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# Model realization and model reduction for quantum systems

**Mohan Sarovar**

Scalable and Secure Systems Research

Sandia National Laboratories, Livermore, USA

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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# Outline

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- **Model realization and system identification**
  - Estimating unknown Hamiltonian parameters

arXiv:1401.5780 [pdf, other]
**Quantum Hamiltonian identification from measurement time traces**
Jun Zhang, Mohan Sarovar
Comments: 6 pages, 2 figures
Subjects: Quantum Physics (quant-ph)

- **Model reduction**
  - Reducing simulation cost for certain many-body quantum systems

arXiv:1406.7069 [pdf, other]
**On model reduction for quantum dynamics: symmetries and invariant subspaces**
Akshat Kumar, Mohan Sarovar
Comments: 24 pages, 2 figures. Comments welcome
Subjects: Quantum Physics (quant-ph); Mathematical Physics (math-ph)

# System Identification

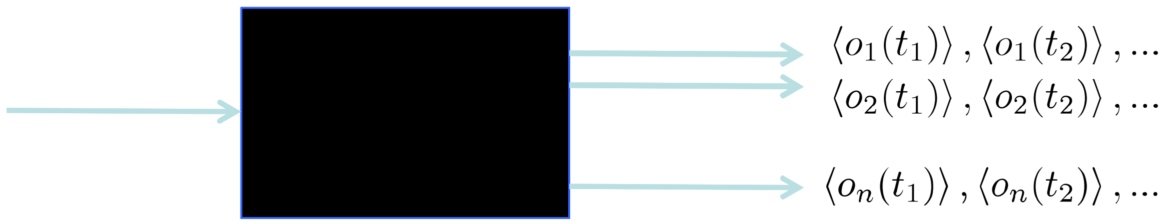
Identify system from input-output behavior

*e.g.* Process tomography: identify process (CP-map, unitary) at a particular time

Alternative: **identify generator/Hamiltonian of system**

# System Identification

How powerful are time traces?

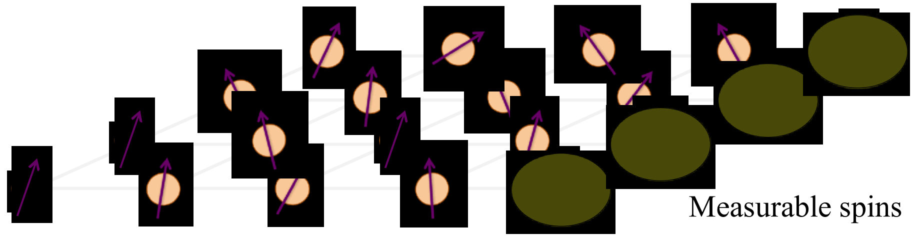



Additional considerations

- Measurements could be restricted
- May have partial information about system

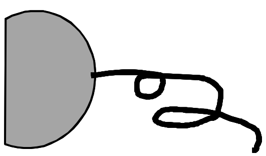
**Assumptions:**
1. system is finite dimensional
2. Hamiltonian dynamics (closed system)

# An example




Parametric Hamiltonian

$$H(\theta_1, \theta_2, \ldots, \theta_M)$$



$$\langle \sigma_z^1(t_0) \rangle, \langle \sigma_z^1(t_1) \rangle, \ldots, \langle \sigma_z^1(t_n) \rangle$$

Time trace of some accessible observable

Can we back out the parameters in the Hamiltonian from just this?

# The setup

Choose an orthogonal operator basis for the linear operator space (e.g. generalized Paulis)

$$[iX_j, iX_k] = \sum_{l=1}^{N^2-1} C_{jkl}(iX_l), \quad j,k = 1,\cdots,N^2-1,$$

Hamiltonian can be expanded in this basis

$$H = \sum_{m=1}^{M} a_m(\theta) X_m$$

**Goal**: to identify $a_m$

Leads to a linear, autonomous equation for state x(t)

$$\frac{\mathrm{d}}{\mathrm{d}t} x_k = \sum_{l=1}^{N^2-1} \left( \sum_{m=1}^{M} C_{mkl} a_m \right) x_l$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{x} = \mathbf{A}\mathbf{x}, \quad x_k(0) = \langle \psi(0) | X_k | \psi(0) \rangle$$

