

Quantum Filtering and Analysis of Multiplicities in Eigenvalue Spectra

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Fine-grained spectral properties of quantum Hamiltonians, including both eigenvalues and their multiplicities, provide useful information for characterizing many-body quantum systems as well as for understanding phenomena such as topological order. Extracting such information with small additive error is #BQP-complete in the worst case. In this work, we introduce QFAMES (quantum filtering and analysis of multiplicities in eigenvalue spectra), a quantum algorithm that efficiently identifies clusters of closely spaced dominant eigenvalues and determines their multiplicities under physically motivated assumptions, which allows us to bypass worst-case complexity barriers. QFAMES also enables the estimation of observable expectation values within targeted energy clusters, providing a powerful tool for studying quantum phase transitions and other physical properties. We validate the effectiveness of QFAMES through numerical demonstrations, including its applications to characterizing quantum phases in the transverse-field Ising model and estimating the ground-state degeneracy of a topologically ordered phase in the two-dimensional toric code model. We also generalize QFAMES to the setting of mixed initial states. Our approach offers rigorous theoretical guarantees and significant advantages over existing subspace-based quantum spectral analysis methods, particularly in terms of the sample complexity and the ability to resolve degeneracies.

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I. INTRODUCTION

Understanding the energy spectrum of a Hamiltonian is a central problem in quantum computing, quantum complexity theory, quantum chemistry, and many-body physics. While estimating the ground-state energy or a few low-lying excitations is a common task, many physical properties require more fine-grained spectral information. For instance, the ground-state degeneracy (GSD) can indicate the presence of topological order—a hallmark of certain condensed matter phases [1] and a key feature for topological quantum computation [2]. More generally, we are interested in estimating both locations and the multiplicities of eigenvalues.

Despite their fundamental physical relevance, extracting such spectral information is computationally challenging: the Hilbert space dimension grows exponentially with

system size, making exact diagonalization infeasible even for modestly sized systems. Indeed, the GSD or eigenstate degeneracy problem is shown to be in the worst case #BQP-complete—the counting version of QMA [3,4]. As a result, we can only hope to solve this problem by leveraging additional assumptions for physically motivated Hamiltonians.

In this work, we tackle this problem by proposing a new quantum algorithm, dubbed quantum filtering and analysis of multiplicities in eigenvalue spectra (QFAMES). Our approach prepares a collection of initial states and leverages their correlated information to estimate the *density of dominant eigenstates* (DODS) defined as

$$\mu_D(E) \propto \sum_{i \in \mathcal{D}} \delta(E - \lambda_i), \quad (1)$$

where $\{\lambda_i\}_{i \in \mathcal{D}}$ denotes the multiset of dominant energy eigenvalues (counting multiplicity), whose corresponding eigenvectors have sufficiently large overlaps with the subspace spanned by the initial states.

To our knowledge, QFAMES is the first quantum algorithm that can provably estimate the DODS with rigorous theoretical guarantees. Specifically, QFAMES identifies clusters of closely spaced dominant eigenvalues and

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determines exactly the number of (possibly degenerate) eigenstates within each cluster with a proper choice of initial states. The algorithm requires only a single-ancilla qubit and employs short-depth circuits, which makes it suitable for the early fault-tolerant regime (see Theorem 2). Furthermore, recent advances [5–9] suggest that even this single-ancilla qubit may be eliminated under additional assumptions (see Sec. VI).

We then extend the algorithm to efficiently estimate expectation values of observables for the dominant eigenstates within a specified cluster. This task may be viewed as a natural generalization of the *eigenstate property estimation* problem [10–13] which focuses solely on a single, isolated eigenstate. Our approach enables probing physical properties within targeted clusters, thereby providing a useful tool for characterizing phenomena such as quantum phase transitions. The proposed framework is applicable to both pure and mixed initial states.

The effectiveness of QFAMES relies on the choice of initial states. Specifically, we require that the overlap between the set of initial states and *any* normalized vector in a dominant eigenspace be uniformly bounded from below. This *uniform overlap condition* generalizes the standard overlap assumption in quantum phase estimation. Moreover, we show that an information-theoretic barrier prevents degeneracy resolution when this condition is not met (see Proposition C1).

That said, there may not be an operationally viable way to directly check the uniform overlap condition in practice, as it requires access to the target eigenspace. In practice, users should choose from a set of physically motivated initial states that are expected to have good coverage of the target eigenspaces. The QFAMES algorithm does not require the initial states to be linearly independent. This allows users to choose a larger, potentially redundant set of initial states (pure or mixed) to satisfy the uniform overlap condition, while avoiding numerical instabilities associated with near-linear dependence. We outline three scenarios where such initial states may be prepared in practice.

First, for molecular quantum chemistry problems, there already exist various practical proposals that prepare low-energy trial state sets, including sums of Slater determinants [14–16], spin flip [17,18], coupled cluster [19, 20], and more general variational Ansätze [21–24]. These protocols can be applied in conjunction with subspace-based quantum eigenvalue estimation methods [23,25–31] to determine ground- and excited-state energies. Starting from these physically motivated initial states, QFAMES (a) provides a theoretical foundation and necessary conditions for subspace-based methods and (b) improves performance compared to previous subspace diagonalization approaches. In particular, it is not plagued by the problem of inverting ill-conditioned overlap matrices. The analysis presented here also sheds light on the conditions

required for initial states in existing subspace diagonalization methods.

Second, tensor network methods, such as matrix product states (MPS) (or projected entangled-pair states in two or higher spatial dimensions) with low bond dimensions, can efficiently prepare initial states that are useful in quantum chemistry and condensed matter systems [16,32–40]. While the bond dimension required to represent the exact ground state of a quantum system may be large, QFAMES only requires that the set of initial states collectively has non-negligible overlap with the ground-state manifold. This relaxes the bond dimension requirements. In this paper, we study the transverse-field Ising model (TFIM), the toric code model, and the anisotropic Heisenberg (XXZ) model, which demonstrate the efficacy of these matrix product initial states when combined with QFAMES.

Third, generalizing QFAMES to mixed initial states (discussed in Sec. VII) opens up new possibilities. For instance, recently developed dissipative algorithms for preparing low-temperature thermal or ground states [41–55] typically yield mixed states, especially when the ground-state manifold is degenerate. Also, the controlled state-preparation oracle is inaccessible due to the irreversibility of the dissipative process. Our construction addresses this by utilizing an additional system register, thereby removing the need for controlled state-preparation circuits. We demonstrate, via a proof-of-principle example, that solving the generalized eigenvalue problem with such mixed states extracts significantly more information about observables within the ground-state manifold than individual measurements alone.

The paper is structured as follows. In Sec. II, we review the related works. In Sec. III, we introduce the problem setup and summarize the main results. Section IV presents the QFAMES algorithm in detail, while Sec. V discusses how to extend the method to extract information of physical observables. Section VI discusses how to implement the QFAMES algorithm in a control-free, ancilla-free setting. The extension of QFAMES to mixed-state case is discussed in Sec. VII. In Sec. VIII, we present numerical simulation results with an illustrative example, the transverse-field Ising model, the toric code model, and the XXZ model. Finally, Sec. IX concludes with a discussion of possible future directions.

II. RELATED WORK

The estimation of Hamiltonian eigenvalues is a fundamental problem in the literature of quantum computation, which can be addressed by a variety of methods collectively known as quantum phase estimation (QPE) algorithms [56–70]. These methods primarily aim at determining the locations of eigenvalues but are inherently incapable of identifying their multiplicities, as they typically

assume access to only a single initial state. A more detailed review of these algorithms is provided in Appendix B.

In the literature, several recent works [71,72] have also explored problems related to estimating Eq. (1), albeit under different oracle models and assumptions. Some of these studies establish a connection between density of states (DOS) estimation and quantum topological data analysis [73–75], where QPE can be employed to sample energies and estimate degeneracies within small energy intervals [71]. In contrast, Ref. [72] reformulates the estimation of ground-state degeneracy as a ground-state preparation task for a specially constructed auxiliary Hamiltonian, which in turn requires efficient ground-state preparation of the auxiliary Hamiltonian.

As will be shown later, our observable eigenstate property estimation problem reduces to a generalized eigenvalue problem, which shares structural similarities with subspace-based quantum eigenvalue estimation methods [23,25–31,76,77]. These subspace methods can be generalized to estimate eigenvalue multiplicities when multiple initial states are used. QFAMES, however, distinguishes itself with the following features:

- (1) *Heisenberg-limited scaling.* Krylov subspace-based methods often require uniform time sampling, which prevents the attainment of Heisenberg-limited scaling in energy estimation, as established in Theorem 1.7 of Ref. [78]. QFAMES circumvents this limitation by utilizing Gaussian sampling of the evolution time.
- (2) *Separation of dominant eigenvalues.* Subspace-based methods usually require high-precision measurements of data matrices due to coherence between different dominant eigenvalues. Although noise can be suppressed via singular value truncation [76,77] as in QFAMES, the resulting complexity remains suboptimal according to state-of-the-art analyses of subspace methods [23,29,30]. QFAMES addresses this by applying a Gaussian energy filter to distinguish distinct dominant eigenvalues and separate them into smaller, well-conditioned singular value decomposition (SVD) subproblems for multiplicity determination.
- (3) *Small data matrix.* The dimension of the data matrix in subspace-based methods often scales with the number of uniformly chosen time points, which is usually proportional to the inverse target precision in energy. In contrast, thanks to the filtering technique, the dimension of the QFAMES data matrix is only determined by the number of initial states, which is independent of the accuracy requirement.

These features allow us to derive stronger theoretical guarantees than those available for standard subspace-based algorithms. To our knowledge, this is also the first work capable of provably estimating eigenvalue multiplicities.

III. SETUP AND MAIN RESULTS

Let us first formally state the DODS estimation problem:

Problem 1 (Density of dominant eigenstates (DODS) estimation). Let H be a Hamiltonian with eigen-decomposition $\{(\lambda_i, |E_i\rangle)\}$, where, after appropriate normalization, the spectrum satisfies $\lambda_i \in [-\pi, \pi]$ for all i . Assume black-box access to controlled time evolution e^{-iHt} for any $t \in \mathbb{R}$, as well as two families of (controlled) state-preparation unitaries $\{U_\ell\}_{\ell \in [L]}$ and $\{V_r\}_{r \in [R]}$ satisfying $U_\ell|0\rangle = |\phi_\ell\rangle$ and $V_r|0\rangle = |\psi_r\rangle$.

We define two overlap matrices $\Phi \in \mathbb{C}^{L \times M}$ and $\Psi \in \mathbb{C}^{R \times M}$,

$$\begin{aligned}\Phi_{l,m} &:= \langle \phi_l | E_m \rangle \quad \forall l \in [L], m \in [M], \\ \Psi_{r,m} &:= \langle \psi_r | E_m \rangle \quad \forall r \in [R], m \in [M].\end{aligned}\tag{2}$$

For each eigenstate $|E_m\rangle$, define its overlap with the initial states as

$$p_m := \|\Phi_{:,m}\|_2 \cdot \|\Psi_{:,m}\|_2.\tag{3}$$

The multiset of *dominant eigenvalues*, indexed by $\mathcal{D}$, consists of those eigenvalues that satisfy the *dominance condition*,

$$\left(p_{\min} := \min_{m \in \mathcal{D}} p_m\right) \gtrsim \left(p_{\text{tail}} := \sum_{m \notin \mathcal{D}} p_m\right).\tag{4}$$

The distinct dominant eigenvalues are denoted by $\{\lambda_i^*\}_{i \in [I]}$, each separated by at least Δ , with corresponding eigenvectors indexed by $\mathcal{D}_i$. The degeneracies $|\mathcal{D}_i|$ satisfy $|\mathcal{D}| = \sum_{i \in [I]} |\mathcal{D}_i|$.

Goal: With high probability, for each $i \in [I]$, estimate the dominant eigenvalue λ_i^* within ϵ -accuracy and exactly determine its dominant degeneracy m_i . These outputs together suffice to approximate the density of dominant eigenstates (DODS) μ_D , as defined in Eq. (1).

The left and right initial states can be either the same or different, depending on the problem setup. When they are different, the left initial states can be viewed as bases for projective measurements. In this work, to ensure that our algorithm can theoretically solve the DODS estimation problem efficiently, we require the dominant eigenvalues to satisfy a *sufficient dominance condition*, namely, that $p_{\min}/p_{\text{tail}}$ be greater than a constant determined by the structure of Φ and Ψ . The precise condition, together with a detailed discussion of the requirement on $p_{\min}/p_{\text{tail}}$, is deferred to Appendix D, Theorem D1, and Remark D1.

If λ_i is a nondegenerate dominant eigenvalue, and there is only one pair of initial states $|\phi\rangle$ and $|\psi\rangle$, then both $|\langle \phi | E_m \rangle|$ and $|\langle \psi | E_m \rangle|$ need to be large enough. Indeed, when $|\phi\rangle = |\psi\rangle$, $p_m = |\langle \phi | E_m \rangle|^2$ is simply the squared

overlap between the initial state and the eigenstate, which is the standard assumption in quantum phase estimation and its variants (see Appendix B). More generally, if λ_i is a nondegenerate dominant eigenvalue but there are multiple pairs of initial states, then both $\sum_{l \in [L]} |\langle \phi_l | E_m \rangle|^2 = \|\Phi_{:,m}\|_2^2$ and $\sum_{r \in [R]} |\langle \psi_r | E_m \rangle|^2 = \|\Psi_{:,m}\|_2^2$ need to be sufficiently large, which states that the eigenstate $|E_m\rangle$ has nonvanishing overlap with at least one initial state in each set. This can be concisely captured by the condition for p_m in Eqs. (3) and (4).

In order to compute the multiplicity of a degenerate dominant eigenvalue λ_i^* , we need a stronger condition to ensure that *all* normalized eigenvectors corresponding to the degenerate eigenvalue λ_i^* in the eigenspace $\mathcal{E}_i := \text{span}\{|E_m\rangle\}_{m \in \mathcal{D}_i}$ have nonvanishing overlap with the set of initial states. In other words, both of the following quantities:

$$\begin{aligned} \min_{|E\rangle \in \mathcal{E}_i, \langle E|E\rangle=1} \sum_{l \in [L]} |\langle \phi_l | E \rangle|^2, \\ \min_{|E\rangle \in \mathcal{E}_i, \langle E|E\rangle=1} \sum_{r \in [R]} |\langle \psi_r | E \rangle|^2, \end{aligned} \quad (5)$$

need to be sufficiently large. This will be formulated more precisely as a *uniform overlap condition* in Assumption C1 of Appendix C. Indeed, if one of the quantities in Eq. (5) vanishes, we prove that there is an *information-theoretic barrier* for resolving the degeneracy (Proposition C1). As a special case, this proves that existing quantum phase estimation algorithms, which typically use only a single initial state, cannot resolve eigenvalue degeneracies.

The uniform overlap condition states that the overlap of all normalized vectors in the eigen-subspace with the initial states should be uniformly bounded from below. However, this does not require the initial states to be well-conditioned. In fact, we do not even require the vectors $\{|\phi_l\rangle\}$ (or $\{|\psi_r\rangle\}$) to be *linearly independent*. This provides significantly enhanced flexibility in choosing the initial states compared to existing subspace methods, which typically require the initial states to be a well-conditioned set of vectors. That said, the initial states should not be chosen randomly. In practical calculations, the initial states should be chosen carefully and in a physically motivated manner, such as low-energy states prepared by variational quantum algorithms [79–81], quantum imaginary-time evolution (QITE) [82–84], and the nonorthogonal Ansatz states used in the nonorthogonal quantum eigensolver [23,26] approach.

The main result of this paper is an efficient quantum algorithm to solve the DODS estimation problem with **rigorous theoretical guarantees**.

Theorem 1 (Main result, Informal version of Theorem 2). There exists a quantum algorithm that repeatedly runs the

quantum circuit in Fig. 1 to collect data with Hamiltonian evolution times $t_1, \dots, t_N \in \mathbb{R}$ such that

- (1) maximal evolution time: $T_{\max} := \max\{|t_n|\} = \tilde{\mathcal{O}}(p_{\text{tail}}\epsilon^{-1}/p_{\min})$;
- (2) total evolution time: $T_{\text{total}} := 2 \sum_{n=1}^N \sum_{l \in [L]} \sum_{r \in [R]} |t_n| = \tilde{\mathcal{O}}((p_{\text{tail}}p_{\min})^{-1}\epsilon^{-1})$.

By classically postprocessing the data, it guarantees that for each distinct dominant eigenvalue,

- (1) its location can be estimated to within ϵ accuracy; and
- (2) its multiplicity can be determined exactly.

According to Eq. (4) and Theorem 1, we have $p_{\text{tail}}/p_{\min} \lesssim 1$, so it suffices to take $T_{\max} = \mathcal{O}(1/\epsilon)$. Moreover, the formal result in Theorem 2 allows greater flexibility in the choice of $T_{\max}$ and T_{total} than Theorem 1. In particular, it suffices to choose $T_{\max} = \tilde{\mathcal{O}}(\delta\epsilon^{-1})$ and $T_{\text{total}} = \tilde{\mathcal{O}}((\delta p_{\min}^2)^{-1}\epsilon^{-1})$ for any $\delta > p_{\text{tail}}/p_{\min}$. When $p_{\text{tail}} \ll p_{\min}$, the constant prefactor of $1/\epsilon$ in $T_{\max}$ can be much smaller than 1, which corresponds to the short-depth regime observed in the literature [62–64,68,70].

Note that our algorithm can also resolve dominant eigenvalues that are **approximately degenerate**, i.e., when there is a cluster of dominant eigenvalues lying in a narrow energy interval around λ_i^* with width $\delta \ll \Delta$. See more discussion in Sec. IV B.

As an extension of the algorithm, we also propose an efficient method (Algorithm 2) for estimating degenerate eigenstate properties in Sec. V. The problem is defined as follows.

