

\[
\tilde{J}_i = J_i - J_i^p \propto U^{-7}
\]

\[
\tilde{K}_i = K_i - K_i^p \propto U^{-14}
\]

Cross validation error \( \propto U^{-14} \)

Estimation is correct up to \( O(1/U^6) \)
From the viewpoint of image compression

We demonstrated the following “image compression”

\[ 4^{10} \times 4^{10} \quad \overset{\sqrt{\_\_\_}}{\longrightarrow} \quad 2^{10} \times 2^{10} \]

trillion pixel image  \quad million pixel image

preserving the 99.9999% of the essential information (for U=10).

original (30 MB) \quad \sqrt{30 \times 10^6} \sim 5 \times 10^3 \quad 5\text{KB} image
Next application: entanglement

Quantum state (w.f.) \( \rightarrow \) ED \( \rightarrow \) entanglement spectrum = spectrum of RDM \( \rightarrow \) \((ED)^{-1}\)

ED

DMRG

e tc.

ED

Physical Hamiltonian

Entanglement Hamiltonian

\[ |\psi\rangle \rightarrow \rho_A = \text{Tr}_B |\psi\rangle \langle \psi| \] reduced density matrix

\[ \lambda_1, \lambda_2, \ldots, \lambda_N \] entanglement spectrum

\[ H_A \] Entanglement Hamiltonian

\[ \rho_A \equiv e^{-H_A} \]
Thermodynamics from pure quantum state

- Reduced density matrix \( \rho_A \)
  \[
  \rho_A = \text{Tr}_B |\psi\rangle \langle \psi| 
  \]

- Entanglement entropy
  \[
  \text{EE} = -\text{tr}_A (\rho_A \log \rho_A) 
  \]
  quantum fluctuation from B

- Gibbs ensemble \( \rho_{\text{Gibbs}} \)
  \[
  \rho_{\text{Gibbs}} = \frac{1}{Z} e^{-\beta H} 
  \]

- Thermodynamic entropy
  \[
  S = -\text{tr}(\rho_{\text{Gibbs}} \log \rho_{\text{Gibbs}}) 
  \]
  thermal fluctuation from the bath

e.g. entangled two-spins

\[
|\psi\rangle_\pm = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A |\downarrow\rangle_B \pm |\downarrow\rangle_A |\uparrow\rangle_B) 
\]

\[
\text{EE} = -\text{tr}_B (\rho_B \log \rho_B) = \log 2 
\]
Entanglement Hamiltonian

Pushing forward the analogy

\[ \rho_{\text{Gibbs}} = \frac{1}{Z} e^{-\beta H} \quad \rightarrow \quad \rho_A \equiv e^{-H_A} \]

Physical Hamiltonian

Entanglement Hamiltonian

e.g. entangled two-spins

\[ |\psi\rangle_\pm = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A |\downarrow\rangle_B \pm |\downarrow\rangle_A |\uparrow\rangle_B) \]

\[ \rightarrow H_A \propto \text{id.} \equiv \text{free spin } s = 1/2 \]

Spectrum of \( \rho_A \)

\[ \lambda_1, \ldots, \lambda_N \]

(ED)\(^{-1}\) \[ \text{“log (matrix)”} \]

\[ H_A \]
Construction of Entanglement Hamiltonian

Short-ranged interactions       Few-body interactions

Symmetries such as U(1), SU(2), ... True for $H_A$ ?

Entanglement-edge correspondence

\[ H_A = H_{\text{edge}} \propto H_{\text{free}} = \text{id.} \]

Similar to physical edge Hamiltonian \( \rightarrow \) EH is local & few-body?