$|\psi\rangle \in \mathbb{C}^N$

$\dim H = N \times N$

$\mathbf{x} \in \mathbb{R}^{(N^2-1)}$

$\dim A = (N^2-1) \times (N^2-1)$

# The setup

Similarly, each directly measured observable can be expanded in the same basis. Resulting in a AC system

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x} = \mathbf{A}\mathbf{x}$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t)$$

But this may be too complex a description. E.g.

$$\mathbf{C} = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & a' & b' \\ 0 & 0 & c' & d' \end{bmatrix}$$

# Filtration to find minimal description

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$$O_i = \sum_j o_j^{(i)} X_j \qquad \mathcal{M} = \{X_{\nu_\mathbf{1}}, X_{\nu_\mathbf{2}}, \ldots, X_{\nu_\mathbf{p}}\}$$

Directly measured set

$$H = \sum_{m=1}^{M} a_m(\theta) X_m \qquad \Delta = \{X_m\}_{m=1}^{M}$$

Hamiltonian set

**Filtration** recursively constructed as:

$$G_0 = \mathcal{M}, \text{ and}$$

$$G_i = [G_{i-1}, \Delta] \cup G_{i-1}$$

where

$$[G_{i-1}, \Delta] \equiv \{X_j : \mathrm{tr}\left(X_j^\dagger [g, h]\right) \neq 0, \text{ where } g \in G_{i-1}, h \in \Delta\}$$

Finite algebra => procedure terminates, resulting in filtration $\bar{G}$

Accessible set

Results in minimal description

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_a = \tilde{\mathbf{A}}\mathbf{x}_a$$

# Sampling and discretization

$$\mathbf{x}_a(j+1) = \tilde{\mathbf{A}}_d \mathbf{x}_a(j) \qquad \tilde{\mathbf{A}}_d = e^{\tilde{\mathbf{A}}\Delta t}$$

$$\mathbf{y}(j) = \tilde{\mathbf{C}} \mathbf{x}_a(j)$$

Note: $\mathbf{x}_a(j) \equiv \mathbf{x}_a(j\Delta t)$

$\mathbf{y}(j) \equiv \mathbf{y}(j\Delta t)$

Explicit solution

$$\mathbf{y}(j) = \tilde{\mathbf{C}} \tilde{\mathbf{A}}_d^j \mathbf{x}_a(0)$$

**Goal:**

Use $\{\mathbf{y}(j)\}_{j=0}^{J}$ to estimate $\{a_m\}_{m=1}^{M}$

Strategy:

1. Find the minimal linear model that generates the collected data
2. Back out the unknown parameters from this model

# Eigenstate realization algorithm

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Step 1: Form Hankel matrix from data

$$\mathbf{H}_{rs}(k) = \begin{bmatrix} \mathbf{y}(k) & \mathbf{y}(k+1) & \cdots & \mathbf{y}(k+(s-1)) \\ \mathbf{y}(j_1+k) & \mathbf{y}(j_1+k+1) & \cdots & \mathbf{y}(j_1+k+(s-1)) \\ \vdots & \vdots & & \vdots \\ \mathbf{y}(j_{r-1}+k) & \mathbf{y}(j_{r-1}+k+1) & \cdots & \mathbf{y}(j_{r-1}+k+(s-1)) \end{bmatrix}$$

Step 2: Take SVD of Hankel matrix at k=0

$$\mathbf{H}_{rs}(0) = P \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} Q^{\mathsf{T}} = \begin{bmatrix} P_1 & P_2 \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^{\mathsf{T}} \\ Q_2^{\mathsf{T}} \end{bmatrix}$$

Step 3: Form realizations of linear model from SVD components

$$\hat{\mathbf{A}}_d = \Sigma^{-\frac{1}{2}} P_1^{\mathsf{T}} \mathbf{H}_{rs}(1) Q_1 \Sigma^{-\frac{1}{2}}, \qquad \hat{\mathbf{C}} = \mathsf{E}_p^{\mathsf{T}} P_1 \Sigma^{\frac{1}{2}},$$

$$\hat{\mathbf{x}}(0) = \Sigma^{\frac{1}{2}} Q_1^{\mathsf{T}} e_1,$$

# Realization to parameter estimation

The triple $(\hat{\mathbf{A}}_d, \hat{\mathbf{C}}, \hat{\mathbf{x}}(0))$ is a realization of the triple $(\tilde{\mathbf{A}}_d, \tilde{\mathbf{C}}, \mathbf{x}_a(0))$

$$\mathbf{y}(j) = \mathbf{C}\tilde{\mathbf{A}}_d^j \mathbf{x}_a(0) = \hat{\mathbf{C}}\hat{\mathbf{A}}_d^j \hat{\mathbf{x}}(0), \quad \text{for all } j \geq 0,$$