Problem 2 (Degenerate eigenstate property estimation). Let O be an observable. For each dominant eigenvalue λ_i^* , estimate the eigenvalues of the projected observable $O_{\mathcal{D}_i}$ in the corresponding subspace,

$$O_{\mathcal{D}_i} := (\langle E_k | O | E_{k'} \rangle)_{k,k' \in \mathcal{D}_i}, \quad \mathcal{D}_i = \{k \in \mathcal{D} : \lambda_k = \lambda_i^*\}. \quad (6)$$

Let us denote the eigenvalues by λ_k^O . We remark that any value within the range $[\min_k \lambda_k^O, \max_k \lambda_k^O]$ can be realized by some linear combination of the degenerate eigenstates. It is thus less useful to estimate $\langle E_m | O | E_m \rangle$ for each individual dominant eigenstate. For example, in the ferromagnetic phase of a spin chain model, there can be two degenerate ground states $|E_0\rangle = |\uparrow\uparrow \cdots \uparrow\rangle$ and $|E_1\rangle = |\downarrow\downarrow \cdots \downarrow\rangle$. The measured ground states can be however $(|E_0\rangle + |E_1\rangle)/\sqrt{2}$ and $(|E_0\rangle - |E_1\rangle)/\sqrt{2}$, both of which yield zero average magnetization.

For simplicity, we provide the resource estimation in the case of no tail eigenvalues (i.e., $p_{\text{tail}} = 0$) and $p_{\min}$ being bounded below by a constant (i.e., $p_{\min} = \Omega(1)$). To

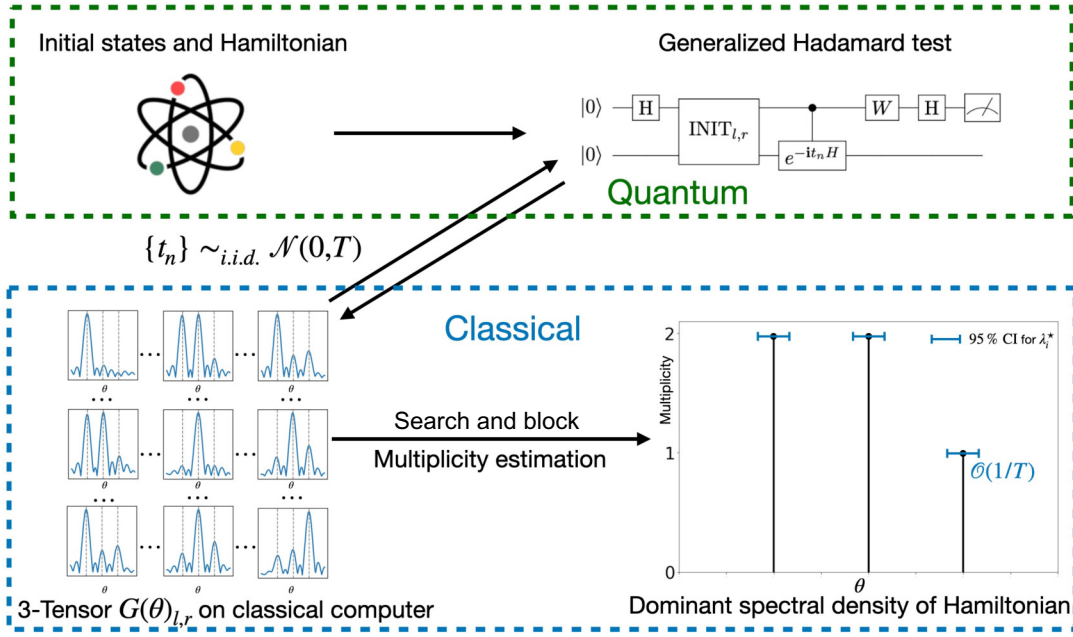


FIG. 1. Illustration of the quantum filtering and analysis of multiplicities in eigenvalue spectra algorithm. Given the Hamiltonian and two sets of initial states prepared by circuits $\{U_l\}_{l \in [L]}$ and $\{V_r\}_{r \in [R]}$, we measure quantities of the form $Z_{l,r}(t_n) = \langle 0|U_l^\dagger e^{-iHt_n} V_r|0\rangle$ using the generalized Hadamard test circuit. The collected quantum data are then processed classically to (1) estimate the locations of energy eigenstate clusters through searching and blocking and (2) compute the multiplicities of the probed clusters.

achieve ϵ_O -accuracy in estimating each eigenvalue of $O_{\mathcal{D}_i}$, it suffices to choose

$$T_{\max} = \tilde{O}(\Delta^{-1}), \quad T_{\text{total}} = \tilde{O}(\Delta^{-1} \epsilon_O^{-2}). \quad (7)$$

Here, for simplicity, we suppress the dependence on the constant $p_{\min}$, since $p_{\min} = \Omega(1)$. The proposition showing this result is Proposition 1 in Sec. V.

IV. QFAMES ALGORITHM AND COMPLEXITY ANALYSIS

In this section, we describe the QFAMES algorithm in Sec. IV A, present its pseudocode, and provide an illustrative example. A detailed complexity analysis follows in Sec. IV B.

A. Algorithmic description

Our goal is to estimate the DODS, including the dominant eigenvalues λ_i^* and corresponding multiplicities m_i . If we assume the eigenvalues are separated by at least Δ , then we can define energy filters of the form $\exp[-(\theta - H)^2 T^2]$ to filter out the energy eigenstates away from the desired dominant eigenvalue, where the filter width is chosen to be $T \gtrsim 1/\Delta$. The filter can be implemented with time evolution operators through sampling from its Fourier transform

$$e^{-(\theta - H)^2 T^2} = \int e^{i(\theta - H)t} a_T(t) dt, \quad (8)$$

where

$$a_T(t) = \frac{1}{2T\sqrt{\pi}} \exp\left(-\frac{t^2}{4T^2}\right) \quad (9)$$

is the probability density function (PDF) for evolution time t [more rigorously, we will sample t from a truncated Gaussian distribution as defined in Eq. (16) to avoid extremely large t_n].

For the given sets of left and right initial states $|\phi_l\rangle$ and $|\psi_r\rangle$, we want to compute the matrix $\mathcal{G}(\theta)$ with matrix elements

$$\mathcal{G}_{l,r}(\theta) = \langle \phi_l | e^{-(\theta - H)^2 T^2} | \psi_r \rangle. \quad (10)$$

At $\theta = \lambda_i^*$, we have

$$\begin{aligned} \mathcal{G}(\lambda_i^*) &= \Phi \cdot \text{diag}\left(\left\{e^{-(\lambda_i^* - \lambda_m)^2 T^2}\right\}_{m \in [M]}\right) \cdot \Psi^\dagger \\ &\approx \Phi_{:, \mathcal{D}_i} \cdot (\Psi_{:, \mathcal{D}_i})^\dagger, \end{aligned} \quad (11)$$

where the matrices Φ and Ψ are defined in Eq. (2), and $\Phi_{:, \mathcal{D}_i}$ and $\Psi_{:, \mathcal{D}_i}$ are the corresponding submatrices that contain the columns of dominant eigenstates with eigenvalue λ_i^* . $\mathcal{D}_i$ denotes the index set of these eigenvalues. Due to the concentration of $\exp(-x^2 T^2)$ around zero, this expression implies that only those eigenvalues that are close to λ_i^* contribute significantly to the matrix $\mathcal{G}(\lambda_i^*)$, and the

- (1) *Location estimation:* We evaluate the **Frobenius norm** of $\mathcal{G}(\theta)$ on a uniform grid of $\theta \in [-\pi, \pi]$, and use a “searching and blocking” strategy to find the peaks θ_i^* of $\|\mathcal{G}(\theta)\|_F$. Each peak corresponds to a distinct dominant eigenvalue λ_i^* .
- (2) *Multiplicity estimation:* For each candidate dominant eigenvalue θ_i^* , we compute the **numerical rank** of $\mathcal{G}(\theta_i^*)$ (the number of singular values above some threshold) as the estimated multiplicity.

Step 1: Generate data. To obtain Eq. (10), we need to measure quantities of the form

$$\mathcal{Z}_{l,r}(t_n) := \langle 0 | U_l^\dagger e^{-iHt_n} V_r | 0 \rangle = \langle \phi_l | e^{-iHt_n} | \psi_r \rangle. \quad (12)$$

$$\text{INIT}_{l,r} = \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{|c|} \hline \text{INIT}_{l,r} \\ \hline \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{|c|} \hline \text{---} \text{---} \text{---} \\ \hline \end{array} \begin{array}{|c|} \hline \text{---} \text{---} \text{---} \\ \hline \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \begin{array}{|c|} \hline U_l \\ \hline \end{array} \begin{array}{|c|} \hline V_r \\ \hline \end{array} \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \quad (14)$$

$$\mathbb{E}[Z_{l,r,n}] = \sum_{m \in [M]} \Phi_{l,m} \cdot e^{-i\lambda_m t_n} \cdot (\Psi_{r,m})^*, \quad (15)$$

The times $t_1, \dots, t_N$ are sampled independently from the Gaussian probabilistic density function $a_T(t)$. In practice,

$$\begin{aligned} a_T^{\text{trunc}}(t) &= \left(1 - \int_{-\sigma T}^{\sigma T} \frac{1}{2T\sqrt{\pi}} \exp\left(-\frac{s^2}{4T^2}\right) ds \right) \delta_0(t) \\ &\quad + \frac{1}{2T\sqrt{\pi}} \exp\left(-\frac{t^2}{4T^2}\right) \mathbf{1}_{[-\sigma T, \sigma T]}(t), \end{aligned} \quad (16)$$

Step 2: Compute the filtered matrix estimator. We can now **contract** the time dimension of the data tensor with the following complex exponential vector:

$$\frac{1}{N} [e^{i\theta t_1} \quad e^{i\theta t_2} \quad \dots \quad e^{i\theta t_N}], \quad (17)$$

$$G(\theta)_{l,r} = \frac{1}{N} \sum_{n=1}^N Z_{l,r,n} e^{i\theta t_n}, \quad l \in [L], r \in [R]. \quad (18)$$
$$\begin{aligned}\mathbb{E}[G(\theta)] &= \mathcal{G}(\theta) \\ &= \Phi \cdot \text{diag} \left(\left\{ \int e^{i(\theta - \lambda_m)t} a_T^{\text{trunc}}(t) dt \right\}_{m \in [M]} \right) \cdot \Psi^\dagger \\ &\approx \Phi \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in [M]} \right) \cdot \Psi^\dagger. \quad (19)\end{aligned}$$

Step 3: Search and block. After computing $G(\theta)$, the dominant eigenvalues are identified as the peaks of $\|G(\theta)\|_F$ and can be located using the search-and-block procedure proposed in Ref. [64]. This strategy consists of two iterative components—the search step and the block step—which are described as follows:

(1) *Search*: In the first step, we find the maximum point θ_1^* of $\|G(\theta)\|_F$, which approximates to one of the dominant eigenvalues.

- (2) *Block*: To approximate the next dominant eigenvalue and avoid repetition, we define a block interval

$$\mathcal{I}_{B,1} = [\theta_1^* - \alpha/T, \theta_1^* + \alpha/T] \quad (20)$$

ALGORITHM 1. Quantum filtering and analysis of multiplicities in eigenvalue spectra

1: **Preparation:**
 Number of data pairs: N ;
 Two initial state sets: $\{\phi_i\}_{i=1}^L$ and $\{\psi_j\}_{j=1}^R$;
 Filter parameter: T ;
 Truncation parameter in a_T^{trunc} : σ ;
 Number of dominant eigenvalues (guess): $\tilde{I}$;
 Singular value decomposition threshold: τ ;
 Searching parameter: q (we search with discrete energy step q/T);
 Block parameter: α (distinct dominant eigenvalues are at least separated by α/T);

2: **Running:**

3: **Stage I: Estimate the location of dominant eigenvalues**

4: ▷ Step 1: Generate data

5: Sample $\{t_n\}$ i.i.d. from the truncated Gaussian distribution $a_T^{\text{trunc}}(t)$ defined in Eq. (16)

6: **for** $l = 1$ to L **do**

7: **for** $r=1$ to R **do**

8: **for** $n = 1$ to N **do**
 Generate data $Z_{l,r,n} \in \{\pm 1 \pm i\}$ using the generalized Hadamard test with (U_l, V_r, t_n)

9: **end for**

10: **end for**

11: **end for**

12: **end for**

13: ▷ Step 2: Compute the filtered density function

14: $J \leftarrow \left\lfloor \frac{2\pi T}{q} \right\rfloor$.

15: Generate discrete candidates: $\theta_j \leftarrow -\pi + \frac{jq}{T}$ for $j = 0, 1, \dots, J$.

16: Calculate

$$\|G(\theta_j)\|_F \leftarrow \left\| \frac{1}{N} \sum_{n=1}^N Z_{:, :, n} \exp(i\theta_j t_n) \right\|_F, \quad 0 \leq j \leq J.$$

17: ▷ Step 3: Search-and-block

18: Block set: $\mathcal{B}_1 \leftarrow \emptyset$.

19: **for** $i = 1$ to $\tilde{I}$ **do**

20: $j_i = \text{argmax}_{\theta_j \notin \mathcal{B}_i} \|G(\theta_j)\|_F$.

21: $\theta_i^* \leftarrow \theta_{j_i}$.

22: $\mathcal{B}_{i+1} \leftarrow \mathcal{B}_i \cup (\theta_i^* - \frac{\alpha}{T}, \theta_i^* + \frac{\alpha}{T})$. ▷ Block interval to avoid finding the same peak

23: **end for**

24: **Output:** *Distinct dominant eigenvalues:* $\{\theta_i^*\}_{i=1}^{\tilde{I}}$

25:

26: **Stage II: Estimate the multiplicity of each dominant eigenvalue**

ALGORITHM 1. (Continued.)

27: ▷ Step 4: Estimate multiplicity

28: **for** $i = 1$ to $\tilde{I}$ **do**

29: Calculate SVD of the data matrix at each θ_i^* :

$$U_i \Sigma_i V_i^\dagger = \text{SVD} \left(\frac{1}{N} \sum_{n=1}^N Z_{:, :, n} \exp(i\theta_i^* t_n) \right)$$

30: $m_i = \# \{j \mid (\Sigma_i)_{j,j} > \tau\}$.

31: **end for**

32: **Output:** *Multiplicities:* $\{m_i\}_{i=1}^{\tilde{I}}$.

for some given constant α . The conditions for α are stated in Theorem 2. In the following steps, we will not find any points from this interval.

- (3) *Second iteration*: In the second iteration, we find the second-largest point θ_2^* of $\|G(\theta)\|_F$ outside the block interval $\mathcal{I}_{B,1} = [\theta_1^* - \alpha/T, \theta_1^* + \alpha/T]$ around θ_1^* ,

$$\theta_2^* = \arg \max_{\theta \in \mathcal{I}_{B,1}^c} \|G(\theta)\|_F. \quad (21)$$

After obtaining θ_2^* , we enlarge the block interval by setting $\mathcal{I}_{B,2} = [\theta_2^* - \alpha/T, \theta_2^* + \alpha/T] \cup \mathcal{I}_{B,1}$, and then identify the third maximum of $\|G(\theta)\|_F$ outside $\mathcal{I}_{B,2}$. This searching and updating process is iteratively repeated until a set of $\tilde{I}$ “maximal” points is discovered. Ultimately, we obtain an approximate candidate set $\{\theta_i^*\}_{i=1}^{\tilde{I}}$ corresponding to the set of dominant eigenvalues $\{\lambda_i^*\}_{i \in [I]}$.

Step 4: Estimate multiplicity. For each $\{\theta_i^*\}_{i=1}^{\tilde{I}}$, we perform the singular value decomposition

$$G(\theta_i^*) = U_i \Sigma_i V_i^\dagger, \quad (22)$$

and define

$$m_i = \# \{j \mid (\Sigma_i)_{j,j} > \tau\} \quad (23)$$

for some given threshold τ , which gives the multiplicity associated with each candidate θ_i^* . If $m_i = 0$, then θ_i^* corresponds to a spurious dominant eigenvalue and should be discarded.

Pseudocode. Figure 2 summarizes the QFAMES workflow as a tensor network. The left/right blocks U_l and V_r prepare two families of initial states. Time evolution e^{-iHt} induces cross-correlations between these families, which (via the generalized Hadamard test) yield the sampled signals $\mathcal{Z}_{l,r}(t_n)$. A time-domain filter $a_T(t)$ and a discrete Fourier transform produce frequency-domain matrices $G(\theta)$, which are then processed classically: a search-and-blocking step estimates the distinct dominant eigenvalues $\{\lambda_i^*\}$, and rank/conditioning tests on submatrices determine

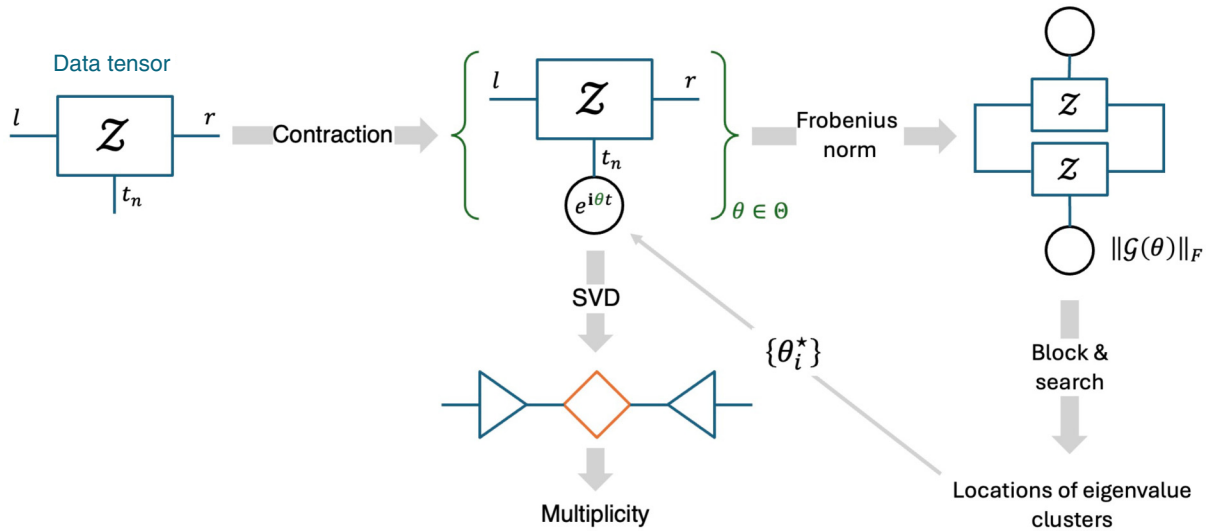


FIG. 2. Diagram of the quantum filtering and analysis of multiplicities in eigenvalue spectra algorithm for postprocessing the 3-tensor generated from quantum data of the generalized Hadamard test circuit. Left/right tensors U_l and V_r prepare initial-state families; the middle leg represents time evolution e^{-iHt} and data acquisition of cross-correlators $\mathcal{Z}_{l,r}(t_n)$. A filter $a_T(t)$ and discrete Fourier transform yield $\mathcal{G}(\theta)$, which is postprocessed by search-and-blocking to locate dominant eigenvalues $\{\lambda_i^*\}$ and by rank tests to determine multiplicities $\{m_i\}$.

multiplicities $\{m_i\}$. An optional branch forms projected observable matrices and solves a generalized eigenvalue problem to obtain the spectrum of $\mathcal{O}_{\mathcal{D}_i}$ for each λ_i^* . The detailed algorithm for eigenvalue and multiplicity estimation is presented in Algorithm 1, while the observable estimation will be discussed in detail in Sec. V.

