Estimating Eigenenergies from Quantum Dynamics: A Unified Noise-Resilient Measurement-Driven Approach

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Introduction

Simulating many body dynamics i.e., we want to find the ground state of many body system energy.

- e.g., If we have some molecules, how do we find the ground state energy?
- We begin by formalising this using the time-independent Schrödinger equation:

$$H|\psi\rangle = E|\psi\rangle$$

- where $H \in \mathbb{C}^{d \times d}$, $d \gg 1$ is the Hamiltonian operator.
- (Takes the form of an eigenvalue problem)

Difficulty/ Our Method

- **Difficulty** The above stated problem is computationally hard to solve for classical computers because it grows exponentially.

- **Method**: Hybrid approach, this finds the eigenenergies by collecting real-time measurements and post-processing them using the machinery of dynamic mode decomposition (DMD).

Previous Methods

- **Variational Quantum Eigensolver (VQE)**: A variational approach that uses a parameterized quantum circuit (ansatz) and classical optimization to minimize the energy expectation value.
- **Ansatz**:

$$|\psi(\theta)\rangle = U(\theta)|0\rangle$$

  where $U(\theta)$ is a parameterized circuit (e.g., hardware-efficient or problem-specific ansatz).

$$\min_{\theta} E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

- **Deficiency**: Sensitive to ansatz choice; Difficult to optimize (barren plateaus).

Introduction to Subspace Methods

- Recent studies have proposed subspace methods.
- These methods project the many-body Schrödinger equation onto a subspace of the Hilbert space.
- The subspace is constructed through real-time evolution.

Generalized Eigenvalue Equations

- These approaches yield generalized eigenvalue equations built from non-orthogonal real-time basis states.
- Subspace Hamiltonian and overlap matrix elements are defined as:

$$H_{ij} = \langle \phi_i | H | \phi_j \rangle = \langle \phi_0 | e^{iHt_i} H e^{-iHt_j} | \phi_0 \rangle , \tag{1}$$

$$S_{ij} = \langle \phi_i | | \phi_j \rangle = \langle \phi_0 | e^{iH(t_i - t_j)} | \phi_0 \rangle . \tag{2}$$

The matrix elements H_{ij} and S_{ij} are obtained through measurements on quantum hardware.

Generalized Eigenvalue Problem

- The resulting projected eigenvalue problem, $H\Psi = \tilde{E}S\Psi$, is then solved classically to estimate approximate energies $\tilde{E}$. Ψ is the column vector

- Examples of methods using this approach include Quantum Filter Diagonalization (QFD) and the Variational Quantum Phase Estimation (VQPE) method, which both use a uniform timestep grid $t_j = j\Delta t$.

Unitary Variational Quantum Phase Estimation (UVQPE)

- **L**ike VQPE, UVQPE solves a generalized eigenvalue problem but employs unitary projections.
- **Deficiency**: Computationally intensive; significant classical resources needed and limitations in resolving low-energy eigenvalues if overlap with initial states is low.

Quantum Complex Exponential Least Squares(QCELS)

- The optimization problem:

$$\tilde{E} = \arg\min_{\theta\in\mathbb{R}} \min_{r\in\mathbb{C}} \frac{1}{N} \sum_{n=0}^{N-1} |Z_n - re^{-it_n\theta}|^2$$

  seeks the best (r, θ) to fit quantum data
- QCELS works well when an initial state $|\phi_0\rangle$ has significant overlap with the desired eigenstates. Under these conditions:
- **Difficulty**: Finding suitable initial states with high eigenstate overlap is challenging.

Quantum Circuit

Time-evolved overlaps of the form $\langle\phi|U|\phi\rangle$ (where U is a unitary operator) can be measured using projective quantum measurements, specifically through the Hadamard test.