Markov parameters – model realization invariants

Define $\hat{\mathbf{A}} = \log \hat{\mathbf{A}}_d / \Delta t$

Expanding the exponential in a power series and equating terms,

$$\mathbf{C}\tilde{\mathbf{A}}^j \mathbf{x}_a(0) = \hat{\mathbf{C}}\hat{\mathbf{A}}^j \hat{\mathbf{x}}(0), \quad \text{for all } j \geq 0$$

*Determined by the data*

*Polynomial equation in unknown parameters*

# Realization to parameter estimation

$$\mathbf{C}\tilde{\mathbf{A}}^j \mathbf{x}_a(0) = \hat{\mathbf{C}}\hat{\mathbf{A}}^j \hat{\mathbf{x}}(0), \quad \text{for all } j \geq 0$$

*Determined by the data*

*Polynomial equation in unknown parameters*

Solving these equations yields estimates of parameters

Notes:

1. Parameter estimates can be non-unique (gauge freedom/symmetries)
2. $\Delta t$ must be small enough

   How small? Smaller than one-over-fastest-frequency

# Example

## XX spin chain


Fukuhara et al. Nature Physics, **9** 235 (2013)

$$H = \sum_{k=1}^{n} \frac{\omega_k}{2}\sigma_z^k + \sum_{k=1}^{n-1} \delta_k \left(\sigma_+^k \sigma_-^{k+1} + \sigma_-^k \sigma_+^{k+1}\right)$$

$$\mathcal{M} = \sigma_x^1$$

Measure end spin

$$\bar{G} = \{2^{-n/2}\sigma_x^1, \quad 2^{-n/2}\sigma_y^1\} \cup \{2^{-n/2}\sigma_z^1 \cdots \sigma_z^{k-1}\sigma_x^k, \quad 2^{-n/2}\sigma_z^1 \cdots \sigma_z^{k-1}\sigma_y^k\}_{k=2}^{n}$$

Filtration (generalized Pauli basis)

$$\tilde{\mathbf{A}} = \begin{bmatrix} 0 & \omega_1 & 0 & -\delta_1 & & & & \\ -\omega_1 & 0 & \delta_1 & 0 & 0 & & & \\ 0 & -\delta_1 & 0 & \omega_2 & 0 & \ddots & & \\ \delta_1 & 0 & -\omega_2 & 0 & \ddots & \ddots & 0 & \\ & 0 & \ddots & \ddots & \ddots & \ddots & \ddots & -\delta_{n-1} \\ & & \ddots & \ddots & \ddots & 0 & \delta_{n-1} & 0 \\ & & & 0 & 0 & -\delta_{n-1} & 0 & \omega_n \\ & & & & \delta_{n-1} & 0 & -\omega_n & 0 \end{bmatrix}$$

Filtered system matrix is *2n x 2n* (as opposed to *$2^n$ x $2^n$*)

$$\mathbf{x}_a = [\bar{x}_1, \bar{y}_1, \ldots, \bar{x}_n, \bar{y}_n]^{\mathsf{T}}$$

$$\bar{x}_1 = \langle \sigma_x^1 \rangle, \bar{y}_1 = \langle \sigma_y^1 \rangle$$

$$\bar{x}_k \equiv \langle \sigma_z^1 \cdots \sigma_z^{k-1} \sigma_x^k \rangle,$$

$$\bar{y}_k \equiv \langle \sigma_z^1 \cdots \sigma_z^{k-1} \sigma_y^k \rangle, \quad k \geq 2$$