In the above algorithm, σT denotes the maximal Hamiltonian simulation time used in the generalized Hadamard test, and N is the number of repetitions for **each** entry estimation. Therefore, the total Hamiltonian simulation time is upper bounded by $LR\sigma TN$. The importance of off-diagonal entries in the data tensor Z for resolving spectral multiplicities is demonstrated through a concrete illustrative example in Sec. VIII A.

Besides Gaussian functions, one may also use the Kaiser windows and the discrete prolate spheroidal sequence (DPSS/Slepian) windows [85–87] to further suppress spectral leakage and sharpen cluster localization. We leave a detailed study of this to future work.

B. Complexity analysis

In this section, we analyze the theoretical complexity of the QFAMES algorithm introduced in Sec. IV A. Recall the overlaps of the dominant eigenvalues and tails defined as Eq. (4),

$$\begin{aligned} p_{\min} &= \min_{m \in \mathcal{D}} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)}, \\ p_{\text{tail}} &= \sum_{m \notin \mathcal{D}} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)}, \end{aligned} \quad (24)$$

The main theorem on the performance guarantees of the QFAMES algorithm is stated as follows:

Theorem 2. Assume the uniform overlap condition (Assumption C1) holds true, $p_{\text{tail}}/p_{\text{min}}$ is sufficiently small, and the parameters in Algorithm 1 satisfy the following conditions:

$$\begin{aligned}
N &= \tilde{\Omega}(LRp_{\text{tail}}^{-2}), \quad T = \tilde{\Omega}(1/\Delta), \\
\sigma &= \tilde{\Omega}(1), \quad \tilde{I} \geq I, \quad \tau = \Theta(p_{\text{tail}}), \\
q &= \mathcal{O}\left(\frac{P_{\text{tail}}}{(1+\sigma)\sqrt{|\mathcal{D}|LR}}\right), \\
\alpha &= \Omega\left(\log\left(\frac{|\mathcal{D}|LR}{p_{\text{tail}}}\right)\right), \quad \alpha = \mathcal{O}(\Delta T).
\end{aligned} \tag{25}$$

Given failure probability $\eta \in (0, 1)$, there exists a permutation $\pi : [I] \rightarrow [I]$ such that, with probability at least $1 - \eta$, we have

$$\lambda_{\pi(i)}^* \in [\theta_i^* - \epsilon, \theta_i^* + \epsilon], \quad \forall 1 \leq i \leq I, \quad (26)$$

where the confidence interval length ϵ is given by

$$\epsilon = \tilde{\mathcal{O}}\left(\frac{p_{\text{tail}}}{p_{\text{min}}} \cdot \frac{1}{T}\right) \quad (27)$$

and

$$m_i = |\mathcal{D}_{\pi(i)}|, \quad 1 \leq i \leq I, \quad m_i = 0, \quad I < i \leq \tilde{I}. \quad (28)$$

We defer a more general and rigorous version of the above theorem, along with its proof, to Appendix D. The

above theorem shows that Algorithm 1 can accurately estimate the locations of the dominant eigenvalues and identify their multiplicities. Note that the conditions on T, N, σ, q , and α are similar to those in Theorem 3.2 of Ref. [64] (see the detailed discussion in Remark D1), and the choice of τ plays an important role in filtering out non-dominant eigenvalues. In practice, exact values for $p_{\min}$ and p_{tail} are often unknown. The parameters T, N, σ, q , and α are flexible, typically subject only to upper or lower bounds, whereas selecting τ requires care to avoid overestimating or underestimating multiplicity. When p_{tail} is unknown, two heuristic methods for selecting the SVD threshold τ are as follows: (1) Noise-based selection: set $\tau \gtrsim \sqrt{LR/N}$. Since each entry of $G(\theta)$ is estimated from N samples, the entry-wise statistical fluctuation is of order $N^{-1/2}$, so the Frobenius norm of the corresponding noise matrix is of order $\sqrt{LR/N}$; (2) Singular value drop: in low-noise regimes, the effective rank deficiency of $G(\theta)$ typically yields a visible separation between the leading singular values and the remainder; in this case, τ can be chosen within this gap.

It can be directly obtained from Theorem 2 that the maximal evolution time $T_{\max} = \sigma T = \tilde{O}(p_{\text{tail}} p_{\min}^{-1} \epsilon^{-1})$, and the total evolution time $T_{\text{total}} = O(NLRT_{\max}) = \tilde{O}(L^2 R^2 (p_{\text{tail}} p_{\min})^{-1} \epsilon^{-1})$. When p_{tail} is close to zero and $p_{\min} = \Omega(1)$, however, the maximal evolution time will instead reach the bound from below as $T_{\max} = \hat{\Omega}(\Delta^{-1})$, where Δ is the spectral gap. In this case, we can use a

looser constant $c = \tilde{\Theta}(\Delta^{-1} \epsilon)$ to replace p_{tail} in the scalings and the total evolution time will consequently scale as $T_{\text{total}} = \tilde{O}(L^2 R^2 \Delta \epsilon^{-2})$. Note that we aim to resolve the gap Δ between distinct dominant eigenvalues, which implicitly indicates that $\Delta > \epsilon$.

Furthermore, our algorithm also applies to the case of approximately degenerate dominant eigenvalues, where a cluster of such eigenvalues lies within a narrow interval of width $\delta \ll \Delta$ around λ_i^* . In this setting, the algorithm can efficiently identify the locations of the clusters and determine the exact number of dominant eigenvalues in each. The corresponding assumptions and results are presented in detail in Appendix D.

V. EXTENSION TO OBSERVABLE MEASUREMENTS

Within each located dominant eigenvalues, other than multiplicity, more meaningful information can be encoded in expectation values of physical observables. In this section, we will show that it can also be extractable under the QFAMES framework.

The main idea is to slightly modify our circuit to include the observables. Given an observable O , it can always be rewritten as the weighted sum of unitary Hermitian operators such as Pauli matrices. We can thus assume O to be unitary without loss of generality. The measurement outcomes $Z_{l,r,n}^O$ of the modified circuit

$$(29)$$

provides an unbiased estimator of

$$\mathbb{E}[Z_{l,r,n}^O] = Z_{l,r,n}^O(t_n, t'_n) := \langle \phi_l | e^{iH t'_n} O e^{-iH t_n} | \psi_r \rangle. \quad (30)$$

Analogous to the QFAMES algorithm, the next step is to contract the time dimension of the 3-tensor $Z_{l,r,n}^O$ with the complex exponential vector

$$\frac{1}{N} \begin{bmatrix} e^{i\theta(t_1 - t'_1)} & e^{i\theta(t_2 - t'_2)} & \dots & e^{i\theta(t_N - t'_N)} \end{bmatrix}, \quad (31)$$

where both $\{t_n\}$ and $\{t'_n\}$ are sampled independently from the truncated Gaussian density distribution $a_{T/\sqrt{2}}^{\text{trunc}}(t)$ defined in Eq. (16). This results in an L -by- R matrix

$$G^O(\theta)_{l,r} = \frac{1}{N} \sum_{n=1}^N Z_{l,r,n}^O e^{i\theta(t_n - t'_n)} \quad \forall l \in [L], r \in [R], \quad (32)$$

whose expectation values are

$$\begin{aligned} \mathbb{E}[G^O(\theta)_{l,r}] &= \mathbb{E} \left[\langle \phi_l | e^{i(H-\theta)t'_n} O e^{-i(H-\theta)t_n} | \psi_r \rangle \right] \\ &= \langle \phi_l | \mathbb{E} \left[e^{i(H-\theta)t'_n} \right] O \mathbb{E} \left[e^{-i(H-\theta)t_n} \right] | \psi_r \rangle \\ &\approx \langle \phi_l | e^{-(\theta-H)^2 T^2 / 2} O e^{-(\theta-H)^2 T^2 / 2} | \psi_r \rangle \\ &= \Phi \cdot \text{diag} \left(\left\{ e^{-(\theta-\lambda_k)^2 T^2 / 2} \right\}_{k \in [M]} \right) \cdot O_{[M]} \\ &\quad \cdot \text{diag} \left(\left\{ e^{-(\theta-\lambda_{k'})^2 T^2 / 2} \right\}_{k' \in [M]} \right) \cdot \Psi^\dagger, \quad (33) \end{aligned}$$

where the matrix $O_{[M]} := (\langle E_k | O | E_{k'} \rangle)_{k,k' \in [M]}$ is written in the Hamiltonian eigenstate basis. In the second equality, we use the fact that t_n, t'_n are independent random variables.

If we use the Gaussian density distribution without truncation, in Eq. (33) the approximately equal sign should be instead an equal sign.

Let us focus on degenerate dominant eigenstates located at θ_i given by Algorithm 1 with multiplicity m_i . Recall that we have obtained the SVD $G(\theta_i) = U_i \Sigma_i V_i^\dagger$ and can thus restrict the matrices $G(\theta_i)$ and $G^O(\theta_i)$ to the large singular value subspace with cutoff threshold τ ,

$$\tilde{G}(\theta_i) = ((U_i)_{:, [m_i]})^\dagger \cdot G(\theta_i) \cdot ((V_i)_{:, [m_i]}) = (\Sigma_i)_{[m_i]}, \quad (34)$$

$$\tilde{G}^O(\theta_i) = ((U_i)_{:, [m_i]})^\dagger \cdot G^O(\theta_i) \cdot ((V_i)_{:, [m_i]}), \quad (35)$$

where $(\Sigma_i)_{[m_i]}$ is the diagonal matrix of m_i singular values of $G(\theta_i)$ that are larger than the SVD threshold τ , and $(U_i)_{:, [m_i]}$ and $(V_i)_{:, [m_i]}$ are the submatrices of U_i and V_i that contain the corresponding columns. The rest is to solve the generalized eigenvalue problem

$$\tilde{G}^O(\theta_i) w = \lambda^O \tilde{G}(\theta_i) w, \quad (36)$$

with regard to a low dimension, full-rank matrix $G(\theta_i)$, and the resulting eigenvalues $\lambda_1^O, \dots, \lambda_{m_i}^O$ will be approximately those of the matrix

$$O_{\mathcal{D}_i} := (\langle E_k | O | E_{k'} \rangle)_{k, k' \in \mathcal{D}_i}, \quad \mathcal{D}_i = \{k \in \mathcal{D} : \lambda_k \in \mathcal{I}_i\}, \quad (37)$$

which is the projection of $O_{[M]}$ onto the subspace spanned by the dominant eigenstates indexed by $\mathcal{D}_i$ with eigenvalue λ_i^* . We note that when the observable O and the Hamiltonian do not commute, there is not a one-to-one correspondence between the generalized eigenvalues λ_k^O and the Hamiltonian eigenstate expectations $\langle E_k | O | E_k \rangle$. Instead, it provides the possible range of expectation values of observable O within the corresponding dominant eigenvector subspace $\mathcal{E}_i$, which is $[\min_k \lambda_k^O, \max_k \lambda_k^O]$.

The correctness of this result can be justified as follows. When T is large enough and the random noise is negligible, we have

$$G(\theta_i) \approx \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\left\{ e^{-(\theta_i - \lambda_k)^2 T^2} \right\}_{k \in \mathcal{D}_i} \right) \cdot (\Psi_{:, \mathcal{D}_i})^\dagger. \quad (38)$$

Thus, there must exist two invertible matrices $P_U \in \mathbb{C}^{|\mathcal{D}_i| \times |\mathcal{D}_i|}$ and $P_V \in \mathbb{C}^{|\mathcal{D}_i| \times |\mathcal{D}_i|}$ such that

$$\Phi_{:, \mathcal{D}_i} = (U_i)_{:, [m_i]} P_U, \quad \Psi_{:, \mathcal{D}_i} = (V_i)_{:, [m_i]} P_V. \quad (39)$$

Plugging this into the formula of $\tilde{G}^O(\theta_i)$ and $\tilde{G}(\theta_i)$, we obtain

$$\tilde{G}^O(\theta_i) = P_U \cdot \text{diag} \left(\left\{ e^{-(\theta_i - \lambda_k)^2 T^2 / 2} \right\}_{k \in \mathcal{D}_i} \right) \cdot O_{\mathcal{D}_i} \cdot \text{diag} \left(\left\{ e^{-(\theta_i - \lambda_{k'})^2 T^2 / 2} \right\}_{k' \in \mathcal{D}_i} \right) \cdot P_V^\dagger \quad (40)$$

and

$$\tilde{G}(\theta_i) = \underbrace{P_U \cdot \text{diag} \left(\left\{ e^{-(\theta_i - \lambda_k)^2 T^2 / 2} \right\}_{k \in \mathcal{D}_i} \right)}_{\text{full rank}} \cdot \underbrace{\text{diag} \left(\left\{ e^{-(\theta_i - \lambda_{k'})^2 T^2 / 2} \right\}_{k' \in \mathcal{D}_i} \right) \cdot P_V^\dagger}_{\text{full rank}}. \quad (41)$$

Comparing the above two formulas, it is straightforward to see that the generalized eigenvalue problem in Eq. (36) will give eigenvalues of $O_{\mathcal{D}_i}$.

Below, we will provide an informal resource analysis for the observable estimation algorithm. For simplicity, we focus on the second regime we discussed at the end of Sec. IV B. The proof is given in Appendix E.

Proposition 1. In addition to the assumption in Theorem 2, assume that $|\mathcal{D}_i|, L, R = \mathcal{O}(1)$, access to a Pauli observable O , and

- (1) $p_{\min} = \Omega(1)$, which is reflected by the SVD threshold τ in the algorithm;

- (2) there are no tail eigenvalues, i.e., $p_{\text{tail}} = 0$.

To achieve ϵ_O -accuracy in estimating eigenvalues of $O_{\mathcal{D}_i}$, it suffices to choose

$$T_{\max} = \tilde{\mathcal{O}}(\Delta^{-1}), \quad N = \tilde{\Omega}(\epsilon_O^{-2}), \quad (42)$$

and the total evolution time

$$T_{\text{total}} = \tilde{\mathcal{O}}(NLRT_{\max}) = \tilde{\mathcal{O}}(\Delta^{-1} \epsilon_O^{-2}). \quad (43)$$

We note that the constant in Proposition 1 depends on polynomially on $p_{\min}^{-1}$, as seen from the proof in Appendix E. Here, we assume $p_{\min} = \Omega(1)$ to avoid this amplification factor and only focus on the scaling with

ALGORITHM 2. Extracting observable expectation values under the quantum filtering and analysis of multiplicities in eigenvalue spectra framework

-
- 1: **Preparation:**
 - Number of data pairs: N ;
 - Two initial state sets: $\{\phi_i\}_{i=1}^L$ and $\{\psi_j\}_{j=1}^R$;
 - Filter parameter: T ;
 - Truncation parameter in a_T^{trunc} : σ ;
 - Unitary observable: O ;
 - Output from Algorithm 1:**
 - Location of degenerate dominant eigenvalue: θ_i ;
 - Degeneracy: m_i ;
 - SVD result of $G(\theta_i)$: $G(\theta_i) = U_i \Sigma_i V_i^\dagger$.
 - 2: **Running:**
 - 3: ▷ Step 1: Generate data
 - 4: Sample $\{t_n\}$ and $\{t'_n\}$ i.i.d. from the truncated Gaussian distribution $a_{T/\sqrt{2}}^{\text{trunc}}(t)$ defined as Eq. (16)
 - 5: **for** $l = 1$ to L **do**
 - 6: **for** $r = 1$ to R **do**
 - 7: **for** $n = 1$ to N **do**
 - Generate $Z_{l,r,n}^O \in \{\pm 1 \pm \mathbf{i}\}$ using generalized Hadamard test in Eq. (29)
 - with (U_l, V_r, t_n, t'_n, O)
 - 8: **end for**
 - 9: **end for**
 - 10: **end for**
 - 11: ▷ Step 2: Solve the generalized eigenvalue problem
 - 12: ▷ Step 2: Solve the generalized eigenvalue problem
 - 13: Calculate

$$G^O(\theta_i) \leftarrow \frac{1}{N} \sum_{n=1}^N Z_{l,r,n}^O \exp(\mathbf{i}\theta_i(t_n - t'_n)).$$

- 14: Calculate matrices

$$\begin{aligned} \tilde{G}^O(\theta_i) &= ((U_i)_{:, [m_i]})^\dagger \cdot G^O(\theta_i) \cdot ((V_i)_{:, [m_i]}) \\ \tilde{G}(\theta_i) &= ((U_i)_{:, [m_i]})^\dagger \cdot G(\theta_i) \cdot ((V_i)_{:, [m_i]}) = (\Sigma_i)_{[m_i]}, \end{aligned}$$

- 15: Solve the generalized eigenvalue problem

$$\tilde{G}^O(\theta_i)w = \lambda^O \tilde{G}(\theta_i)w.$$

- 16: **Output:** *Eigenvalues:* $\{\lambda_k^O\}_{k=1}^{m_i}$ that provide estimations of eigenvalues of $O_{\mathcal{D}_i}$.
-

respect to ϵ_O and Δ . It is instructive to contrast the generalized eigenvalue problem in Eq. (36) with those arising in quantum subspace methods for eigenvalue estimation [23,25–31]. According to Theorem 2.7 of Ref. [29], if each entry of the projected Hamiltonian and overlap matrices is estimated using N_s samples, then the statistical error per entry scales as $\mathcal{O}(N_s^{-1/2})$. The corresponding error in the eigenvalue of interest scales as $\mathcal{O}(N_s^{-1/(2(1+\gamma))})$, where $0 \leq \gamma \leq \frac{1}{2}$ arises from a weighted geometric mean inequality for the projected matrices. Thus, the convergence can be slower than the shot-noise-limited scaling

$\mathcal{O}(N_s^{-1/2})$ whenever $\gamma > 0$. Moreover, the error bound in Ref. [29] includes additional amplification factors that depend polynomially on the subspace dimension D (the dimension of the data matrix); in practice, D is therefore typically kept small. In our setting, the generalized eigenvalue problem in Eq. (36) involves an $L \times R$ matrix, so the relevant dimension is $D = \max(L, R)$. In the regime of Proposition 1, L and R are constants, and improved accuracy is obtained by increasing the maximal evolution time T_{max} and the number of samples used to estimate each matrix entry, rather than by enlarging the data matrix dimension.