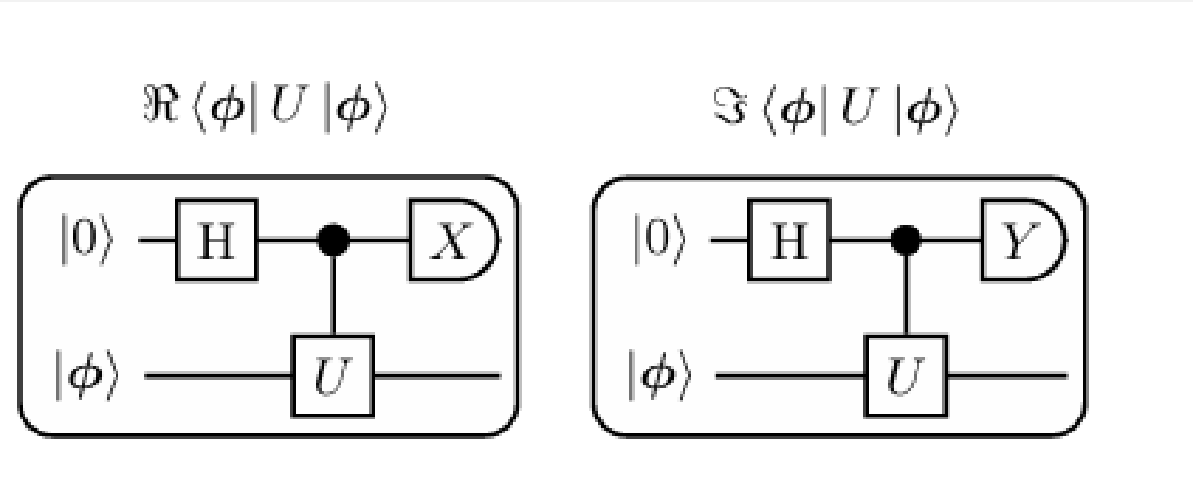

Figure: Hadamard testt circuit

The ancilla is measured in the Pauli-X basis to get the real part of $\langle\phi|U|\phi\rangle$, and in the Pauli-$Y$ basis to get the imaginary part.

More details on circuit

The Hadamard operator H is given by:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

The Pauli-X measurement basis states are:

$$|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle)$$

The Y-basis gate are:

$$|i\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm i|1\rangle)$$

For the probability $p(+)$ of measuring $|+\rangle$, we have:

$$p(+) = \langle\psi|P_+|\psi\rangle, \quad \text{where} \quad P_+ = |+\rangle\langle+|$$

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle \otimes |\phi\rangle + |1\rangle \otimes U|\phi\rangle)$$

DMD: Approximating Nonlinear Dynamics with a Linear Model

Goal: Approximate a nonlinear dynamical system

$$\frac{d\vec{x}}{dt} = f(\vec{x}), \quad \vec{x} \in \mathbb{C}^n,$$

with a linear system

$$\frac{d\vec{x}}{dt} \approx A\vec{x}.$$

- We seek the best linear operator A to capture the dynamics of $\vec{x}$.

Assumption: Access to Full State Measurements

Assume we can directly measure the full state $\vec{x}$ at discrete times t_j:

$$\vec{x}_j = \vec{x}(t_j), \quad \vec{x}_j \in \mathbb{C}^n.$$

Snapshot Matrices: Organize measurements into:

$$X = \begin{bmatrix} \vec{x}_1 & \vec{x}_2 & \dots & \vec{x}_{m-1} \end{bmatrix}, \quad X' = \begin{bmatrix} \vec{x}_2 & \vec{x}_3 & \dots & \vec{x}_m \end{bmatrix}.$$

Finding the Best-Fit Matrix A

Solve for A in $AX = X'$ by minimizing the residual $\|X' - AX\|_F$:

$$A = X'X^+,$$

where X^+ is the pseudoinverse of X.