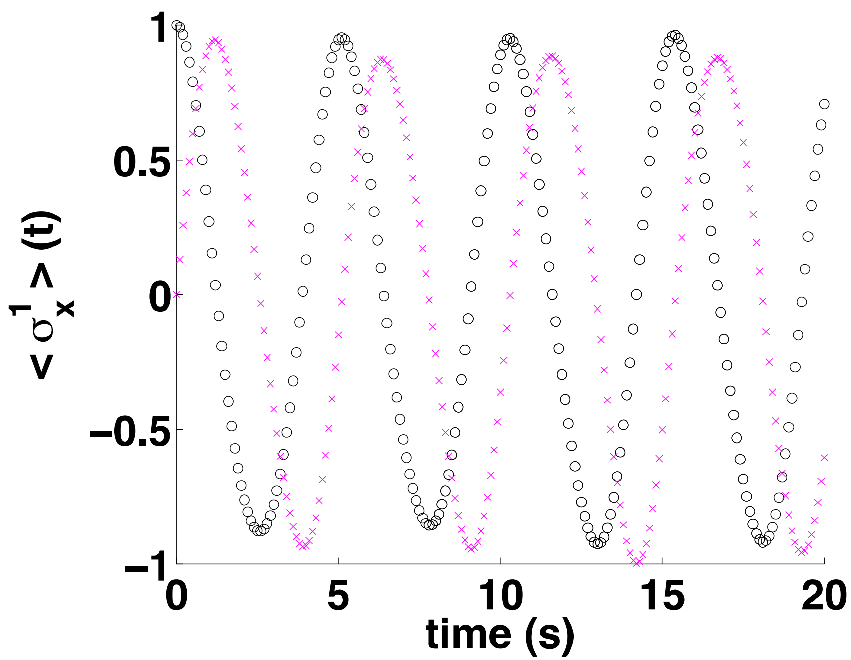
# Example



**XX spin chain (*n*=3 qubits)**

$$H = \sum_{k=1}^{3} \frac{\omega_k}{2} \sigma_z^k + \sum_{k=1}^{2} \delta_k \left( \sigma_+^k \sigma_-^{k+1} + \sigma_-^k \sigma_+^{k+1} \right)$$

$$\omega_1 = 1.3, \omega_2 = 2.4, \omega_3 = 1.7, \delta_1 = 0.3, \delta_2 = 0.2$$




○ $\frac{|0\rangle + |1\rangle}{\sqrt{2}}|00\rangle$

✖ $\frac{|0\rangle + i|1\rangle}{\sqrt{2}}|00\rangle$

# Example

**XX spin chain (*n*=3 qubits)**

$$H = \sum_{k=1}^{3} \frac{\omega_k}{2} \sigma_z^k + \sum_{k=1}^{2} \delta_k \left( \sigma_+^k \sigma_-^{k+1} + \sigma_-^k \sigma_+^{k+1} \right)$$

$$\omega_1 = 1.3, \omega_2 = 2.4, \omega_3 = 1.7, \delta_1 = 0.3, \delta_2 = 0.2$$

Construct Hankel matrix with $r$=100, $s$=100 and all $j_i$=1

$$\begin{aligned}
\omega_1 &= & \hat{\mathbf{C}}_2 \hat{\mathbf{A}}_2 \hat{\mathbf{x}}_2(0) &= & 1.3 \\
\omega_1^2 + \delta_1^2 &= & -\hat{\mathbf{C}}_1 \hat{\mathbf{A}}_1^2 \hat{\mathbf{x}}_1(0) &= & 1.78 \\
\omega_1^3 + \delta_1^2(2\omega_1 + \omega_2) &= & -\hat{\mathbf{C}}_2 \hat{\mathbf{A}}_2^3 \hat{\mathbf{x}}_2(0) &= & 2.647 \\
\omega_1^4 + \delta_1^2(3\omega_1^2 + 2\omega_1\omega_2 + \omega_2^2 + \delta_1^2 + \delta_2^2) &= & \hat{\mathbf{C}}_1 \hat{\mathbf{A}}_1^4 \hat{\mathbf{x}}_1(0) &= & 4.4041 \\
\delta_1^4 (3\omega_1 + 2\omega_2) + \delta_1^2 \left( \delta_2^2 (2\omega_1 + 2\omega_2 + \omega_3) + 4\omega_1^3 + 3\omega_2\omega_1^2 + 2\omega_2^2\omega_1 + \omega_2^3 \right) + \omega_1^5 &= & \hat{\mathbf{C}}_2 \hat{\mathbf{A}}_2^5 \hat{\mathbf{x}}_2(0) &= & 8.2942
\end{aligned}$$

