Quantum Krylov Diagonalization

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1 Introduction

Eigenvalue problem is crucial in high energy physics, condensed matter physics, quantum chemistry, and nuclear physics. There are two main type of quantum-classical eigensolver algorithms out there.

1. Variational Quantum Eigensolver(VQE) which utilizes the quantum computer estimate a physical observable, then classically optimize quantum circuit's parameters.
2. Quantum Krylov Diagonalization(QKD) which utilizes quantum computer to approximate the projection of the Hamiltonian into a Krylov subspace and classically diagonalize that Hamiltonian.

2 Krylov subspace

3 Non-Orthogonal QKD

The Hamiltonian H obeys the standard eigenvalue equation, $H|\psi_k\rangle = E_k|\psi_k\rangle$, with the energy eigenvalue E_k and corresponding eigenvector $|\psi_k\rangle$, assumed to satisfy the orthonormality condition, $\langle\psi_k|\psi_{k'}\rangle = \delta_{kk'}$. General functions of the Hamiltonian $f(H)$ will also obey the eigenvalue equation:

$$f(H)|\psi_k\rangle = f(E_k)|\psi_k\rangle . \tag{1}$$

We want to use quantum computer to calculate the projection of the Hamiltonian H into a Krylov subspace $\mathcal{K}$. Initially, we have some initial or reference state $|\psi_0\rangle$ and a Hamiltonian H. The Krylov subspace basis is defined below:

$$\mathcal{K} = \text{span}\{|\psi_0\rangle, e^{iHdt}|\psi_0\rangle, e^{i2Hdt}|\psi_0\rangle \ldots, e^{iH(n-1)dt}|\psi_0\rangle\}$$

Each basis is written as the following:

$$|\psi_j\rangle = U_j|\psi_0\rangle = e^{ijHdt}|\psi_0\rangle, \quad j = 0, 1, \ldots, n-1$$

U_j is the time evolution operator and can be approximated as a quantum circuit using Trotterization. Note, Krylov basis might be non-orthogonal and this is where the name is coming from (QKD), any eigenstate $|\phi_j\rangle$ of H can be represented with the Krylov basis as:

$$\begin{aligned} |\phi_j\rangle &= \sum_{i=0} c_i |\psi_i\rangle \\ &= Vc \end{aligned}$$

V is a matrix, its ith column contains the ith Krylov basis. c is a column vector which contains $[c_0, c_1, \ldots, c_{M-1}]^T$.

Now, let's plug this into eq. (1), then we will have the following:

$$\begin{aligned} f(H) \sum_{i=0} c_i |\psi_i\rangle &= f(E_k) \sum_{i=0} c_i |\psi_i\rangle \\ f(H)Vc &= f(E_k)Vc \end{aligned}$$

Multiply both sides by $\langle\psi_{k'}|$ to make it into a generalized eigenvalue problem:

$$\begin{aligned} \langle\psi_{k'}| f(H) \sum_{i=0} c_i |\psi_i\rangle &= f(E_k) \sum_{i=0} c_i \langle\psi_{k'}|\psi_i\rangle \\ V^\dagger f(H)Vc &= f(E_k)V^\dagger Vc \end{aligned}$$

Let $F(H) = V^\dagger f(H)V$ and $V^\dagger V = S$, then:

$$F(H)c = f(E_k)Sc$$

$F(H)$ and S are the two linear transformations, c is the generalized eigenvector, and $f(E_k)$ is the generalized eigenvalue of $(F(H), S)$.

We can use Krylov subspace's basis to construct a low-dimensional Hamiltonian $\tilde{H}$ to approximate the eigenvalue of the original Hamiltonian H. The matrix element of $\tilde{H}$ is defined as the following:

$$\tilde{H}_{jk} := \langle\psi_j| \tilde{H} |\psi_k\rangle, \quad \tilde{S}_{jk} := \langle\psi_j|\psi_k\rangle$$

$\tilde{S}$ is a Gram matrix. Its element is the inner product of basis vector $|\psi_j\rangle$ and $|\psi_k\rangle$, and this forms a Hermitian matrix S.

A convenient shorthand is to represent the Krylov basis as a matrix V whose columns are the vectors $|\psi_j\rangle$: then

$$\tilde{H} = V^\dagger HV, \quad \tilde{S} = V^\dagger V$$

The job of the classical post-processing is then to find the lowest eigenvalue of the matrix pencil (He , Se), which means solving the generalized eigenvalue problem Eq. (2) in the main text, which we also reproduce here for convenience:

4 Orthogonal QKD