VI. ANCILLA-FREE ALTERNATIVE TO THE GENERALIZED HADAMARD TEST

In the QFAMES algorithm, the generalized Hadamard test circuits (13) and (29) are used to generate the quantum data $Z_{l,r,n}$, and for observables, $Z_{l,r,n}^O$, which requires controlled Hamiltonian evolution and initial state-preparation circuits. Such controlled operations can be challenging to implement on near-term and even early fault-tolerant quantum devices. To address this limitation, several alternatives to the generalized Hadamard test have recently been proposed that are either ancilla-free [5–7,9,88] or substantially reduce the requirements of controlled operations [8]. The method in Ref. [5] is particularly suitable for QFAMES, as it

- (1) exactly allows to measure $\mathcal{Z}_{l,r}(t) = \langle \phi_l | e^{-\mathbf{i}Ht} | \psi_r \rangle$ with different left and right initial states $|\phi_l\rangle$ and $|\psi_r\rangle$;
- (2) can produce the data for t in the time interval $[0, \sigma T]$ in a single execution of the algorithm;
- (3) can be easily generalized to the cases involving multiple time evolutions, thereby allowing access to measuring $\mathcal{Z}_{l,r}^O(t, t')$ in the observable version of QFAMES.

Below we will briefly introduce this algorithm. A key observation is that the main difficulty of measuring $\mathcal{Z}_{l,r}(t) = r(t)e^{\mathbf{i}\varphi(t)}$ lies in the phase $\varphi(t)$ rather than the absolute value $r(t)$, and these two quantities are related via complex analysis. Notice that for a bounded Hamiltonian, the analytic continuation $\mathcal{Z}_{l,r}(z) = \langle \phi_l | e^{-\mathbf{i}Hz} | \psi_r \rangle$ is a holomorphic function on the complex plane $z = t - \mathbf{i}\beta$, and so is $\ln \mathcal{Z}_{l,r}(z) = \ln r(z) + \mathbf{i}\varphi(z)$ when $\mathcal{Z}_{l,r}(z) \neq 0$. Therefore, the Cauchy-Riemann equation connects the absolute value and phase as

$$\frac{d\varphi(t)}{dt} = \left. \frac{\partial \ln r(z)}{\partial \beta} \right|_{\beta=0} \approx \frac{1}{2h} [\ln r(t - \mathbf{i}h) - \ln r(t + \mathbf{i}h)].$$

The last step is the finite difference approximation and h is a small constant. Assuming knowledge of $\varphi(0)$, one

can obtain the phases $\varphi(t)$ for t in the desired interval by integrating Eq. (44). Thus it is only required to measure the quantities $r(t) = |\langle \phi_l | e^{-iHt} | \psi_r \rangle|$ and $r(t \pm ih) = |\langle \phi_l | e^{-iHt} e^{\pm hH} | \psi_r \rangle|$. The corresponding circuits are

$$|0\rangle \xrightarrow{V_r} \xrightarrow{e^{-itH}} \xrightarrow{U_l^\dagger} \text{---} \text{---} \text{---} |0\rangle \quad (44)$$

$$|0\rangle \xrightarrow{V_r} \xrightarrow{e^{\pm hH}/c_{\psi_r,\pm}} \xrightarrow{e^{-itH}} \xrightarrow{U_l^\dagger} \text{---} \text{---} \text{---} |0\rangle \quad (45)$$

which provide unbiased estimations of $r(t)^2$ and $r(t \pm ih)^2 / c_{\psi_r,\pm}^2$, respectively. In addition to the necessary state preparations and real-time evolutions, these circuits require at most *a single short step* of imaginary-time evolution to one side of the initial states, and the last step is a projective measurement onto computational basis state $|0\rangle$.

Note that the imaginary-time evolution is nonunitary and thus a precomputed normalization factor $c_{\psi_r,\pm} = \sqrt{\langle \psi_r | e^{\pm 2hH} | \psi_r \rangle}$ is required in the quantum circuit. When the initial state $|\psi_r\rangle = V_r |0\rangle$ has short correlation length and the Hamiltonian H is local, the single step of imaginary-time evolution can be approximated by local unitary evolution operators times $c_{\psi_r,\pm}$, as shown in the QITE algorithm [82]. If it is not the case, there also exist alternatives to QITE. For example, one can introduce a single auxiliary qubit to implement the single-step imaginary-time evolution via probabilistic imaginary-time evolution algorithms [83,89], while still avoiding the requirement for controlled long real-time evolutions.

To measure $Z_{l,r}^O(t, t')$, we just need to view t and t' as two separate variables and perform the algorithm from both sides. The modified circuits are as follows:

$$|0\rangle \xrightarrow{V_r} \xrightarrow{e^{-itH}} \xrightarrow{O} \xrightarrow{e^{it'H}} \xrightarrow{U_l^\dagger} \text{---} \text{---} \text{---} |0\rangle \quad |Z_{l,r}^O(t, t')|^2 \quad (46)$$

$$|0\rangle \xrightarrow{V_r} \xrightarrow{e^{\pm hH}/c_{\psi_r,\pm}} \xrightarrow{e^{-itH}} \xrightarrow{O} \xrightarrow{e^{it'H}} \xrightarrow{U_l^\dagger} \text{---} \text{---} \text{---} |0\rangle \quad |Z_{l,r}^O(t \pm ih, t')|^2 / c_{\psi_r,\pm}^2 \quad (47)$$

$$|0\rangle \xrightarrow{V_r} \xrightarrow{e^{-itH}} \xrightarrow{O} \xrightarrow{e^{it'H}} \xrightarrow{e^{\pm hH}/c_{\phi_l,\pm}} \xrightarrow{U_l^\dagger} \text{---} \text{---} \text{---} |0\rangle \quad |Z_{l,r}^O(t, t' \pm ih)|^2 / c_{\phi_l,\pm}^2 \quad (48)$$

VII. QFAMES WITH MIXED-STATE INPUTS

We have presented QFAMES assuming that the initial states are pure states and we have access to the controlled unitary operators that prepare these states. In this section, we generalize the observable version to mixed states and remove the requirement for controlled state-preparation gates. Note that the multiplicity estimation version of QFAMES can be naturally embedded in the observable version of QFAMES. For simplicity, we only present the observable version of QFAMES with mixed-state inputs

We first introduce the algorithm. Assume that we have access to a set of mixed states $\{\rho_l\}_{l \in [L]}$ and $\{\sigma_r\}_{r \in [R]}$.

Step 1: Generate data. Analogous to the case of pure initial states, we aim to measure quantities of the form

$$\begin{aligned} Z_{l,r}^{\text{mixed}}(t_n, t'_n) &:= \text{tr} \left(\rho_l e^{-iH t_n} \sigma_r e^{-iH t'_n} \right), \\ Z_{l,r}^{O,\text{mixed}}(t_n, t'_n, t''_n) &:= \text{tr} \left(\rho_l e^{-iH t_n} O e^{-iH t'_n} \sigma_r e^{-iH t''_n} \right). \end{aligned} \quad (49)$$

Their unbiased estimates can be obtained through the following circuits using a swap test:

$$Z_{l,r,n}^{\text{mixed}} : \quad \begin{array}{c} |0\rangle \xrightarrow{H} \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} W \xrightarrow{H} \text{---} \text{---} \text{---} \\ \rho_l \xrightarrow{\quad} \xrightarrow{e^{-it'_n H}} \text{---} \times \text{---} \\ \sigma_r \xrightarrow{\quad} \xrightarrow{e^{-it_n H}} \text{---} \times \text{---} \end{array} \quad (50)$$

$$(51)$$

Both circuits only require the ability to prepare the mixed states ρ_l and σ_r and do not require controlled state-preparation gates, which might be of independent interest.

Step 2: Construct filtered data matrices. The second step is to contract the time dimensions of the 3-tensors $Z_{l,r,n}^{\text{mixed}}$ and $Z_{l,r,n}^{O,\text{mixed}}$ with element-wise products of complex exponential vectors of the form $e^{i\theta t_n}$,

$$[f_n(\theta, T, \{t_n\})] := [e^{i\theta t_n}], \quad (52)$$

where the set $\{t_n\}$ are sampled independently from the truncated Gaussian density distribution $a_T^{\text{trunc}}(t)$. Similar to the pure state case, we define

$$\begin{aligned} G_{l,r}^{\text{mixed}}(\theta) &= \frac{1}{N} \sum_{n=1}^N Z_{l,r,n}^{\text{mixed}} f_n(\theta, T, \{t_n\}) f_n(\theta, T, \{t'_n\}), \\ G_{l,r}^{O,\text{mixed}}(\theta) &= \frac{1}{N} \sum_{n=1}^N Z_{l,r,n}^{O,\text{mixed}} f_n\left(\theta, \frac{T}{\sqrt{2}}, \{t_n\}\right) \\ &\quad f_n\left(\theta, \frac{T}{\sqrt{2}}, \{t'_n\}\right) f_n(\theta, T, \{t'_n\}). \end{aligned} \quad (53)$$

When N is sufficiently large, we have

$$\begin{aligned} G_{l,r}^{\text{mixed}}(\theta) &\approx \mathbb{E}[G_{l,r}^{\text{mixed}}(\theta)] = \text{tr}(\rho_l(\theta, T) \sigma_r(\theta, T)), \\ G_{l,r}^{O,\text{mixed}}(\theta) &\approx \mathbb{E}[G_{l,r}^{O,\text{mixed}}(\theta)] = \text{tr}(\rho_l(\theta, T) O \sigma_r(\theta, T)), \end{aligned} \quad (54)$$

where $\rho(\theta, T) := e^{-(\theta-H)^2 T^2/2} \rho e^{-(\theta-H)^2 T^2/2}$ denotes the filtered density matrix of a given mixed state ρ . If we vectorize the density matrices as $\rho \rightarrow |\rho\rangle$, we obtain

$$\begin{aligned} G_{l,r}^{\text{mixed}}(\theta) &\approx \langle\langle \rho_l(\theta, T) | \sigma_r(\theta, T) \rangle\rangle \\ &= \sum_{i,j} (\rho_l)_{i,j} (\sigma_r)_{j,i} \exp(-((\theta - \lambda_j)^2 + (\theta - \lambda_i)^2) T^2), \\ G_{l,r}^{O,\text{mixed}}(\theta) &\approx \langle\langle \rho_l(\theta, T) | \mathbb{I} \otimes O | \sigma_r(\theta, T) \rangle\rangle. \end{aligned} \quad (55)$$

Step 3: Estimate dominant eigenvalues and multiplicities. According to Eq. (55), $\|G^{\text{mixed}}(\theta)\|_F$ peaks when θ is close to the dominant eigenvalues of H . Similar to

the pure state case, in the third step, we find the dominant eigenvalues $\{\theta_k^*\}$ by locating the peaks of the function $\|G^{\text{mixed}}(\theta)\|_F$ over θ following the same *search and block* strategy (Sec. IV A) as in the pure state case.

Step 4: Observable estimation. For each identified dominant eigenvalue θ_k^* , we solve the following generalized eigenvalue problem:

$$G^{O,\text{mixed}}(\theta_k^*) w = \lambda^O G^{\text{mixed}}(\theta_k^*) w, \quad (56)$$

to obtain estimates of the extremal eigenvalues (after taking the maximal/minimal generalized eigenvalues λ^O of the observable O within the (nearly) degenerate dominant eigenspace of H . As in Sec. V, one may first restrict $G^{\text{mixed}}(\theta_k^*)$ and $G^{O,\text{mixed}}(\theta_k^*)$ to the large singular value subspace of $G^{\text{mixed}}(\theta_k^*)$ (using the cutoff threshold τ) to obtain a low-dimensional, full-rank generalized eigenvalue problem. We note that, because θ_k^* is close to the dominant eigenvalue λ_k^* of H , the filtered density matrices $\rho_l(\theta_k^*, T)$ and $\sigma_r(\theta_k^*, T)$ are approximately supported on the subspace spanned by the (nearly) degenerate dominant eigenvectors of H . Let Π_k denote the spectral projector onto the (nearly) degenerate dominant subspace associated with the cluster centered at θ_k^* . The physically meaningful range of the expectation values of O within this manifold is

$$\lambda_{\min}(\Pi_k O \Pi_k), \quad \lambda_{\max}(\Pi_k O \Pi_k). \quad (57)$$

Under the condition that the projection of $G_{l,r}^{\text{mixed}}(\theta_k^*)$ onto the degenerate eigenspace maintains sufficient rank [see Eq. (63)], the generalized eigenvalue problem (56) yields consistent estimates of these extremal eigenvalues, which is the same as in the pure state case in Sec. V. For example, in the case when $L = R$ and $\rho_l = \sigma_l$ for all l , and the vectors $\{|\rho_l(\theta_k^*, T)\rangle\}_{l \in [L]}$ span the degenerate dominant eigenspace in the vectorized representation, the maximal eigenvalue problem Eq. (57) can be formulated as

$$\begin{aligned} \max_{|\psi\rangle \in \text{Ran}(\Pi_k)} \frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle} &= \max_{|\psi\rangle \in \text{Ran}(\Pi_k)} \frac{\text{tr}(|\psi\rangle\langle\psi|O)}{\langle\psi|\psi\rangle} \\ &= \max_{|\psi\rangle \in \text{Ran}(\Pi_k)} \frac{\text{Tr}(|\psi\rangle\langle\psi|O|\psi\rangle\langle\psi|)}{\text{Tr}(|\psi\rangle\langle\psi||\psi\rangle\langle\psi|)} \\ &= \max_{\sum_i |c_i|^2 = 1} \frac{\sum_{j,k} c_j^* c_k \text{tr}(\rho_j O \rho_k)}{\sum_{j,k} c_j^* c_k \text{tr}(\rho_j \rho_k)} = \max_i \lambda_i^O, \end{aligned} \quad (58)$$

where

$$G^{O,\text{mixed}}(\theta_k^*)w = \lambda_i^O G^{\text{mixed}}(\theta_k^*)w. \quad (59)$$

Analogous to the pure state case, the observable structure is better characterized by the pairing of mixed states ρ_l and σ_r , which yields information inaccessible through direct measurements of O on the individual states. Here, we provide a simple toy example to illustrate this. Assume that there is a twofold degenerate ground state $\{|0\rangle, |1\rangle\}$. In this ground-state subspace an observable Z has the form $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. Assume access to four density matrices, which are after the filtering process projected onto the ground-state subspace as

$$\begin{aligned} \rho_1 &= \begin{bmatrix} 0.6 & 0 \\ 0 & 0.4 \end{bmatrix}, \\ \rho_2 &= \begin{bmatrix} 0.4 & 0 \\ 0 & 0.6 \end{bmatrix}, \\ \rho_3 &= |+\rangle\langle +| = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \\ \rho_4 &= |+\rangle\langle +| = \frac{1}{2} \begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}. \end{aligned} \quad (60)$$

Here $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$. Direct measurements of the observable Z with these four density matrices yield

$$\text{tr}(\rho_{1,2}Z) = \pm 0.2, \quad \text{tr}(\rho_{3,4}Z) = 0, \quad (61)$$

which cannot fully capture the “ferromagnetic” feature of the ground-state manifold with regard to $O = Z$. However, in the mixed-state version of the QFAMES algorithm, we have

$$\begin{aligned} G_{l,r}^{\text{mixed}} &= \text{tr}(\rho_l \rho_r) = \begin{bmatrix} 0.52 & 0.48 & 0.5 & 0.5 \\ 0.48 & 0.52 & 0.5 & 0.5 \\ 0.5 & 0.5 & 1 & 0.5 \\ 0.5 & 0.5 & 0.5 & 1 \end{bmatrix}, \\ G_{l,r}^{O,\text{mixed}} &= \text{tr}(\rho_l O \rho_r) = \begin{bmatrix} 0.2 & 0 & 0.1 & 0.1 \\ 0 & -0.2 & -0.1 & -0.1 \\ 0.1 & -0.1 & 0 & -0.5i \\ 0.1 & -0.1 & 0.5i & 0 \end{bmatrix}. \end{aligned} \quad (62)$$

Solve the generalized eigenvalue problem $G_{l,r}^{O,\text{mixed}}w = \lambda^O G_{l,r}^{\text{mixed}}w$, and we can correctly obtain $\min \lambda^O = -1$ and $\max \lambda^O = 1$.

The detailed algorithm is summarized in Algorithm 3.

As previously noted, the success of mixed-state QFAMES requires that the initial mixed states have sufficient overlap with the (nearly) degenerate dominant

eigenvectors of H . Under the assumption $\{\rho_l\} = \{\sigma_r\}$, this requirement is characterized by the following condition:

$$\min_{H|\psi\rangle = \lambda_k^*|\psi\rangle} \max_{\substack{p_i \geq 0 \\ \sum_i p_i = 1}} \left\langle \psi \left| \sum_i p_i \rho_i \right| \psi \right\rangle = \omega(1). \quad (63)$$

When the goal is to estimate the extremal eigenvalues of O within the low-energy subspace of H , there is extensive literature on preparing such mixed states using recently developed dissipative algorithms for low-temperature thermal state or ground-state preparation [41–44, 46–48, 50, 53, 55, 90–102]. For example, certain physically interesting systems exhibit metastable states, often arising from

ALGORITHM 3. Extracting observable expectation values under quantum filtering and analysis of multiplicities in eigenvalue spectra with mixed-state inputs.