Coupling parameters only occur up to even order (symmetry) => can only be determined up to sign

# Summary

- System identification through model realization
- Most useful when
  - measurements are restricted
  - prior information about process is available
- Continuing work:
  - Noisy measurements
    - Use a different model realization invariant (transfer function)
  - Markovian open-system evolution

# Outline

- **Model realization and system identification**
  - Estimating unknown Hamiltonian parameters
- **Model reduction**
  - Reducing simulation cost for certain many-body quantum systems

arXiv:1406.7069 [pdf, other]

**On model reduction for quantum dynamics: symmetries and invariant subspaces**

Akshat Kumar, Mohan Sarovar

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# Outline

## Quantum state space: exponential

- Full-scale simulation of quantum systems very difficult
  - "Hilbert space is a big place" – Carl Caves

- Formal state is exponentially large in the number of particles

$$\rho_1 \in \mathcal{H}_1 \qquad \dim\mathcal{H}_1 = n_1$$

$$\rho_2 \in \mathcal{H}_2 \qquad \dim\mathcal{H}_2 = n_2$$

$$\rho_c \in \mathcal{H}_1 \otimes \mathcal{H}_2 \qquad \dim\mathcal{H}_1 \otimes \mathcal{H}_2 = n_1 n_2 \neq n_1 + n_2$$

# Outline

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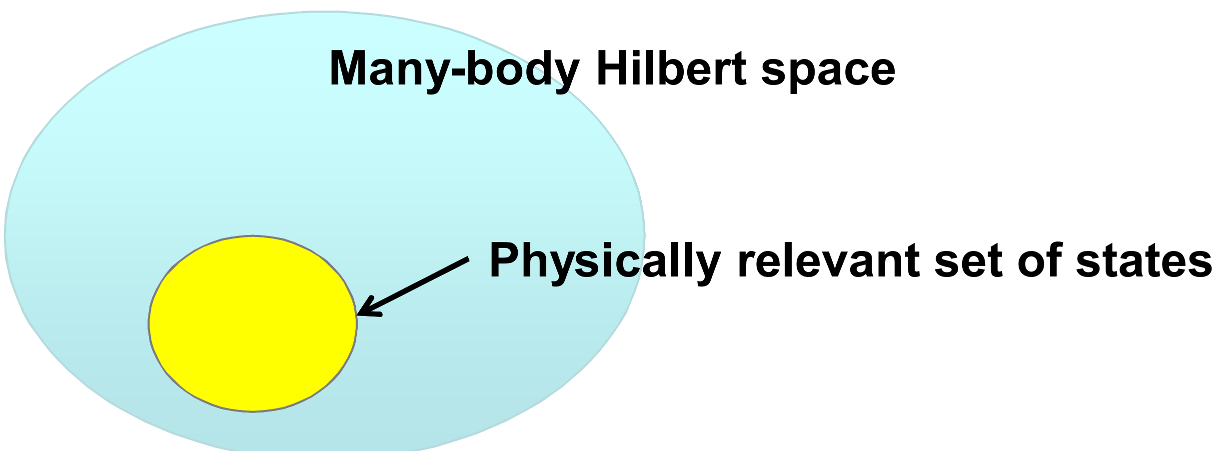
## Quantum state space: not really exponential?

- For most practical systems, this exponential scaling is only formal

PRL **106,** 170501 (2011) PHYSICAL REVIEW LETTERS week ending 29 APRIL 2011

**Quantum Simulation of Time-Dependent Hamiltonians and the Convenient Illusion of Hilbert Space**

David Poulin,[1] Angie Qarry,[2,3] Rolando Somma,[4] and Frank Verstraete[2]

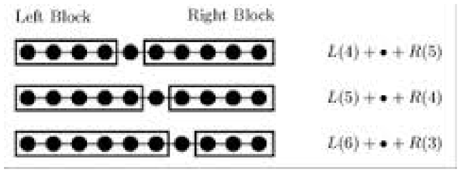


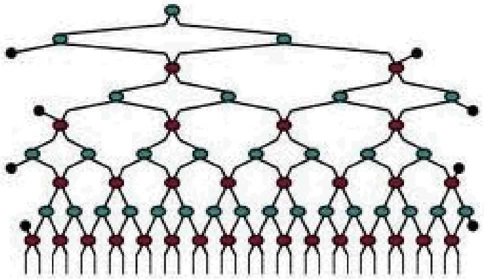

- Identifying this set of relevant states is difficult

# Identifying reduced order models

**Techniques in physics:**

- static: DMRG, MPS, etc.