Quantum Mechanics Analogy

In Quantum Mechanics: The time-dependent Schrödinger equation:

$$i\hbar \frac{d\psi(t)}{dt} = H\psi(t),$$

describes the evolution under Hamiltonian H.
But we don't have full access to $\psi(t)$, i.e, we do not have direct access to the full many-body quantum state. Instead, we can only access the state of a quantum system via measurement sampling of observables

Dynamic Mode Decomposition (DMD)

- **Origins:** DMD, initially developed in numerical fluid dynamics, approximates the temporal progression of dynamical systems by analyzing measurement snapshots over time.
- **Purpose:** DMD constructs an efficient representation of the full trajectory of an N-dimensional system state manifold $\mathbb{C}^N$ using snapshots at intervals Δt.
- **Least-Squares (LS) Approximation:**

$$\phi_{k+1} \approx A_k \phi_k \tag{3}$$

  where $A_k \in \mathbb{C}^{N \times N}$ minimizes the residual $\|\phi_{k+1} - A_k \phi_k\|$.
- **Extended to Sequence of Snapshots:**

$$\begin{bmatrix} \phi_1 & \dots & \phi_{K+1} \end{bmatrix} \approx A \begin{bmatrix} \phi_0 & \dots & \phi_K \end{bmatrix} \tag{4}$$

- **Temporal Dynamics:** The approximate dynamics $\phi_{\text{DMD}}(t) = A^{t/\Delta t} \phi_0$ are governed by the **eigenvalues** and **eigenvectors** of A, which define the system's evolution modes.

Takens' Embedding Theorem

Theorem Statement

Takens' Embedding Theorem: For pairs (ϕ, y), where $\phi : M \to M$ is a smooth diffeomorphism and $y : M \to \mathbb{R}$ is a smooth function, it is generically possible to embed the manifold M in $\mathbb{R}^{2d+1}$ using the delay-coordinate map:

$$\Phi_{(\phi,y)}(x) = \left(y(x), y(\phi(x)), y(\phi^2(x)), \ldots, y(\phi^{2d}(x))\right),$$

where d is the dimension of M. This embedding allows the reconstruction of the state space from a time series of observations.

here, "smooth" means at least C^2

Comparison Between Classical and Quantum Takens' Theorem

Feature	**Classical Takens' Theorem**	**Quantum Adaptation**
System	Classical dynamical system on a manifold M	Quantum system evolving in a Hilbert space
Transformation	Smooth diffeomorphism $\phi : M \to M$	Unitary time evolution e^{-iHt} governed by a Hamiltonian H
Observable	Single smooth function $y : M \to \mathbb{R}$	Single quantum observable function $o(t) = o[\phi(t)]$, where $\phi(t)$ represents the evolving state
Embedding Map	$\Phi_{(\phi,y)}(x) = (y(x), y(\phi(x)), \ldots, y(\phi^{2d}(x)))$	$o_{t,d^*} = [o(t), o(t+\Delta\tau), \ldots, o(t+(d^*-1)$
Goal	Reconstruct the state space M using delay-coordinate map	Approximate quantum state dynamics using time-delayed observable overlaps
Key Insight	Time-delayed measurements reconstruct M	Observable trajectories capture quantum dynamics without full state access

$$d* \leq 2N + 1$$

Observable Dynamic Mode Decomposition (ODMD) - Time Delay and Measurement Steps

Setting the Time Delay

To efficiently leverage near-term quantum resources, we set the time delay in Takens' embedding to match the DMD time interval, $\Delta\tau = \Delta t$.

Measurement Steps and Observable Trajectories

We measure the system at time steps $\{t_k = k\Delta t\}_{k=0}^{K+1}$, constructing observable trajectories $\mathbf{o}_{t_k,d}$ of length $d \leq d*$:

$$\mathbf{o}_{t_k,d} = \begin{bmatrix} o(t_k) \\ o(t_{k+1}) \\ \vdots \\ o(t_{k+d-1}) \end{bmatrix}, \quad 0 \leq k \leq K+1.$$

Observable Dynamic Mode Decomposition (ODMD) - Hankel Matrix and Linear Flow Approximation

Hankel Matrix Form

By construction, the first $d-1$ entries of $\mathbf{o}_{t_k,d}$ are identical to the last $d-1$ entries of $\mathbf{o}_{t_{k-1},d}$. Arranging successive trajectories as columns forms a Hankel matrix $X_{k_1:k_2}$:

$$X_{k_1:k_2} = \begin{bmatrix} \mathbf{o}_{t_{k_1},d} & \mathbf{o}_{t_{k_1+1},d} & \cdots & \mathbf{o}_{t_{k_2},d} \end{bmatrix},$$

where each anti-diagonal contains equal elements.