1: **Preparation:**

Number of time samples: N ;
Two sets of initial mixed states: $\{\rho_l\}_{l=1}^L$ and $\{\sigma_r\}_{r=1}^R$;
Filter parameter: T ;
Truncation parameter in a_T^{trunc} : σ ;
Number of dominant eigenvalues (guess): $\tilde{I}$;
Singular value decomposition threshold: τ ;
Searching parameter: q (we search with discrete energy step q/T);
Block parameter: α (distinct dominant eigenvalues are at least separated by α/T);

2: **Running:**

3: ▷ **Stage I: Estimate the location of dominant eigenvalues**

4: Sample $\{t_n, t'_n\}$ i.i.d. from the truncated Gaussian distribution $a_T^{\text{trunc}}(t)$ defined in Eq. (16).

5: **for** $l = 1$ to L **do**

6: **for** $r = 1$ to R **do**

7: **for** $n = 1$ to N **do**

8: Generate data $Z_{l,r,n}^{\text{mixed}}$ using (50).

9: **end for**

10: **end for**

11: **end for**

12: $J \leftarrow \left\lfloor \frac{2\pi T}{q} \right\rfloor$.

13: Generate discrete candidates: $\theta_j \leftarrow -\pi + \frac{jq}{T}$ for $j = 0, 1, \dots, J$.

14: Calculate (53) for $0 \leq j \leq J$:

$$\|G^{\text{mixed}}(\theta_j)\|_F \leftarrow \left\| \frac{1}{N} \sum_{n=1}^N Z_{:, :, n}^{\text{mixed}} e^{i\theta_j t_n} e^{i\theta_j t'_n} \right\|_F.$$

15: Running the search-and-block procedure with α in Algorithm 1 to estimate the dominant eigenvalues.

16: **Output:** Distinct dominant eigenvalues: $\{\theta_i^*\}_{i=1}^{\tilde{I}}$.

ALGORITHM 3. (Continued.)

```

17: ▷ Stage II: Estimate observable expectation values
18: Sample  $\{t_n, t'_n\}$  i.i.d. from the truncated Gaussian
    distribution  $a_{T/\sqrt{2}}^{\text{trunc}}(t)$  defined as Eq. (16) and  $\{t''_n\}$ 
    i.i.d. from  $a_T^{\text{trunc}}(t)$ .
19: for  $l = 1$  to  $L$  do
20:   for  $r=1$  to  $R$  do
21:     for  $n = 1$  to  $N$  do
22:       Generate  $Z_{l,r,n}^{O,\text{mixed}}$  using (51).
23:     end for
24:   end for
25: end for
26: Calculate

```

$$G^{O,\text{mixed}}(\theta_i^*) \leftarrow \frac{1}{N} \sum_{n=1}^N Z_{l,r,n}^{O,\text{mixed}} \exp(i\theta_i^* t_n) \exp(i\theta_i^* t'_n) \exp(i\theta_i^* t''_n), \quad 0 \leq i \leq \tilde{I}.$$

27: Solve the generalized eigenvalue problem

$$G^{O,\text{mixed}}(\theta_i^*) w = \lambda^O G^{\text{mixed}}(\theta_i^*) w.$$

28: **Output:** *Eigenvalues:* $\{\lambda_k^O\}_{k=1}^{m_i}$ that provide estimates of eigenvalues of $O_{\mathcal{D}_i}$.

energy or entropy bottlenecks in the dissipative dynamics [103–106]. Characterizing the physical observables of these states is of significant interest in condensed matter physics and quantum materials science [107–112]. While reaching the true global thermal equilibrium in such systems typically requires exponential time, relaxing to a specific low-temperature metastable state is often a polynomial-time process [113–118]. Consequently, starting from a random initial state allows one to efficiently populate the underlying metastable subspace, thereby making the condition in Eq. (63) achievable.

VIII. NUMERICAL RESULTS

In this section, we numerically demonstrate the efficiency of QFAMES by applying it to four models: (1) A simple illustrative example in Sec. VIII A; (2) A TFIM in Sec. VIII B; (3) 2D toric code example in Sec. VIII C; (4) XXZ model in Sec. VIII D. For simplicity, we set the left and right initial states to be the same. In the first case, we provide three simple initial states that are not orthogonal to each other to estimate the multiplicity of the ground states. For the TFIM, we take five low-energy matrix product states with bond dimension 2 as the initial states. We not only compute the ground-state degeneracies but also probe ground-state properties of different quantum phases by measuring observable expectation values. In the third example, we employ an increasing number of random initial states to estimate the ground-state degeneracy of a

model with topological order, thereby demonstrating that QFAMES is applicable in a broad range of settings. All codes and data needed to produce the results in this section are available online [119].

A. Illustrative example

To illustrate the effectiveness of QFAMES, we consider a simple Hamiltonian with three eigenvalues: $\lambda_0 = \lambda_1 = 0$ and $\lambda_2 = 0.1$. There are only two distinct eigenvalues: $\lambda_0^* = 0$ and $\lambda_1^* = 0.1$. The Hamiltonian is given by

$$H = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0.1 \end{bmatrix}, \quad (64)$$

and we assume access to three initial states $|\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle$ with overlap matrix

$$\Phi = \Psi = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix}. \quad (65)$$

In this case, the tail overlap $p_{\text{tail}} = 0$ and all eigenvalues are dominant. A single initial-state approach would only yield an estimate of the location of λ_0^* and λ_1^* but fail to resolve the degeneracy of λ_0^* . Moreover, because the overlaps with λ_2 (λ_1^*) are not sufficiently dominant compared to those with λ_0, λ_1 (λ_0^*), single-state approaches might not reliably estimate the location of λ_2 (λ_1^*).

To resolve the degeneracy at λ_0^* , it is essential to utilize the off-diagonal entries of the data tensor, which encode important information about the spectral structure. We can check that the $\mathcal{Z}$ matrix has the form

$$\mathcal{Z}(t) = \frac{1}{3} \begin{bmatrix} 2 + e^{-i0.1t} & e^{-i0.1t} & 2 - e^{-i0.1t} \\ e^{-i0.1t} & 2 + e^{-i0.1t} & -e^{-i0.1t} \\ 2 - e^{-i0.1t} & -e^{-i0.1t} & 2 + e^{-i0.1t} \end{bmatrix}. \quad (66)$$

The off-diagonal entry $\mathcal{Z}_{0,1}(t) = \frac{1}{3}e^{-i0.1t}$, for example, reveals two key pieces of information:

- (1) $\lambda_2 = 0.1$ must be one of the dominant eigenvalues, as it is the only effective frequency present in the signal;
- (2) The degeneracy of dominant eigenvalue λ_0^* must be at least two, since the signal corresponding to the frequency $\lambda \approx 0$ vanishes in this off-diagonal entry.

The first point allows for a more accurate estimation of the location of λ_2 , while the second provides insight into the multiplicity of λ_0^* .

Now we perform numerical simulations to demonstrate the main ideas of QFAMES. We independently sample $\{t_n\}_{n=1}^N$ with $N = 2000$ from the truncated Gaussian distribution $a_T^{\text{trunc}}(t)$ defined in Eq. (16) with truncation

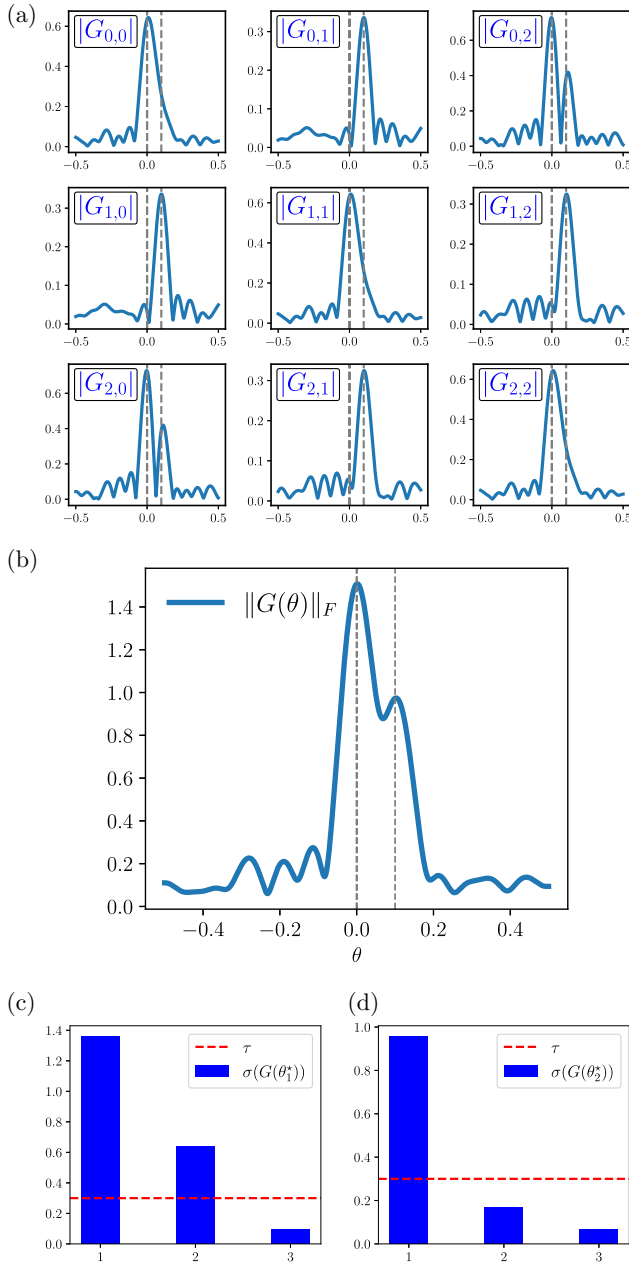


FIG. 3. Illustration of the quantum filtering and analysis of multiplicities in eigenvalue spectra algorithm on the illustrative example. (a) The magnitude of $G_{ij}(\theta) = (1/N) \sum_{n=1}^N Z_{i,j,n} e^{i\theta t_n}$ for each $0 \leq i, j \leq 2$. The x -axis stands for θ . The gray dashed lines indicate the positions of the eigenvalues. (b) The Frobenius norm $\|G(\theta)\|_F$, which clearly identifies the two distinct dominant eigenvalues. (c) and (d) The singular values of $G(\theta)$ at each λ_i^* , correctly indicating the corresponding multiplicities when the threshold $\tau = 0.1\sqrt{LR} = 0.3$.

parameter $\sigma = 1$, and generate each Z_n using a single-shot generalized Hadamard test. In Fig. 3(a), we plot the magnitude of each entry of $G(\theta)$ for $T = 40$. The diagonal entries exhibit a prominent peak corresponding to λ_0^* , while the second peak near λ_2 is not clearly identifiable. As a result,

the standard QPE-based approach described in Appendix B cannot locate λ_2 and fails to reveal the multiplicity of λ_0^* . Although the diagonal landscapes are the same in Fig. 3(a), if we focus on the off-diagonal landscapes, it is evident that there exists one dominant eigenvalue near $\lambda_2 = 0.1$. This can be more systematically observed in the plot of the Frobenius norm $\|G(\theta)\|_F$ in Fig. 3(b), which clearly reveals two distinct dominant eigenvalues, including an “amplified” peak near $\lambda_0 = \lambda_1 = 0$. Note that the artificial peaks in Figs. 3(a) and 3(b) are due to noises that can be suppressed as we increase the number of samples N . Figures 3(c) and 3(d) show the singular values of $G(\theta)$ at $\theta = 0$ and $\theta = 0.1$, respectively. They exactly recover the multiplicities: two states associated with the dominant eigenvalue near zero and one state associated with the dominant eigenvalue near 0.1.

In Fig. 4, we show the accuracy of the QFAMES algorithm in locating dominant eigenvalues as a function of $T_{\max}$, T_{total} . The parameters are chosen as follows: SVD threshold $\tau = 0.1\sqrt{LR}$, block parameter $\alpha = 5$, search parameter $q = 0.005$, and T takes values 40, 50, 60, 80, 100, 200, 400, and 800. The error is defined as

$$\text{Error} = \max_i |\theta_i^* - \lambda_i^*|. \quad (67)$$

In Fig. 4, we also include a comparison with the Quantum Multiple Eigenvalue Gaussian filter Search (QMEGS) algorithm [64], using the same parameters as QFAMES except for $N = 6000$, which ensures the total number of Hamiltonian simulations is the same. From the graph, we observe that QFAMES achieves significantly lower error than QMEGS when $T_{\max} < 100$, while the errors of both methods become comparable for larger $T_{\max}$. This demonstrates the advantage of QFAMES in identifying dominant eigenvalues when $T_{\max}$ is not sufficiently large, aided by the use of off-diagonal entries in $G(\theta)$. Furthermore, we note that QMEGS cannot identify the multiplicity of λ_0^* , as it relies solely on the diagonal entries of $G(\theta)$, whereas QFAMES accurately estimates the multiplicities of both dominant eigenvalues.

B. Transverse-field Ising model (TFIM)

Here we consider the transverse-field Ising model on a spin chain of length N_{spin} ,

$$H = - \sum_{i=1}^{N_{\text{spin}}-1} Z_i Z_{i+1} - g \sum_{i=1}^{N_{\text{spin}}} X_i, \quad (68)$$

where Z_i and X_i are the Pauli operators acting on the i th qubit and g is the coupling coefficient. The ground state of the TFIM lies in the ferromagnetic phase for $g < 1$ and undergoes a quantum phase transition at $g = 1$ to the paramagnetic phase for $g > 1$. Note that in the thermodynamic

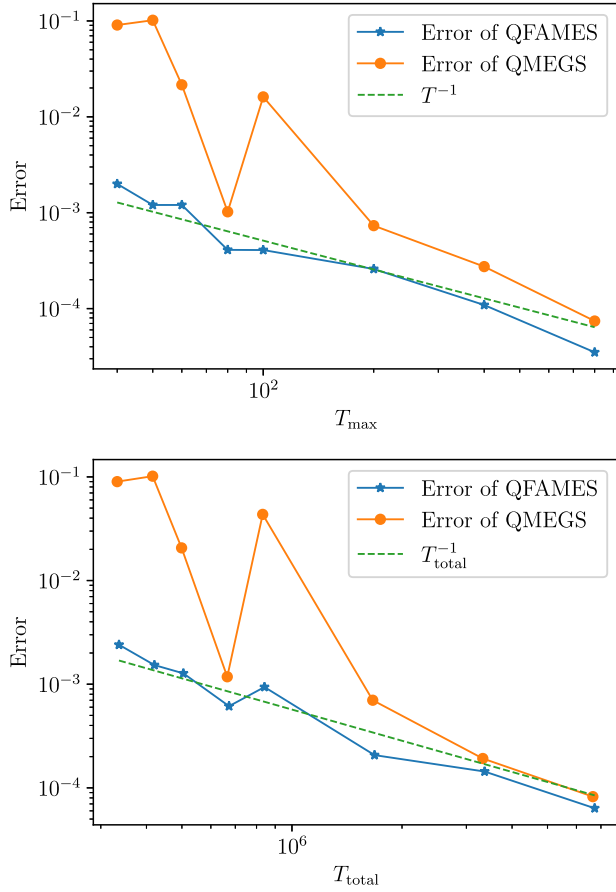


FIG. 4. Quantum filtering and analysis of multiplicities in eigenvalue spectra (Algorithm 1) vs QMEGS [64] in the illustrative example as a function of (upper): max evolution time $T_{\max} = \sigma T$, and (lower): total evolution time T_{total} . The dashed line stands for the fitted error proportional to $1/T$, as predicted by Eq. (27).

limit, the GSD is 2 in the ferromagnetic phase, 1 in the paramagnetic phase, and the system is gapless at the phase transition point.

In our test, we set system size $N_{\text{spin}} = 20$ and $g = 0.5, 0.8, 0.9, 0.95, 1, 1.05, 1.1, 1.2, 1.5$. For each g , the set of initial states is chosen to be five MPS of bond dimension 2 that are orthogonal to each other and have approximately the lowest energies. We first run density matrix renormalizing group (DMRG) with bond dimension 2 to find the MPS $|\psi_0\rangle$. The states $|\psi_i\rangle$ ($i > 0$) are then sequentially obtained by running DMRG with the projected Hamiltonian

$$H_i = \left(1 - \sum_{j=0}^{i-1} |\psi_j\rangle \langle \psi_j|\right) H \left(1 - \sum_{j=0}^{i-1} |\psi_j\rangle \langle \psi_j|\right).$$

We simulate the time evolutions with the time-evolving block decimation algorithm [120] with maximum MPS bond dimension $\chi = 100$. The Gaussian filter parameter $T/\sqrt{2} = 2.5$. For simplicity, for the time parameters t_n

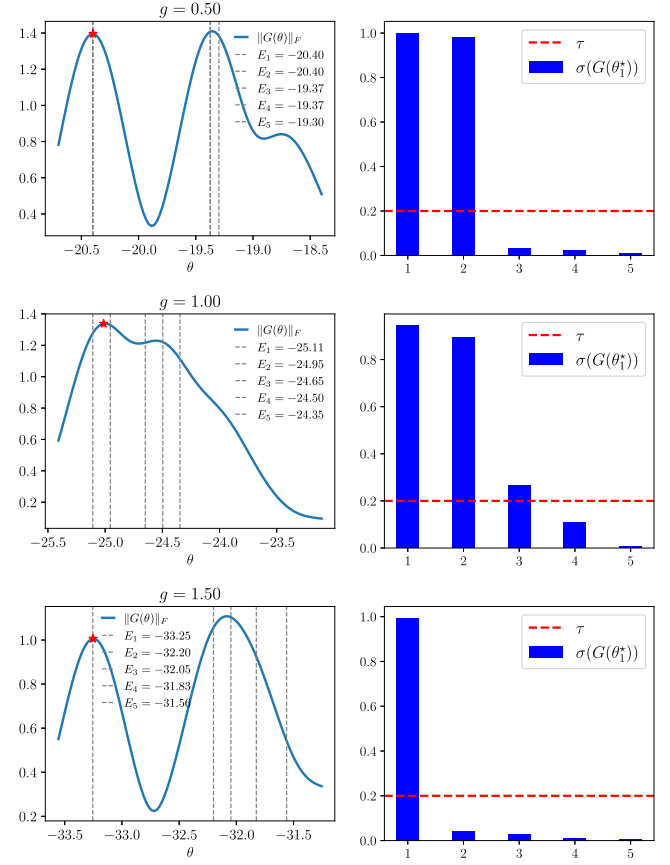


FIG. 5. Illustration of the quantum filtering and analysis of multiplicities in eigenvalue spectra algorithm on the transverse-field Ising model. The left column shows the Frobenius norm of $G(\theta)$ around the ground state energy for $g = 0.5, 1.0$ and 1.5 , from up to down. The gray vertical dashed lines stand for the five lowest-lying energy eigenvalues. The right column shows the singular values of the $G(\theta_1^*)$, where θ_1^* is the leftmost peak found in corresponding Frobenius norm (marked with red stars). The SVD cutoff threshold is set to be 0.2.

and t'_n in Eq. (30), we choose $(t_n, t'_n) \in \mathcal{T}_{\text{sample}} \times \mathcal{T}_{\text{sample}}$, where $\mathcal{T}_{\text{sample}}$ consist of $N = 100$ samples drawn from Gaussian density distribution $a_{T/\sqrt{2}}(t)$. This choice will effectively generate $N^2 = 10^4$ samples to compress measurement error. In Fig. 5 we demonstrate how QFAMES can be applied to resolve the near-ground-state multiplicity of TFIM. When $g = 0.5$, we can clearly see a near-degenerate pair. When $g = 1$, we are in the gapless phase, and more states around the ground state are detected with a moderate choice of T . While when $g = 1.5$, the ground state is found to be unique.