- dynamic: Nakajima-Zwanzig (statistical), Bloch equations, Glauber dynamics

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P}x(t) = {} & \mathbf{PAP}x(t) + \mathbf{PB}u(t) \\
& + \mathbf{PA}\mathcal{G}(t,0)\mathbf{Q}x(0) \\
& + \int_0^t \mathbf{PA}\mathcal{G}(t,s)\mathbf{QAP}x(s)ds \\
& + \int_0^t \mathbf{PA}\mathcal{G}(t,s)\mathbf{QB}u(s)ds.
\end{aligned}
$$

# Model reduction

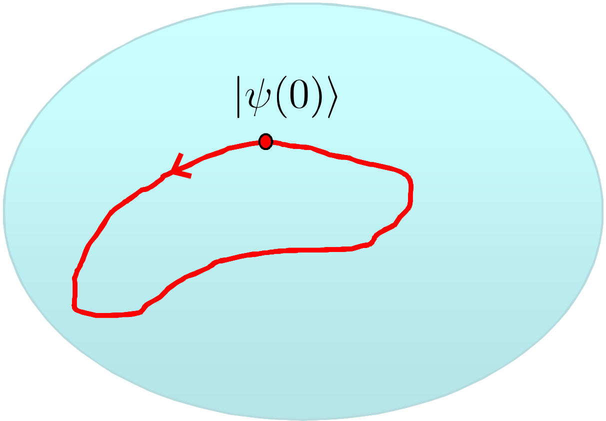
| Resources available / Desired Output | State snapshots | Input-output map | Dynamical model |
|---|---|---|---|
| Full state vector<br>want to reproduce $\|\psi(t)\rangle$ | Proper orthogonal decomposition (POD) | - | Identify invariant subspaces |
| Input-output map<br>want to reproduce *y(t)* | Empirical balanced truncation (BPOD) | Minimal model realization algorithms | Balanced truncation |

# Compressible dynamics

$$|\psi(t)\rangle = e^{iHt}\,|\psi(0)\rangle$$

$$H = \sum_i \lambda_i h_i$$

e.g. adiabatic QC




**Problem:**

Identify subspace of Hilbert space that contains $|\psi(0)\rangle$

and is invariant under Hamiltonian for all choices of $\lambda$

Projective model reduction: columns of P are basis vectors in this invariant subspace

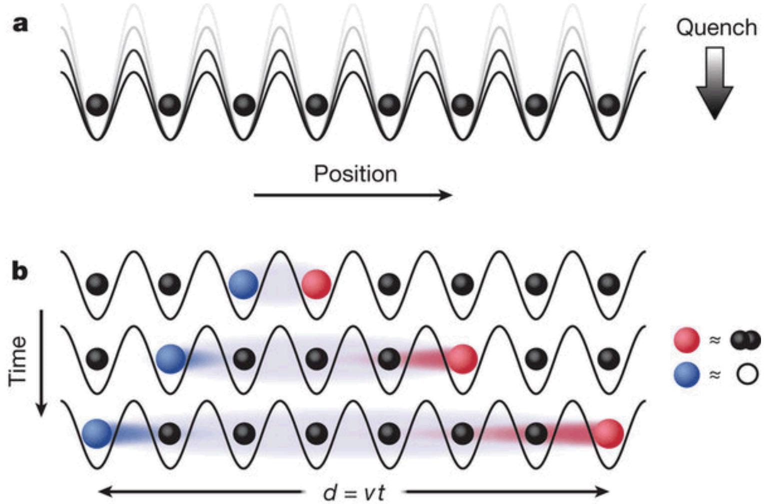
$$\frac{\mathrm{d}}{\mathrm{d}t} P\,|\psi(t)\rangle = P^\dagger H P\,|\psi(t)\rangle \qquad \mathrm{dim} P = N \times q, \quad q \ll N$$

q x q compressed description

# *E.g.* Quench dynamics

Can identify many important features of many-body model by looking at dynamics after quench