As long as the ent-edge corresp. holds, we can estimate EH

Comparison with other method

Full diag. of RDM: exact but computationally hard

- need all the eigenvectors of the RDM \( \rho_A \equiv e^{-H_A} \)
  
  \( \rightarrow \) strong constraint: memory size < matrix dimension

Our method: approximate but computationally cheap

- only a small number of eigenvalues \( \rightarrow \) memory efficient algos. (e.g. Lanczos)
- use of symmetry

\[ \text{e.g. magnetization conservation} \]  
\[ \text{High-spin sector} \rightarrow \text{small Hilb. space} \]

\[ \text{We can reduce dim. as long as} \]
\[ \# \text{ of evals.} > \# \text{ of params.} \]

![Graph showing Hilbert space dimension vs. number of up spins](image)

\[ \text{dim}(S^z_A = 0) = 184756 \]
\[ \text{dim}(S^z_A = 8) = 190 \]

- \( L = 20 \) \( s = 1/2 \) chain

Computational cost

\[ \text{RDM} \rightarrow \text{EH} ~ O(e^L) \]

\[ \text{RDM} \rightarrow \text{ES} ~ O(L^n) \text{ w/o transl. symm.} \]

\[ \text{ES} \rightarrow \text{EH} ~ O(1) \text{ w/ transl. symm.} \]
Not just a “Hello, World”!

Entanglement hamiltonian and entanglement contour in inhomogeneous 1D critical systems

Erik Tonni$^1$, Javier Rodríguez-Laguna$^2$ and Germán Sierra$^3$

1 SISSA and INFN, via Bonomea 265, 34136 Trieste, Italy.
2 Departamento de Física Fundamental, UNED, Madrid, Spain.
3 Instituto de Física Teórica, UAM/CSIC, Madrid, Spain.

Our analytic expressions is the rainbow model. A numerical analysis is performed for this inhomogeneous critical chain by adapting the method of [33] for the entanglement hamiltonian and the method of [27] for the contour function for the entanglement.

The Glassy Phase of Optimal Quantum Control

Alexandre G.R. Day,$^{1,\ast}$ Marin Bukov,$^2,\dagger$ Phillip Weinberg,$^1$ Pankaj Mehta,$^1$ and Dries Sels$^{1,3,4}$

$^1$Department of Physics, Boston University, 590 Commonwealth Ave., Boston, MA 02215, USA
$^2$ Department of Physics, University of California, Berkeley, CA 94720, USA
$^3$Department of Physics, Harvard University, 17 Oxford St., Cambridge, MA 02138, USA
$^4$Theory of quantum and complex systems, Universiteit Antwerpen, B-2610 Antwerpen, Belgium
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Low-energy manifold of classical spin models). Based on this data, we employ ideas from Machine Learning to learn only those properties of the coupling of the exact effective spin-energy model $H_{\text{eff}}(T)$[56, 61, 62], which influence the
Outlook: Materials design for exotic quantum states

Models written with **emergent d.o.f** (e.g. Majoranas, dimers, lattice gauge fields)

- e.g. Q. dimer model
  \[ H(V,t) = \sum V(\begin{array}{c} 1 \end{array} 1 \begin{array}{c} 2 \end{array} 1 + 1 1 \begin{array}{c} 2 \end{array} 1) - t(\begin{array}{c} 1 \end{array} 1 \begin{array}{c} 2 \end{array} 1 + 1 1 \begin{array}{c} 2 \end{array} 1) \]

- e.g. string-net condensation (lattice gauge)
  \[ H = - \sum I Q_I - \sum B_p, \quad B_p = \sum_{s=0}^{N} a_s B_p^s \]

Levin-Wen (2005)

Model of emergent d.o.f with exotic quantum state

- e.g. Majorana fermion

Energy spectrum
- = low energy spectrum of unknown parent Hamiltonian

\[ (ED)^{-1} \]

Parent Hamiltonian written with physical d.o.f (electrons, spins)

- e.g. Kitaev model

Materials design
- e.g. Honeycomb iridates
We propose a scheme to construct Hamiltonians from a given spectrum $E_1, E_2, \ldots, E_N \rightarrow H$

Energy spectrum

Entanglement spectrum

Low energy Hamiltonian

Parent Hamiltonian

Entanglement Hamiltonian