We can further obtain the ground-state properties of each phase by applying Algorithm 2. The observable we choose is

$$S^z = \frac{1}{2N_{\text{spin}}} \sum_{i=1}^{N_{\text{spin}}} Z_i, \quad (69)$$

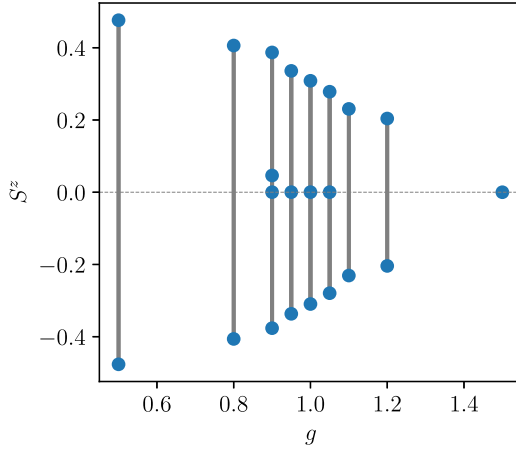


FIG. 6. Illustration of Algorithm 2 on the transverse-field Ising model. The observable is $S^z = (1/2N_{\text{spin}}) \sum_{i=1}^{N_{\text{spin}}} Z_i$. In the manifold of near-ground-state cluster, the possible ranges of observable expectation values are shown by the gray lines. A transition from ferromagnetic to paramagnetic phase can be observed when g increases from 0.5 to 1.5.

and the results are illustrated in Fig. 6. When $g = 0.5$, the solutions to the generalized eigenvalue problem, which serve as an estimation of eigenvalues of $(\langle E_k | S^z | E_{k'} \rangle)_{k,k' \in [m_i]}$, are close to ± 0.5 , showing the near-ground-state cluster lies in the ferromagnetic phase. As g increases, the possible range of expectation values of S^z in the near-ground-state cluster manifold reduces and finally reaches 0 at $g = 1.5$, corresponding to the paramagnetic phase. Note that the blue dots, which represent the eigenvalues of $(\langle E_k | S^z | E_{k'} \rangle)_{k,k' \in [m_i]}$, do not have to be symmetric about 0 (for example at $g = 0.9$), since they are extracted from the near-ground-state cluster identified at finite T rather than from an exact symmetry-resolved eigenspace.

C. 2D toric code

In many-body systems, GSD is a hallmark of topological order and depends only on the global topology of the system. For stabilizer Hamiltonians, the GSD is exactly 2^k , where k is the number of logical qubits encoded by the code. In this section, we estimate the ground-state degeneracy of the 2D toric code Hamiltonians [121] as an example. The Toric code ground state is known to exhibit $\mathbb{Z}_2$ topological order, which has been realized on a quantum computer based on the prior knowledge of its explicit form [122]. In contrast, our numerical experiment starts with a collection of random initial states. Specifically, the toric code Hamiltonian on a 2D lattice is given by

$$H = - \sum_v A_v - \sum_p B_p, \quad (70)$$

where v denotes the vertices and p the plaquettes of the lattice. Qubits live on the edges, with $i \in v$ labeling the

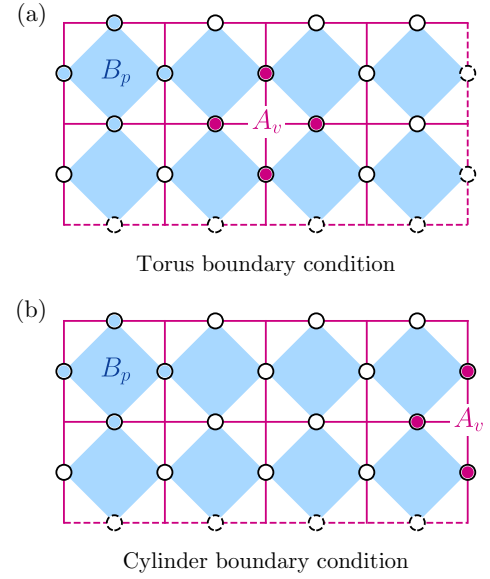


FIG. 7. 2D toric codes on a 2-by-4 lattice with (a) torus and (b) cylinder boundary conditions. Dashed lines stand for periodic boundary conditions in the corresponding directions. The models consist of 16 and 18 qubits, respectively, represented by the small circles.

edges touching a vertex v , and $i \in p$ labeling the edges surrounding a plaquette p . The corresponding stabilizer operators are $A_v = \prod_{i \in v} X_i$ and $B_p = \prod_{i \in p} Z_i$. We study the toric code model on a 2-by-4 lattice with torus and cylinder boundary conditions, as demonstrated in Fig. 7. Their GSDs are *four* and *two*, respectively. The numerical experiment proceeds as follows:

- (1) We randomly sample vectors from the Haar distribution and apply imaginary-time evolution $\exp(-\beta H)$ to enhance their overlap with the ground-state subspace.
- (2) We then apply QFAMES to these boosted vectors to estimate the multiplicity of the cluster corresponding to the smallest eigenvalue.

We find that in the first step of the algorithm, it is necessary to generate a sufficient number of initial states such that the ground-state subspace is contained within their linear span. This condition is essential for correctly estimating the ground-state multiplicity. We also remark that imaginary-time evolution is generally not efficient for large-scale, general Hamiltonians on a quantum computer, and is used here primarily for illustrative purposes. In practical applications, one would need to employ more quantum-friendly methods for generating random low-energy states.

We use $N = 300$ samples, and set circuit depth parameter $T = 10$, the Gaussian truncation parameter $\sigma = 1$, and

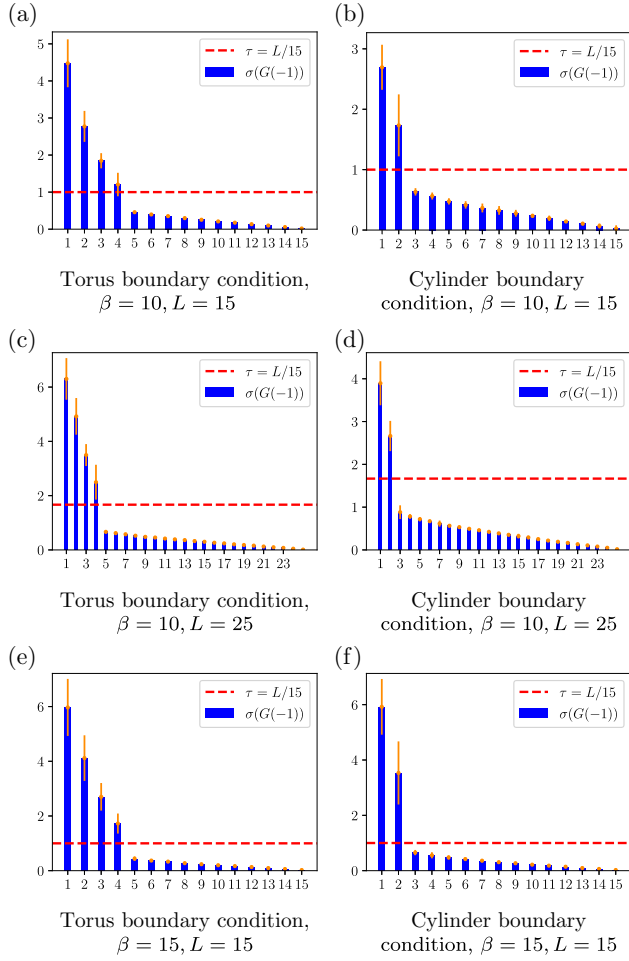


FIG. 8. Illustration of ground-state degeneracy estimation for 2D toric code models with (left) torus and (right) cylinder boundary conditions. The spectra are rescaled to $[-1, 1]$ and we plot the averaged singular values of $G(-1)$. The orange lines are the error bars representing the standard deviation over ten trials for each parameter configuration. Four and two large singular values can be clearly identified, respectively. In the second row, we increase the number of initial states L compared with the first row. In the third row, we increase the imaginary evolution time β . (a) Torus boundary condition, $\beta = 10, L = 15$. (b) cylinder boundary condition, $\beta = 10, L = 15$. (c) Torus boundary condition, $\beta = 10, L = 25$. (d) Cylinder boundary condition, $\beta = 10, L = 25$. (e) Torus boundary condition, $\beta = 15, L = 15$. (f) Cylinder boundary condition, $\beta = 15, L = 15$.

SVD threshold $\tau = \sqrt{LR}/15 = L/15$. For inverse temperature β and the number of states L , we consider different configurations: $(\beta = 10, L = 15)$ and $(\beta = 10, L = 25)$, and $(\beta = 15, L = 15)$. Each setup is repeated ten times, and the averaged singular values are output. Results are shown in Fig. 8. Four and two large singular values can respectively be identified for the two boundary conditions. The performance of the algorithm is also shown to be enhanced by (1) increasing the number of initial states L (the second row in Fig. 8 compared with the first

one), which strengthens the uniform overlap condition, (2) or increasing the imaginary evolution time β (the third row compared with the first one), which reinforces the sufficient dominance condition in Eq. (4).

D. XXZ model

We also consider the spin-1/2 XXZ chain in the presence of an external magnetic field, whose Hamiltonian is

$$H = \sum_{i=1}^{N_{\text{spin}}-1} (X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}) + h \sum_{i=1}^{N_{\text{spin}}} Z_i. \quad (71)$$

The phase diagram of this model has been extensively studied (see, for example, Refs. [123–125]). Its distinct phases can be characterized by the correlation functions, $\langle Z_i Z_{i+r} \rangle$, evaluated at the center of the chain.

Similar to TFIM, we set the system size $N_{\text{spin}} = 20$ and choose five initial states to be orthogonal, low-energy MPS with bond dimension $D = 3$, which is sufficient to obtain large overlaps with the ground state and first several excited states, and $T/\sqrt{2} = 5$. The rest of the parameters are the same as the TFIM experiment. We perform QFAMES with the following sets of parameters (Δ, h) :

- (1) $(\Delta, h) = (-1, 0)$ [Fig. 9(a)]. It is unitarily equivalent to the isotropic ferromagnetic (FM) Heisenberg model, which has $N_{\text{spin}} + 1$ degenerate ferromagnetic ground states due to $SU(2)$ symmetry. Five of them are detected here, limited by the number of initial states provided. The values of correlators in z direction vary depending on the specific ground-state orientation, whereas they all exhibit ferromagnetic behaviors.
- (2) $(\Delta, h) = (-1, 1)$ [Fig. 9(b)]. The ground-state degeneracy is lifted by the magnetic field, such that the system has a unique ground state $|\downarrow \cdots \downarrow\rangle$ and $\langle Z_i Z_{i+r} \rangle = 1$ for all r .
- (3) $(\Delta, h) = (0, 0)$ [Fig. 9(c)] and $(1, 0)$ [Fig. 9(d)]. They correspond to the XY and Heisenberg models, respectively. Both of them are in a gapless, antiferromagnetic (AFM) phase, where the correlation functions are quasi-long range that decay algebraically in r . With our choice of T , we detect a couple of energy eigenstates around the first peak of $\|G(\theta)\|_F$, as expected for a gapless spectrum. Red crosses indicate exact values for ground-state correlation functions $\langle Z_i Z_{i+r} \rangle$ of both the XY model [126] and isotropic Heisenberg model [127, 128], which lie within the ranges obtained with Algorithm 2 (solid gray lines).
- (4) $(\Delta, h) = (2, 0)$ [Fig. 9(e)]. The system is in an AFM gapped phase. When the system size N_{spin} is

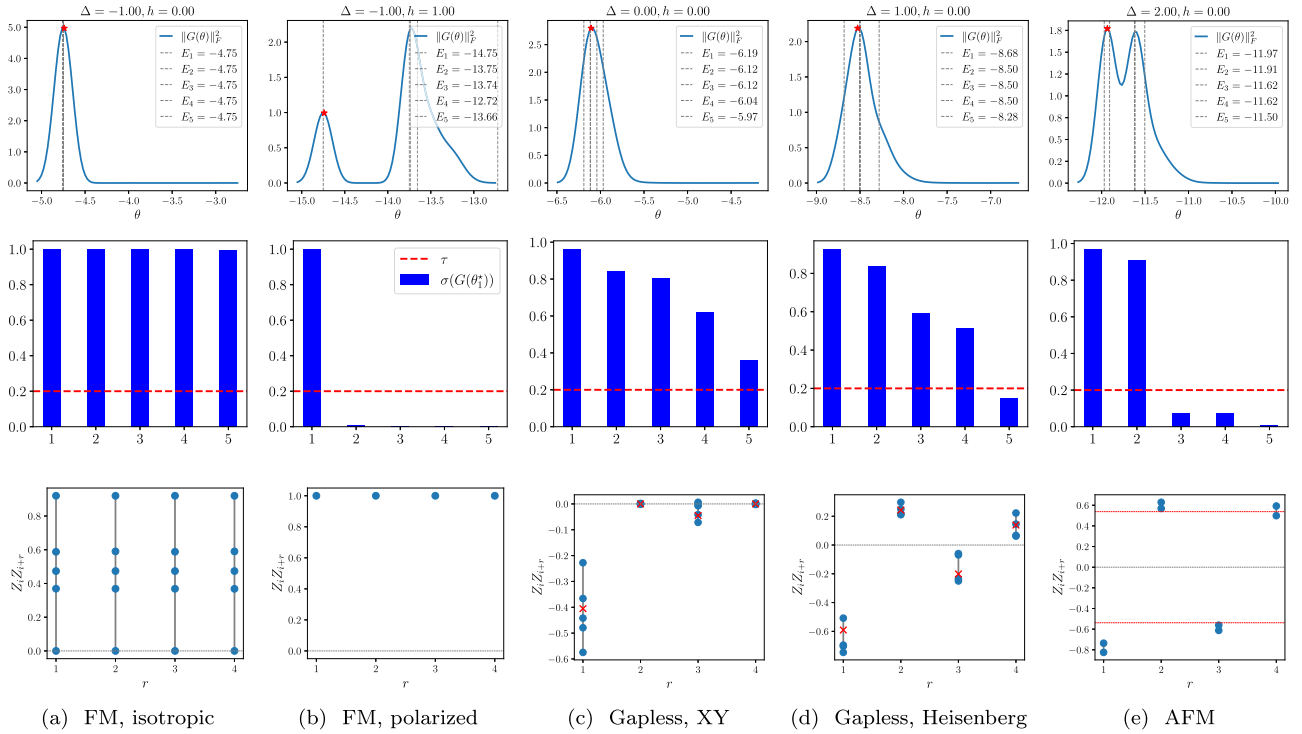


FIG. 9. Illustration of the quantum filtering and analysis of multiplicities in eigenvalue spectra algorithm on the anisotropic Heisenberg model. The top row shows the Frobenius norm of $G(\theta)$ around the ground-state energy for $(\Delta, h) = (-1, 0)$, $(-1, 1)$, $(0, 0)$, $(1, 0)$ and $(2, 0)$, from left to right. In the top row, the gray vertical dashed lines indicate the five lowest-lying energy eigenvalues. The middle row shows the singular values of $G(\theta^*)$, where θ^* is the leftmost peak found in the corresponding Frobenius norm plot (marked with red stars). The SVD cutoff threshold is set to be 0.2. The bottom row shows the estimated ranges of the correlation function $\langle Z_i Z_{i+r} \rangle$ in the center of the chain obtained with Algorithm 2, where $1 \leq r \leq 4$. The red crosses in (c) and (d) represent exact values for ground-state correlation functions, and the red dashed lines in (e) indicate the asymptotic staggered correlation $\pm \lim_{r \rightarrow \infty} \lim_{N_{\text{spin}} \rightarrow \infty} |\langle Z_i Z_{i+r} \rangle|$. (a) Ferromagnetic, isotropic. (b) Ferromagnetic, polarized. (c) Gapless, XY. (d) Gapless, Heisenberg. (e) Antiferromagnetic.

even, the two lowest-energy states form a quasi-degenerate pair [129], with a splitting that decreases rapidly as N_{spin} increases. This quasi-degeneracy can be observed with QFAMES. The ground states exhibit long-range antiferromagnetic order [130], and the corresponding asymptotic staggered correlation $\pm \lim_{r \rightarrow \infty} \lim_{N_{\text{spin}} \rightarrow \infty} |\langle Z_i Z_{i+r} \rangle|$ is indicated by red dashed lines.