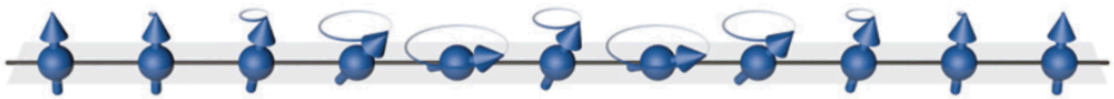
Especially relevant now with cold-atom quantum simulators that are capable of quenched dynamics




Cheneau et al. Nature, **481** 484 (2012)

# *E.g.* Quench dynamics

## Quantum Ising model




Fukuhara et al. Nature Physics, **9** 235 (2013)

$$H = -B \sum_i \sigma_x^i - J \sum_{<i,j>} \sigma_z^i \sigma_z^j$$

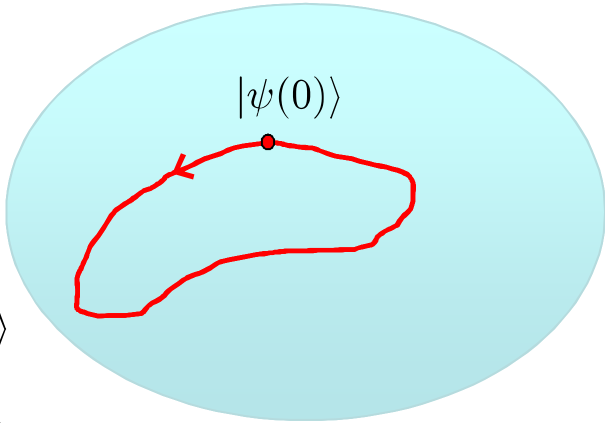
- Basic model for magnetism in crystalline material
- Competition between B and J results in phase transition behavior
- Can be emulated using cold atoms
- As a result: intense interest in dynamical phase transitions, quenching dynamics

Quenching dynamics:

1. Prepare ground state of $H^0 = -B^0 \sum_i \sigma_x^i - J \sum_{<i,j>} \sigma_z^i \sigma_z^j$
1. Rapidly change B and evolve system under $H^1 = -B^1 \sum_i \sigma_x^i - J \sum_{<i,j>} \sigma_z^i \sigma_z^j$
1. The resulting dynamics is very informative; *e.g.* contains information about static phases of system

# Compressible dynamics

$$H = \sum_i \lambda_i h_i$$




**Problem:**

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**Assumptions:**

1. system is finite dimensional
2. Hamiltonian dynamics (closed system)

1. Certificates
   1. Is this dynamics compressible?
2. Computing reduced order models
   1. What is the invariant subspace and moreover, what is the compressed dynamical model?

# Certificate

$$H = \sum_i \lambda_i h_i$$

$$H \in L(\mathcal{H}) \qquad \dim \mathcal{H} = N$$

$$\mathrm{Coeff}(H) \equiv \{h_i\}$$

Theorem: (algebraic certificate)

The Hamiltonian acting on $\mathcal{H}$ keeps invariant a non-trivial proper subspace iff the subalgebra generated by $\mathrm{Coeff}(H)$ is a proper subalgebra of $L(\mathcal{H})$.

Intuition:

$$|\psi(t)\rangle = \exp\{i(\lambda_1 h_1 + \lambda_2 h_2)t\}\, |\psi(0)\rangle$$

$$|\psi(t)\rangle = \sum_n \frac{(it)^n}{n!} (\lambda_1 h_1 + \lambda_2 h_2)^n \, |\psi(0)\rangle$$

Products of $h_i$ generate an algebra. If the full operator algebra is not generated, there are directions not explored in state space