Linear Flow Approximation

In the embedding space, we approximate the system's linear flow using least-squares:

$$X_{1:K+1} \approx A X_{0:K} \Rightarrow A = X_{1:K+1} \left(X_{0:K}\right)^{+},$$

where $(\cdot)^{+}$ denotes the Moore–Penrose pseudo-inverse. The matrix A takes a companion form with d free parameters, representing the system dynamics. This approach is called **Observable Dynamic Mode Decomposition (ODMD)**.

Estimating the Ground State Energy with ODMD

Setup and Observable Matrices

For a quantum system with Hamiltonian H and eigenenergies $E_0 \leq E_1 \leq \cdots \leq E_{N-1}$, the system dynamics follow the time evolution operator e^{-iHt} (using $\hbar = 1$). We define the observable overlap:

$$s(k\Delta t) = \langle \phi_0 | e^{-iHk\Delta t} | \phi_0 \rangle,$$

where $\mathrm{Re}(s)$ and $\mathrm{Im}(s)$ can be measured using techniques like the Hadamard test.

Constructing Observable Matrices

Arrange the delayed overlaps into data matrices X and X' as follows:

$$X = X_{0:K}, \quad X' = X_{1:K+1} \quad \text{with } X, X' \in \mathbb{C}^{d \times (K+1)}.$$

Here, we choose $d = \lfloor \alpha(K+1) \rfloor$ with $\alpha = \frac{1}{2}$.

$$X' = \begin{bmatrix} s(t_1) & s(t_2) & \cdots & s(t_K) \\ s(t_2) & s(t_3) & \cdots & s(t_{K+1}) \\ \vdots & \vdots & \ddots & \vdots \\ s(t_d) & s(t_{d+1}) & \cdots & s(t_{K+d-1}) \end{bmatrix}$$

Solving for Eigenenergies

Eigenvalue Problem

The Hamiltonian's eigenenergies are estimated by solving the eigenvalue problem:

$$A\Psi_\ell = \tilde{\lambda}_\ell \Psi_\ell,$$

where $A = X'X^+$ and $(\cdot)^+$ denotes the Moore–Penrose pseudo-inverse.

Extracting Ground State Energy

The eigenvalues $\tilde{\lambda}_\ell$ of A provide energy estimates through their phases:
Under mild assumptions on Δt, the eigenvalue $\tilde{\lambda}_0$ of A with $\arg(\tilde{\lambda}_0) = \max_\ell \arg(\tilde{\lambda}_\ell)$ converges to the true ground state phase λ_0 as the size of X and X' increases. The ground state energy is estimated as