IX. DISCUSSION

We presented QFAMES, a quantum spectral filtering framework that estimates dominant eigenvalues and their multiplicities by jointly processing cross-correlations from multiple initial states. By exploiting off-diagonal information through generalized Hadamard tests, QFAMES recovers spectral structures that are inaccessible to phase estimation from a single initial state and extends naturally to observable estimation within identified clusters. The algorithm admits rigorous efficiency guarantees.

The quantum data produced by QFAMES naturally form an order-3 tensor. One could attempt to solve the DODS problem using general tensor-decomposition techniques

[131–136] or approaches tailored to high-order time series [137,138]. However, to the best of our knowledge, none of these algorithms provide provable efficiency guarantees in the high-noise or overcomplete regime, and it remains unclear how to extend the existing theoretical results to this setting. In contrast, our analysis gives a simple estimator that is tailored to the QFAMES tensor structure, yields provable efficiency and robustness to measurement noise, and provides exact multiplicity recovery under the stated assumptions. We expect these ideas to be useful beyond the present setting.

The QFAMES algorithm has broad potential applications. For instance, it can be employed to probe the ground-state manifolds of models with topological orders that are difficult to analyze with classical algorithms, such as those exhibiting the fractional quantum Hall effect [139,140]. In addition, although the DOS at finite temperatures typically scales exponentially with system size, QFAMES remains of physical interest for specialized applications, such as the study of quantum many-body scars [112,141,142]. These scars represent a set of rare energy eigenstates in nonintegrable systems that avoid thermalization. Unlike typical eigenstates at finite energy densities,

which exhibit volume-law entanglement, scar states usually possess sub-volume-law entanglement. Consequently, they can be well captured by tractable Ansätze such as the low-bond-dimension MPS demonstrated in this work. This enables QFAMES to be applied to characterize their properties.

A particularly promising direction, enabled by the mixed-state extension in Sec. VII, is to interface QFAMES with state-preparation procedures that are intrinsically dissipative and therefore naturally output mixed states and/or do not admit a controlled, reversible state-preparation oracle. This setting arises in several recent proposals for dissipative Gibbs-state and ground-state preparation. In this regime, our method based on swap-test-based estimators of mixed-state cross-correlators (and their observable-decorated counterparts) provides a practical route to estimating dominant eigenvalues and their multiplicities, as well as extremal observable values within a (nearly) degenerate manifold. Importantly, pairing families of mixed states through cross-correlations can reveal information that is not accessible by measuring the observable on each individual mixed state alone (cf. the toy example in Sec. VII).

This perspective is especially relevant for metastability in open-system dynamics. In many physically interesting models, dissipative dynamics can exhibit long-lived metastable manifolds induced by energetic or entropic bottlenecks, with polynomial-time relaxation into a metastable subspace but potentially exponentially slow convergence to the true global equilibrium [103–112, 116]. Mixed-state QFAMES offers a diagnostic tool in this context: by filtering around a target low-energy cluster

and analyzing the resulting effective rank and generalized eigenvalue extrema, one can characterize the dimension of the metastable subspace and bound physically meaningful observables within it, providing quantitative probes of metastable phases and long-lived prethermal or glassy regimes that are of broad interest in condensed matter physics and quantum materials science [107–112].

These examples, together with the availability of control-free, ancilla-free implementations (Sec. VI), highlight the versatility of QFAMES as a general and efficient tool for uncovering spectral properties across diverse quantum systems, in particular on early fault-tolerant quantum devices.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [119].

APPENDIX A: COLLECTION OF NOTATION

$[n]$ The index set $\{0, 1, \dots, n-1\}$

Hamiltonian notations

$H = \sum_{m \in [M]} \lambda_m E_m\rangle \langle E_m $	Hamiltonian of interest and its spectral decomposition
$\mathcal{D} \subset [M]$	Index set of dominant eigenvalues
$I \in \mathbb{N}_+$	The number of distinct dominant eigenvalues
$\{\lambda_i^*\} \subset \mathbb{R}$	The distinct dominant eigenvalues
$\mathcal{D}_i \subset \mathcal{D}$	The index set of dominant eigenvectors with eigenvalue λ_i^*
$\Delta \in \mathbb{R}_+$	The minimum separation between distinct dominant eigenvalues

Initial-state notations

$L, R \in \mathbb{N}_+$	Number of initial states
$\{U_l\}_{l \in [L]}, \{V_r\}_{r \in [R]}$	Initial-state preparation unitaries

$\{ \phi_l\rangle\}_{l \in [L]}, \{ \psi_r\rangle\}_{r \in [R]}$	Initial states prepared by U_l and V_r
$\Phi \in \mathbb{C}^{L \times M}$	Overlaps between $\{ \phi_l\rangle\}$ and $\{ E_m\rangle\}$
$\Psi \in \mathbb{C}^{R \times M}$	Overlaps between $\{ \psi_r\rangle\}$ and $\{ E_m\rangle\}$
$p_{\text{tail}} \in \mathbb{R}$	Total overlaps with the nondominant eigenvectors
$p_{\text{min}} \in \mathbb{R}$	Minimum overlap with a dominant eigenvector
$\chi \in \mathbb{R}_+$	Uniform overlap condition parameter

Hamiltonian evolution times notations

$N \in \mathbb{N}_+$	Number of evolution times
$\{t_n\}_{n \in [N]} \subset \mathbb{R}$	Evolution time samples
$a_T^{\text{trunc}}(t)$	PDF of the truncated Gaussian distribution
$F(x)$	Fourier transform of $a(t)$; $F(x) = \int_{-\infty}^{\infty} e^{ixt} a(t) dt$
$T \in \mathbb{R}$	Circuit depth parameter
$\sigma \in \mathbb{R}$	Gaussian truncation parameter such that $a_T(t)$ is supported over $[-\sigma T, \sigma T]$

Tensor notations

$Z \in \mathbb{C}^{L \times R \times N}$	Data tensor collected from the measurement outcomes for DODS estimation
$Z_n \in \mathbb{C}^{L \times R}$	A slice of Z defined as $Z_{::,n}$
$Z_{l,r}(t) \in \mathbb{C}$	The expectation $\langle \phi_l e^{-iHt} \psi_r \rangle$
$G(\theta) \in \mathbb{C}^{L \times R}$	The contraction of Z along the third coordinate with the vector $(e^{i\theta t_n})_{n \in [N]}$
$Z^O \in \mathbb{C}^{L \times R \times N}$	Data tensor collected from the measurement outcomes for observable estimation
$G^O(\theta) \in \mathbb{C}^{L \times R}$	The contraction of Z^O along the third coordinate

Algorithm notations

$q \in \mathbb{R}$	The grid-search parameter such that the grid width is q/T
$J \in \mathbb{N}_+$	The number of grid points
$\{\theta_j\} \subset \mathbb{R}$	The grid points
$\mathcal{W}_j$	$\ G(\theta_j)\ _F$ evaluated at each grid point
$\alpha \in \mathbb{R}$	Width of the block
$\{\mathcal{B}_i\}$	Blocked grid points around each peak
$\eta \in [0, 1]$	The failure probability of the algorithm
$\tilde{I} \in \mathbb{N}_+$	Estimated number of distinct dominant eigenvalues
$\{\theta_j^*\}_{j \in [\tilde{I}]} \subset [-\pi, \pi]$	Estimated dominant eigenvalues
$\tau \in \mathbb{R}$	The threshold for the singular values
$\{m_i\} \subset \mathbb{N}_+$	Estimated multiplicities

APPENDIX B: QUANTUM PHASE ESTIMATION AND LIMITATION

The standard quantum phase estimation (QPE) algorithm estimates eigenvalues of a Hamiltonian H by applying the quantum Fourier transform (QFT) to an initial state. Recently, a class of “post-Kitaev” phase estimation algorithms (see e.g., Refs. [60–64,66,67]) has been proposed for early fault-tolerant quantum computers. These algorithms build upon the original single-ancilla Kitaev algorithm [57], which utilizes the output from the Hadamard test circuit. However, they differ in their strategies for selecting Hamiltonian simulation times and in their use of advanced classical signal-processing techniques to handle noisy quantum data.

Unlike QFT-based algorithms, post-Kitaev methods require only a single-ancilla qubit while still achieving Heisenberg-limited scaling. Moreover, they are capable of simultaneously estimating *multiple* eigenvalues, making them particularly advantageous for early fault-tolerant quantum devices. We first briefly review the structure of post-Kitaev phase estimation algorithms, which can be organized within the following three-step framework:

- (1) Generate a sequence of real numbers $\{t_n\}_{n \in [N]}$ as the Hamiltonian evolution times.
- (2) Apply Hadamard test circuit (Fig. 10) to the initial state $|\phi\rangle$ for each time t_n , and collect the measurement outcomes to form a dataset $\{(t_n, \xi_n)\}_{n \in [N]}$, where $\xi_n \in \{\pm 1 \pm 1\}$.

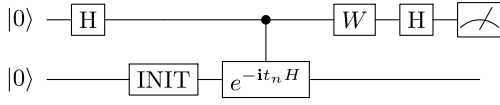


FIG. 10. Hadamard test circuit. W is either the identity or the phase gate $S^\dagger$. Here $\text{INIT } |0\rangle = |\phi\rangle$.

- (3) Perform classical postprocessing on the dataset $\{(t_n, \xi_n)\}_{n \in [N]}$ to estimate the dominant eigenvalues $\{\lambda_m\}_{m \in \mathcal{D}}$.

For each n , the Hadamard test circuit guarantees that

$$\mathbb{E}[\xi_n] = \langle \phi | e^{-iHt_n} | \phi \rangle = \sum_{m \in [M]} \underbrace{|\langle \phi | E_m \rangle|^2}_{:=p_m} \cdot e^{-i\lambda_m t_n}. \quad (\text{B1})$$

Thus, the dataset $\{(t_n, \xi_n)\}_{n \in [N]}$ corresponds to unbiased noisy samples of the Fourier signal

$$x(t) = \sum_{m \in [M]} p_m \exp(-i\lambda_m t). \quad (\text{B2})$$

Estimating the dominant eigenvalues $\{\lambda_m\}_{m \in \mathcal{D}}$ from these samples is then equivalent to the classical spectral estimation problem, which has been extensively studied in signal processing. Different post-Kitaev phase estimation algorithms primarily vary in the choice of t_n in the first step and the classical spectral estimation technique used in the third step to extract the dominant eigenvalues $\{\lambda_m\}_{m \in \mathcal{D}}$ from these samples. Examples include complex exponential least squares [62,63,65], robust phase estimation [68], Gaussian filtering and searching [64,69], ESPRIT [70,78], compressed sensing [66,67], to name a few.

Theoretical analyses have demonstrated that state-of-the-art post-Kitaev algorithms can achieve Heisenberg-limited scaling. Specifically, for a target precision ϵ , the total Hamiltonian evolution time required scales as $1/\epsilon$, ensuring that the algorithm estimates each dominant eigenvalue to within ϵ -accuracy [63,64,70]. Moreover, these algorithms achieve “short” circuit depths: for well-separated dominant eigenvalues, the maximal evolution time scales as p_{tail}/ϵ . These properties, along with other advantages (see Ref. [64]), make post-Kitaev methods particularly suitable for early fault-tolerant quantum devices.

However, QPE and post-Kitaev phase estimation algorithms encounter fundamental limitations when it comes to resolving closely spaced eigenvalues or determining the multiplicities of degenerate eigenvalues. In the nearly degenerate case, although these algorithms guarantee that the output is close to one of the dominant eigenvalues, they cannot distinguish eigenvalues separated by extremely small gaps. For instance, if a Hamiltonian has two dominant eigenvalues with an arbitrarily small separation, the

algorithm may return a single estimate that is ϵ -close to both, without revealing their multiplicities. In the degenerate case, when access is restricted to a single initial state, these algorithms are incapable of producing the correct multiplicity. This limitation is formalized in Proposition C1.

APPENDIX C: UNIFORM OVERLAP CONDITION FOR THE QFAMES ALGORITHM

For a matrix $A \in \mathbb{C}^{m \times n}$ with $m \geq n$, denote its singular values as $\{s_i\}_{i \in [n]}$. Then we define $s_{\min}(A) = \min_i s_i$ to be the smallest singular value of A . We also define

$$s_{\text{avg}}(A) = \sqrt{\frac{\sum_i s_i^2}{n}} = \frac{\|A\|_F}{\sqrt{n}} \quad (\text{C1})$$

to be the average singular value of A , where $\|A\|_F$ is the Frobenius norm of A .

In this Appendix, we formally present the uniform overlap condition for the QFAMES algorithm.

Assumption C1 (Uniform overlap condition). For each $i \in [I]$, let $\mathcal{D}_i := \{m \in \mathcal{D} | \lambda_m = \lambda_i^*\}$ denote the index set of dominant eigenvectors with the same eigenvalue λ_i^* . We assume there exists a constant $\chi > 0$ such that, for every $i \in [I]$, the following inequalities hold:

$$s_{\min}(\Phi_{:, \mathcal{D}_i}) > \frac{s_{\text{avg}}(\Phi_{:, \mathcal{D}_i})}{1 + \chi}, \quad s_{\min}(\Psi_{:, \mathcal{D}_i}) > \frac{s_{\text{avg}}(\Psi_{:, \mathcal{D}_i})}{1 + \chi}. \quad (\text{C2})$$

Recall from Eq. (5) that

$$\begin{aligned} \min_{|E\rangle \in \mathcal{E}_i, \langle E|E\rangle=1} \sum_{l \in [L]} |\langle \phi_l | E \rangle|^2 &= \min_{\|u\|=1} \|\Phi_{:, \mathcal{D}_i} u\|^2 \\ &= s_{\min}(\Phi_{:, \mathcal{D}_i})^2. \end{aligned} \quad (\text{C3})$$

Then the uniform overlap condition states that the smallest singular value must be $(1 + \chi)^{-1}$ times larger than the average singular value, for both $\Phi_{:, \mathcal{D}_i}$ and $\Psi_{:, \mathcal{D}_i}$.

The uniform overlap condition implies that $\Phi_{:, \mathcal{D}_i}$ and $\Psi_{:, \mathcal{D}_i}$ have full column rank. The latter is a *necessary* condition for any algorithm in this access model to correctly estimate multiplicities. This is summarized in the following proposition. As a corollary, when there is only a single initial state, it is impossible to resolve eigenstate degeneracy in the setting of Proposition C1, which corresponds to the case of QPE and post-Kitaev phase estimation algorithms.

Proposition C1 (Information-theoretic indistinguishability). Assume that we only have access to data produced

by the Hadamard test with controlled Hamiltonian evolution $\exp(-iHt)$ and left and right initial states with overlap matrices Φ and Ψ as defined in Eq. (2). Let $\mathcal{D}_i$ denote the indices of a degenerate energy eigenvalue subspace. There exists no classical signal-processing algorithm that can reliably determine the multiplicity $|\mathcal{D}_i|$, if $\text{rank}(\Phi_{:, \mathcal{D}_i}) < |\mathcal{D}_i|$ or $\text{rank}(\Psi_{:, \mathcal{D}_i}) < |\mathcal{D}_i|$.

Proof. For simplicity, we assume λ^* is the only eigenvalue of H with degenerate eigenvectors indexed by $\mathcal{D}$, meaning $H = \lambda^* \sum_{i \in \mathcal{D}} |\varphi_i\rangle \langle \varphi_i|$. According to the assumptions, when the noise is negligible, we have access to quantities of the form

$$\mathcal{Z}_{l,r}(t) = \langle \phi_l | e^{-iHt} | \psi_r \rangle = e^{-i\lambda^* t} \sum_{m \in \mathcal{D}} \Phi_{l,m} \Psi_{r,m}^* \quad (\text{C4})$$

The corresponding data matrix is $\Phi\Psi^\dagger$. If $\text{rank}(\Phi) = k < |\mathcal{D}|$, consider the singular value decomposition of $\Phi = USV^\dagger$, where the singular values $s_j = S_{j,j}$ are sorted in descending order. Therefore $(\Phi V)_{:,j} = (US)_{:,j} = 0$ for any $j \geq k$ (assume the column vectors are indexed by $j \in [|\mathcal{D}|] = \{0, 1, \dots, |\mathcal{D}| - 1\}$). Let us take $\tilde{\Phi} \in \mathbb{C}^{L \times (k+1)}$ and $\tilde{\Psi} \in \mathbb{C}^{R \times (k+1)}$ defined as

$$\begin{aligned} \tilde{\Phi}_{:,j} &:= (\Phi V)_{:,j}, \quad \tilde{\Psi}_{:,j} := (\Psi V)_{:,j}, \quad \text{for } j \in [k]; \\ \tilde{\Phi}_{:,k} &:= 0, \quad \tilde{\Psi}_{r,k} := \sqrt{1 - \sum_{j \in [k]} |\tilde{\Psi}_{r,j}|^2}, \quad \text{for } r \in [R]. \end{aligned} \quad (\text{C5})$$

$\tilde{\Phi}, \tilde{\Psi}$ correspond to the overlap matrices generated by a different Hamiltonian $\tilde{H}$ that has only multiplicity k at the dominant eigenvalue λ^* , and an additional eigenvector $|E_k\rangle$ with a different eigenvalue. $|E_k\rangle$ is defined to ensure the normalization conditions for the overlap matrices: $\|\tilde{\Phi}_{l,:}\| = \|\tilde{\Psi}_{r,:}\| = 1$, for $l \in [L]$ and $r \in [R]$.

Since by construction

$$\tilde{\Phi}\tilde{\Psi}^\dagger = \tilde{\Phi}_{:, [k]} \tilde{\Psi}_{:, [k]}^\dagger = \Phi_{:, \mathcal{D}} V V^\dagger \Psi_{:, \mathcal{D}}^\dagger = \Phi\Psi^\dagger, \quad (\text{C6})$$

we cannot distinguish the signals generated by H and $\tilde{H}$, and hence cannot correctly resolve the multiplicity. The case for $\text{rank}(\Psi_{:, \mathcal{D}}) < |\mathcal{D}|$ is analogous. ■

In our proof of the main theorem (Theorem D1), the uniform overlap condition plays an important role in two aspects:

- (1) In eigenvalue estimation, the condition (C2) is applied in Eq. (D25) to ensure that

$$\left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \right\|_F^2 \quad \text{and} \quad \|\mathcal{G}(\theta \approx \lambda_{\pi_\theta}^*)\|_F$$

admit sufficiently large lower bounds. This guarantees that the dominant eigenvalues can be detected by identifying the peaks of $\|\mathcal{G}(\theta)\|_F$.