# Certificate
## Special case: Pauli Hamiltonian

$$H = \sum_i \lambda_i \sigma_i$$

$$H \in L(\mathcal{H}) \qquad \mathcal{H} = \mathbb{C}^{2n}$$

$$\text{Coeff}(H) \equiv \{h_i\} \qquad \dim \mathcal{H} = 2^n$$

$$\sigma_i : \sigma_x^{(1)} \otimes \mathbf{1} \otimes \ldots \otimes \sigma_y^{(n)}$$

Theorem: (Pauli algebraic certificate)

Any Pauli Hamiltonian acting on n qubits with fewer than 2n terms has a non-trivial proper invariant subspace.

e.g. Quantum (transverse field) Ising model with random couplings and energies

# Example: quench dynamics

## Quantum Ising model


Fukuhara et al. Nature Physics, **9** 235 (2013)

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1. The resulting dynamics is very informative; *e.g.* contains information about static phases of system

# Example

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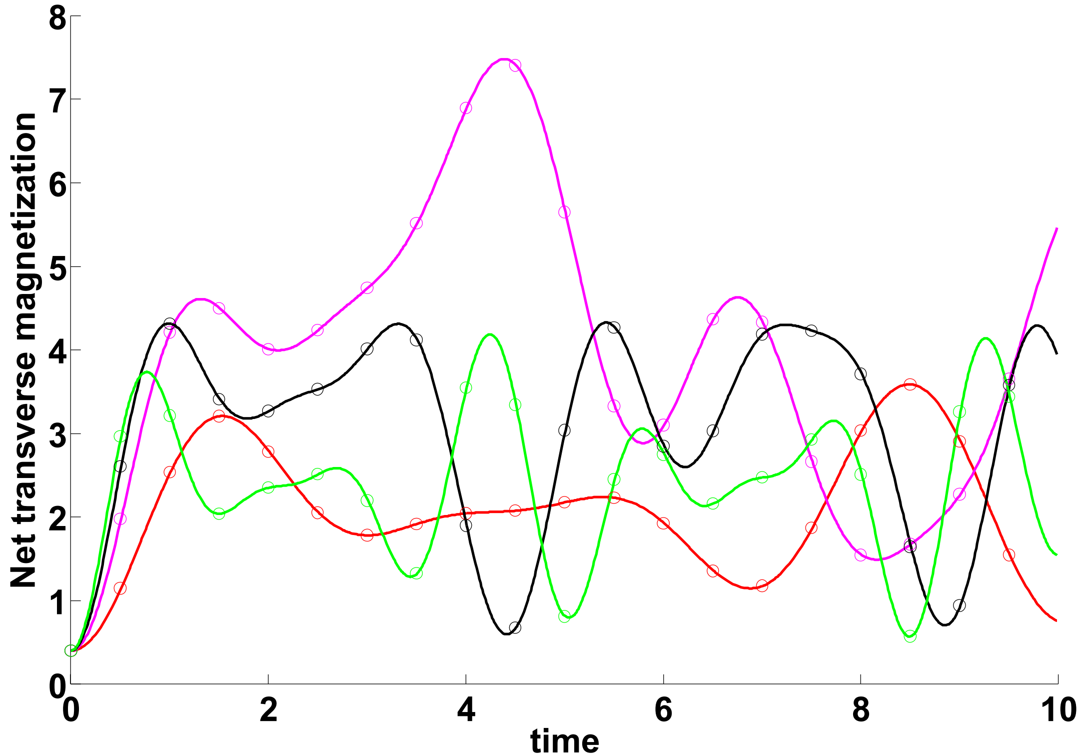
## POD-based model reduction to simulate quenching dynamics of the quantum Ising model

Simulation of quench dynamics in quantum Ising model
(Circles: full model, lines: reduced order model)

Quenches to different parameters are indicated by different colors




N=8 qubits

Full order model:
$2^8$-1 = 255 complex numbers

Reduced order model:
23 complex numbers

Order of magnitude improvement in simulation complexity

# Conclusions and continuing work

- The exponentially scaling of simulation complexity of many-body quantum dynamics may be an “illusion” in many cases

- Model reduction techniques can identify the relevant set of states

- In extreme cases, there may be invariant subspaces
  - Have developed certificates to identify such cases

- Continuing work
  - Develop practical methods for constructing reduced order models
  - Develop code to implement model reduction techniques

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**Model reduction**

Akshat Kumar
Kevin Carlberg
Sandia National Laboratories, Livermore

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