Mitigating Errors in Quantum Krylov Subspace Diagonalization

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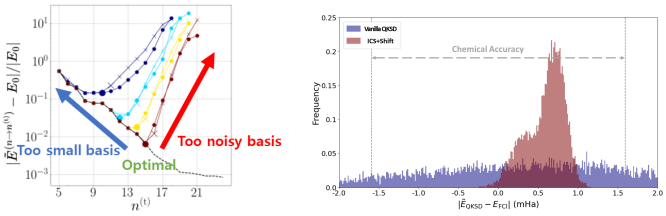
Quantum Krylov subspace diagonalization (QKSD) is an emerging method used in place of quantum phase estimation in the early fault-tolerant era. Within the quantum Krylov subspace, the ansatz is defined as a trigonometric polynomial of Hamiltonian $|\Psi(\boldsymbol{c})\rangle = \sum_{k=0}^{n-1} c_k e^{-i\hat{H}k} |\phi_0\rangle$, where $\boldsymbol{c} \in \mathbb{C}^n$, $|\phi_0\rangle$ is a reference state with a finite overlap with the ground state, and n is the dimension of the Krylov subspace. This ansatz is appealing because of its exponentially fast convergence to the ground state. Once the projection onto the subspace is performed by quantum computers, the classical diagonalization becomes feasible, as the dimension grows only logarithmically with the inverse of accuracy.

In contrast to the classical Krylov subspace diagonalization (KSD) or the Lanczos method, QKSD leverages quantum computers to efficiently estimate the eigenvalues of large Hamiltonians through a faster Krylov projection. However, unlike classical KSD—where machine precision is the primary concern —QKSD is inherently subject to sampling errors that decay more slowly. Given the limitation of the early fault-tolerant quantum device, a simple amplitude estimation algorithm, such as Hadamard test, is employed. These errors are bounded by the standard quantum limits of $\epsilon = O(1/\sqrt{M})$, which are less favorable than the Heisenberg limit. Moreover, due to the difficulty establishing an artificial orthogonal basis, ill-conditioning problems are often encountered, rendering the solution vulnerable to noise.

In this work, we analyze the relationship between the sampling noise and its impact on eigenvalue estimation within the Krylov subspace. We also propose techniques to mitigate sampling errors and to address ill-conditioned bases. First, *basis thresholding* removes the ineffective bases and establishes a trade-off between the loss of information about the subspace and the suppression of noise[1]. The optimal trade-off point is identified through an accurate perturbation analysis, as illustrated in Fig.1a. Second, we introduce a novel measurement technique for QKSD, called shifting operator, which eliminates redundant Hamiltonian terms during the measurement[2]. In electronic structure problems with small-molecules, the measurement cost is reduced by the factor of 20-500, as shown in Fig.1b.



(a) Thresholding (b) Shifting

FIG. 1. (a) QKSD perturbation error with basis thresholding applied. $n^{(t)}$ denotes the number of basis vectors remaining after thresholding. The threshold points identified by our proposed method are highlighted as larger markers, showing near-optimal performance. (b) Error histogram before and after applying shifting technique and iterative coefficient splitting.

[1] G. Lee, D. Lee, and J. Huh, Sampling Error Analysis in Quantum Krylov Subspace Diagonalization, Quantum **8**, 1477 (2024).
[2] G. Lee, S. Choi, J. Huh, and A. F. Izmaylov, Efficient strategies for reducing sampling error in quantum krylov subspace diagonalization (2024), arXiv:2409.02504 [quant-ph].