$$E_0 = -\frac{\arg(\tilde{\lambda}_0)}{\Delta t}.$$

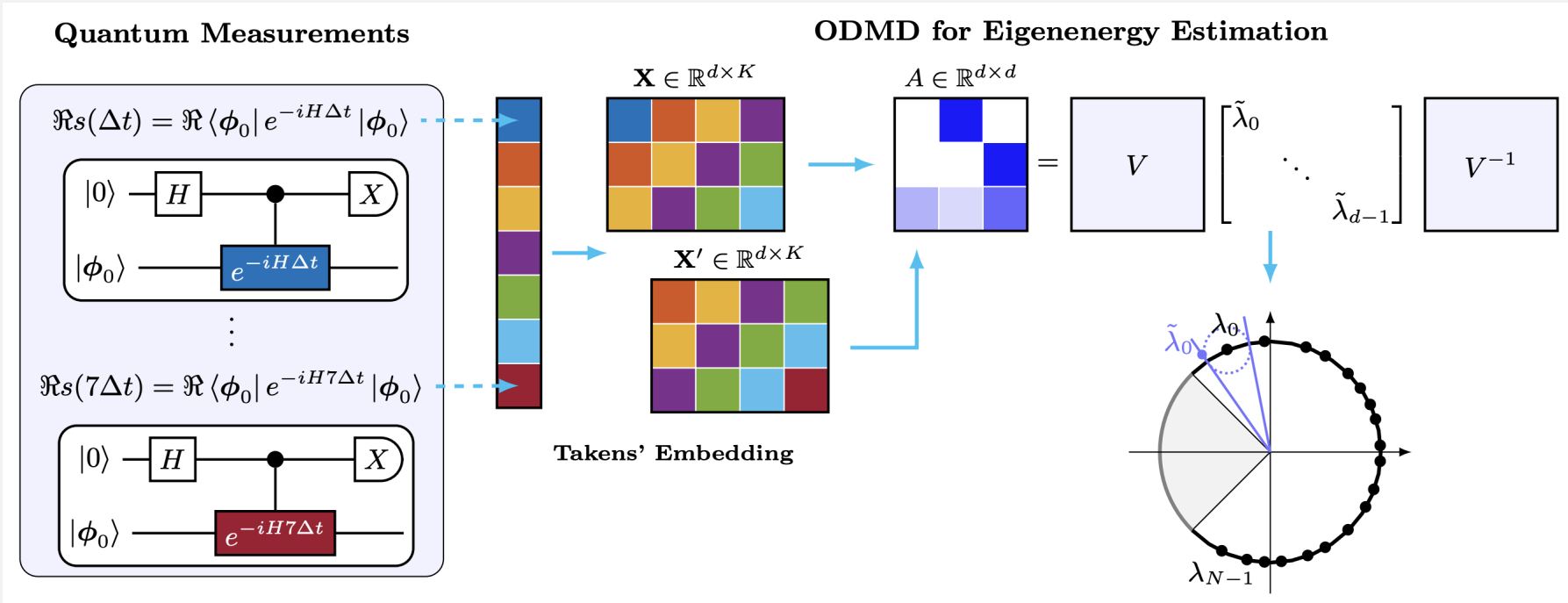

Figure: FIG. 2. ODMD applied to eigenenergy estimation

Regularization for Noise Resilience in ODMD

Singular Value Decomposition (SVD)

To improve conditioning, we use the Singular Value Decomposition (SVD) of X:

$$X = \sum_{\ell=0}^{d-1} \sigma_\ell u_\ell v_\ell^\dagger,$$

where $\sigma_\ell > 0$ are the singular values, and (u_ℓ, v_ℓ) are the associated left and right singular vectors.

Thresholding Small Singular Values

We apply a thresholding procedure to filter out small, noise-sensitive singular values: - Singular values smaller than $\tilde{\delta}\sigma_{\max}$ are truncated, where:

$$\tilde{X}_{\tilde{\delta}} = \sum_{\ell:\sigma_\ell > \tilde{\delta}\sigma_{\max}} \sigma_\ell u_\ell v_\ell^\dagger.$$

- Here, $\sigma_{\max} = \max_\ell \sigma_\ell$ is the largest singular value, and $\tilde{\delta} > 0$ is a relative threshold chosen to control noise.

Algorithm 1: ODMD Ground State Energy Estimation

Input

Time step Δt, noise threshold $\tilde{\delta}$.

Output

Estimated ground state energy $\tilde{E}_0$.

1. Initialize $k \leftarrow 0$
2. **while** not converged **do**
   1. $s_k \leftarrow \Re(s(k\Delta t))$ // quantum measurement
   2. Construct Hankel matrices $X, X' \leftarrow \text{Hankel}(s_0, s_1, \ldots, s_k)$
   3. Apply least-squares regularization: $X_{\tilde{\delta}} \leftarrow X$
   4. Update system matrix $A \leftarrow X' X_{\tilde{\delta}}^{+}$
   5. Update ground state energy $\tilde{E}_0 \Delta t \leftarrow -\max_{1 \le \ell \le d_k} \Im(\log(\tilde{\lambda}_\ell))$
   6. $k \leftarrow k + 1$
3. **end while**