- (2) In multiplicity estimation, the condition ensures that the overlap matrix

$$\Phi_{:, \mathcal{D}_{\pi_\theta}} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger$$

has rank equal to the corresponding degeneracy. This property is then quantitatively exploited in Eq. (D50) to establish a lower bound on the singular values of $\mathcal{G}(\theta \approx \theta_{\pi_i}^*)$.

APPENDIX D: RIGOROUS VERSION OF THEOREM 2 AND PROOF

In this Appendix, we introduce and prove a generalized and rigorous version of Theorem 2. In the more general setting, we consider the case where each dominant eigenvalue is not exactly degenerate but instead lies within a small interval of width δ that is centered at λ_i^* . This motivates the following definition:

Definition D1 (Dominant eigenvalue clusters). There exist parameters $\Delta \gg \delta > 0$ and $I \in \mathbb{N}_+$ such that:

- (1) The dominant eigenvalues $\{\lambda_m\}_{m \in \mathcal{D}}$ are covered by I disjoint cluster intervals $\{\mathcal{I}_i\}_{i=1}^I$ that are centered at $\{\lambda_i^*\}_{i=1}^I$.
- (2) Each cluster interval has length at most δ .
- (3) The cluster intervals are Δ -well-separated. That is, for all $i \neq j \in [I]$, $\text{dis}(\mathcal{I}_i, \mathcal{I}_j) \geq \Delta$.

Here, I is the number of dominant cluster intervals, δ is the maximum width of each interval, and Δ is the minimum pairwise separation between intervals.

We note that Theorem 2 corresponds to the special case $\delta = 0$, where each cluster reduces to a single dominant eigenvalue with exact degeneracy. In the more general setting, a dominant eigenvalue cluster may be viewed as an *approximately degenerate* eigenvalue, and our goal is to estimate both the center of each cluster and the number of dominant eigenvalues it contains. (We slightly abuse notation and use λ_i^* to denote the center of the i th cluster $\mathcal{I}_i$.) The QFAMES algorithm (Algorithm 1) applies directly to this case.

We are now ready to state a generalized and rigorous version of Theorem 2:

Theorem D1 (General version of Theorem 2). Suppose Assumption C1 hold with $\chi = \mathcal{O}(1)$, and the dominant eigenvalue cluster length parameter δ is sufficiently small. Given failure probability $\eta \in (0, 1)$, if the parameters satisfy the following conditions: $\tilde{I} \geq I$,

$$T = \Omega\left(\frac{1}{\Delta} \log\left(\frac{KLR}{p_{\text{tail}}}\right)\right), \quad N = \Omega\left(\frac{LR}{p_{\text{tail}}^2} \log\left((J+K) \frac{LR}{\eta}\right)\right), \quad \sigma = \Omega\left(\log^{1/2}\left(\frac{\sqrt{LR}}{p_{\text{tail}}}\right)\right), \quad (\text{D1})$$

$$q = \mathcal{O}\left(\frac{p_{\text{tail}}}{(1+\sigma)\sqrt{KLR}}\right), \quad q = \mathcal{O}\left(\sqrt{\log\left(\frac{1+2\chi}{1+\chi}\right)}\right), \quad \alpha = \mathcal{O}(\Delta \cdot T), \quad (\text{D2})$$

and

$$T = \mathcal{O}\left(\frac{1}{\delta} \min\left\{\frac{p_{\text{tail}}}{(1+\sigma)\sqrt{KLR}}, \frac{p_{\text{tail}}^2}{KLR}\right\}\right), \quad \alpha = \Omega(\delta \cdot T), \quad (\text{D3})$$

$$\frac{p_{\min}}{p_{\text{tail}}} > 6(1+2\chi). \quad (\text{D4})$$

Here $K = |\mathcal{D}|$, and $J = \lfloor 2\pi T/q \rfloor$ is the number of candidate locations of cluster centers $\{\theta_i\}$ in the block and searching algorithm.

Then, with probability at least $1 - \eta$, there exists a permutation $\pi : [I] \rightarrow [I]$ such that the output of Algorithm 1 $\{(\theta_j^*, m_j)\}_{j \in [I]}$ satisfies the following guarantees:

$$\sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi(j)}^*| = \mathcal{O}\left((1+\sigma) \frac{p_{\text{tail}}}{p_{\min}} \frac{1}{T}\right). \quad (\text{D5})$$

Furthermore, if $p_{\text{tail}}/p_{\min}, \delta$ are sufficiently small so that

$$\frac{1 - \mathcal{O}\left(\frac{((1+\sigma)p_{\text{tail}}/p_{\min} + \delta \cdot T)^2}{(1+\chi)^2}\right)}{(1+\chi)^2} = \Omega\left(\frac{p_{\text{tail}}}{p_{\min}}\right), \quad (\text{D6})$$

we can choose $\tau = \Theta(p_{\text{tail}})$, and $\alpha = \Omega(\log(KLR/p_{\text{tail}}))$ to ensure that, with probability at least $1 - \eta$, we have

$$m_j = |\mathcal{D}_{\pi(j)}|, \quad 1 \leq j \leq I, \quad m_j = 0, \quad j > I. \quad (\text{D7})$$

Remark D1. Here, we give some comments about the conditions and assumptions in the above theorem:

- (1) The conditions (D1) and (D2) are similar to those in Theorem 3.2 of Ref. [64], which ensure the algorithm can identify each cluster separately.
- (2) In the above theorem, Eq. (D3) essentially requires that δ is sufficiently small so that all dominant eigenvalues within a cluster can be approximated by a single output. When $T = \Theta(\alpha/\delta)$, the analysis becomes more involved, as a single cluster may yield multiple outputs, making the second step of the algorithm difficult to track.
- (3) Equation (D4) can be referred to as the sufficient domination condition, defined after Problem 1.

- (4) Although the condition (D6) appears technical, it essentially requires that χ and p_{tail} are small so that the right-hand side is close to 1. This condition ensures a separation between the singular values of $\mathcal{W}_j$, which is necessary for accurately counting the number of dominant eigenvalues in each cluster.

Remark D2. Together, the outputs of the location and multiplicity estimation define an approximate density $\tilde{\mu}$ which approximates the true density μ_D up to a small error in Wasserstein distance. Let θ_i^* be the estimated center of $\mathcal{I}_i$. Define

$$\begin{aligned} \tilde{\mu}(E) &:= \frac{1}{|\mathcal{D}|} \sum_{i=1}^I m_i \delta(E - \theta_i^*), \\ \mu_D(E) &:= \frac{1}{|\mathcal{D}|} \sum_{i \in \mathcal{D}} \delta(E - \lambda_i). \end{aligned} \quad (\text{D8})$$

Let $\epsilon := \sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi(j)}^*|$. Consider a transport map that transports each atom at λ_j in $\mathcal{I}_i$ to θ_i^* . The cost is

$$|\lambda_j - \theta_i^*| \leq |\lambda_j - \lambda_i^*| + |\lambda_i^* - \theta_i^*| \leq \epsilon + \frac{\delta}{2}. \quad (\text{D9})$$

Averaging over the $|\mathcal{D}|$ atoms gives that

$$W_1(\mu_D, \tilde{\mu}) \leq \epsilon + \frac{\delta}{2}. \quad (\text{D10})$$

Proof. The proof strategy of Theorem D1 is similar to the proof of Theorem 3.2 of Ref. [64]. We first show a rough estimation for the location of the clusters and then refine it to get a more accurate estimation. First of all, let us define the exact filter matrix $\mathcal{F}(\theta)$, the data matrix $G(\theta)$ that approximates $\mathcal{F}(\theta)$, the error matrix $E(\theta)$, and the computed filter value function $\mathcal{W}(\theta)$,

$$\begin{aligned}\mathcal{F}(\theta) &:= \Phi \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in [M]} \right) \\ &\quad \cdot \Psi^\dagger \in \mathbb{C}^{L \times R}, \\ G(\theta) &:= \frac{1}{N} \sum_{n=1}^N Z_n \exp(i\theta t_n) \in \mathbb{C}^{L \times R}, \\ \mathcal{E}(\theta) &:= G(\theta) - \mathcal{F}(\theta) \in \mathbb{C}^{L \times R}, \\ \mathcal{W}(\theta) &:= \|G(\theta)\|_F \in \mathbb{R}.\end{aligned}\tag{D11}$$

Step 0: We show that the computed filter value function $\mathcal{W}(\theta)$ well approximates $\|\mathcal{F}(\theta)\|_F$.

Since $\sigma = \Omega \left(\log^{1/2} \left(\sqrt{LR}/p_{\text{tail}} \right) \right)$ and $N = \Omega \left((LR/p_{\text{tail}}^2) \log((J+K)(LR/\eta)) \right)$, according to Lemma D1 with $\beta = p_{\text{tail}}/8$, we have

$$\sup_{\theta_j} |\mathcal{W}(\theta_j) - \|\mathcal{F}(\theta_j)\|_F| \leq \sup_{\theta_j} \|\mathcal{E}(\theta_j)\|_F \leq \frac{p_{\text{tail}}}{8},\tag{D12}$$

with probability at least $1 - \eta/2$. For simplicity, we only consider the case when Eq. (D12) is satisfied, which is true with probability at least $1 - \eta/2$.

Step 1: For each θ_j^* , let $\pi_j = \arg \min_i \left\{ \text{dist}(\theta_j^*, \mathcal{I}_i) \right\}$. We show

$$\sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi_j}^*| \leq \sqrt{\log \left(\frac{2(1+2\chi)}{1+\chi} \right)} \frac{1}{T}\tag{D13}$$

when Eq. (D12) holds true. To achieve this, we need to prove lower and upper bounds for $\mathcal{W}(\theta)$:

(1) If $\theta \in (\cup_i [\lambda_i^* - q/2T, \lambda_i^* + q/2T]) \cap \{\theta_j\}_{j=1}^J$, there exists π_θ (index of the cluster that θ belongs to) such that

$$\begin{aligned}\max_m \{|\theta - \lambda_m| : m \in \mathcal{D}_{\pi_\theta}\} &\leq \frac{q}{2T} + \frac{\delta}{2}, \\ \min_m \{|\theta - \lambda_m| : m \in \mathcal{D} \setminus \mathcal{D}_{\pi_\theta}\} &\geq \Delta - \frac{q}{2T} \geq \Delta/2,\end{aligned}\tag{D14}$$

where we use $T \geq q/\Delta$ to ensure the second inequality holds. This implies that θ lies within a single cluster and is at least a distance of $\Delta/2$ from any other cluster.

Using Eq. (D12) and the triangle inequality for the Frobenius norm, we observe that

$$\begin{aligned}\mathcal{W}(\theta) &\geq \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}_{\pi_\theta}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F \\ &\quad - \sum_{i \neq \pi_\theta} \left\| \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}_i} \right) \cdot (\Psi_{:, \mathcal{D}_i})^\dagger \right\|_F \\ &\quad - \left\| \Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}^c} \right) \cdot (\Psi_{:, \mathcal{D}^c})^\dagger \right\|_F - \frac{p_{\text{tail}}}{8}.\end{aligned}\tag{D15}$$

For the second term, using the second inequality of Eq. (D14) and Lemma D2, Eq. (D64), we have

$$\begin{aligned}
& \sum_{i \neq \pi_\theta} \left\| \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right) \cdot (\Psi_{:, \mathcal{D}_i})^\dagger \right\|_F \\
& \leq \exp(-\Delta^2 T^2 / 4) \sum_{i \neq \pi_\theta} \sum_{m \in \mathcal{D}_i} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)} \\
& \leq \exp(-\Delta^2 T^2 / 4) \sqrt{K-1} \sqrt{\sum_{i \neq \pi_\theta} \sum_{m \in \mathcal{D}_i} \left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)} \\
& \leq \exp(-\Delta^2 T^2 / 4) \sqrt{K-1} \sqrt{\sum_{i \neq \pi_\theta} \sum_{m \in \mathcal{D}_i} \sum_{l=1}^L |\Phi_{l,m}|^2 R} \\
& \leq \sqrt{KLR} \exp(-\Delta^2 T^2 / 4) \leq \frac{p_{\text{tail}}}{8}, \tag{D16}
\end{aligned}$$

where we use Hölder's inequality in the second inequality and $T = \Omega((1/\Delta) \log(KLR/p_{\text{tail}}))$ in the last inequality. Similarly, for the third term, we have

$$\begin{aligned}
& \left\| \Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}^c} \right) \cdot (\Psi_{:, \mathcal{D}^c})^\dagger \right\|_F \\
& \leq \sum_{m \in \mathcal{D}^c} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)} = p_{\text{tail}}. \tag{D17}
\end{aligned}$$

Plugging these two inequalities into Eq. (D15), we have

$$\mathcal{W}(\theta) \geq \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_\theta}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F - \frac{5}{4} p_{\text{tail}}. \tag{D18}$$

For the first term, we notice that $|\lambda_m - \lambda_{\pi_\theta}^*| \leq \delta$ when $m \in \mathcal{D}_{\pi_\theta}$. Combining this and Lemma D2, Eq. (D64) we have

$$\begin{aligned}
& \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) - \exp(-(\theta - \lambda_{\pi_\theta}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_\theta}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F \\
& \leq \delta \cdot T \sum_{m \in [\mathcal{D}_{\pi_\theta}]} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)} \leq \delta \cdot T \sqrt{KLR} \leq \frac{p_{\text{tail}}}{4}, \tag{D19}
\end{aligned}$$

where we use $\delta = \mathcal{O}(p_{\text{tail}}/(\sqrt{KLRT}))$ in the last equality. This gives

$$\begin{aligned}
& \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_\theta}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F \\
& \geq \left\| \underbrace{\Phi_{:, \mathcal{D}_{\pi_\theta}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_{\pi_\theta}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_\theta}} \right)}_{\text{constant diagonal}} \cdot (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F - \frac{p_{\text{tail}}}{4} \\
& \geq \exp \left(- \left(\frac{q}{2T} \right)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F - \frac{p_{\text{tail}}}{4} \\
& \geq \frac{1 + \chi}{1 + 2\chi} \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} (\Psi_{:, \mathcal{D}_{\pi_\theta}})^\dagger \right\|_F - \frac{p_{\text{tail}}}{4}, \tag{D20}
\end{aligned}$$

where we use the fact $q = \mathcal{O}\left(\sqrt{\log((1+2\chi)/(1+\chi))}\right)$ in the last inequality. Finally, plugging this into Eq. (D18), we obtain that

$$\mathcal{W}(\theta) \geq \frac{1+\chi}{1+2\chi} \left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \right\|_F - \frac{3}{2} p_{\text{tail}}. \quad (\text{D21})$$

This gives a lower bound of $\mathcal{W}(\theta)$ if $\theta \in (\cup_i [\lambda_i^* - q/2T, \lambda_i^* + q/2T]) \cap \{\theta_j\}_{j=1}^J$.

- (2) Similar to the above calculation and using Eq. (D12), Eq. (D19), and Lemma D2, Eq. (D64) for the first term, we have

$$\begin{aligned} \mathcal{W}(\theta_j^*) &\leq \left\| \Phi_{:, \mathcal{D}_{\pi_j}} \cdot \text{diag} \left(\left\{ \exp(-(\theta_j^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_j}} \right) \cdot \left(\Psi_{:, \mathcal{D}_{\pi_j}} \right)^\dagger \right\|_F \\ &\quad + \underbrace{\sum_{i \neq \pi_j} \left\| \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\left\{ \exp(-(\theta_j^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right) \cdot \left(\Psi_{:, \mathcal{D}_i} \right)^\dagger \right\|_F}_{\leq \sqrt{KLR} \exp(-\Delta^2 T^2 / 4) \leq \frac{p_{\text{tail}}}{8}} \\ &\quad + \underbrace{\left\| \Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\left\{ \exp(-(\theta_j^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}^c} \right) \cdot \left(\Psi_{:, \mathcal{D}^c} \right)^\dagger \right\|_F}_{\leq p_{\text{tail}}} + \frac{p_{\text{tail}}}{8} \\ &\leq \left\| \Phi_{:, \mathcal{D}_{\pi_j}} \cdot \text{diag} \left(\left\{ \exp(-(\theta_j^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_j}} \right) \cdot \left(\Psi_{:, \mathcal{D}_{\pi_j}} \right)^\dagger \right\|_F + \frac{5}{4} p_{\text{tail}} \\ &\leq \exp \left(-(\theta_j^* - \lambda_{\pi_j}^*)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_j}} \left(\Psi_{:, \mathcal{D}_{\pi_j}} \right)^\dagger \right\|_F + \frac{3}{2} p_{\text{tail}}. \end{aligned} \quad (\text{D22})$$

This gives an upper bound of $\mathcal{W}(\theta_j^*)$.

According to Eqs. (D21) and (D22), when $j = 1$, because $\mathcal{W}(\theta_1^*)$ takes the maximal value, we have

$$\exp \left(-(\theta_1^* - \lambda_{\pi_1}^*)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F + \frac{3}{2} p_{\text{tail}} \geq \mathcal{W}(\theta_1^*) \geq \frac{1+\chi}{1+2\chi} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F - \frac{3}{2} p_{\text{tail}}, \quad (\text{D23})$$

where the second inequality holds since there must exist some grid point θ_1 such that $\theta_1 \in [\lambda_{\pi_1}^* - \frac{q}{2T}, \lambda_{\pi_1}^* + \frac{q}{2T}]$ and $\mathcal{W}(\theta_1^*) \geq \mathcal{W}(\theta_1)$ by definition. Thus,

$$\begin{aligned} \exp \left(-(\theta_1^* - \lambda_{\pi_1}^*)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F + \frac{3}{2} p_{\text{tail}} &\geq \frac{1+\chi}{1+2\chi} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F - \frac{3}{2} p_{\text{tail}} \\ \implies |\theta_1^* - \lambda_{\pi_1}^*| &\leq \log^{1/2} \left(\frac{1}{\frac{1+\chi}{2+\chi} - 3p_{\text{tail}} / \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F} \right) \frac{1}{T}. \end{aligned} \quad (\text{D24})$$

We further note that

$$\begin{aligned}
\left\| \Phi_{:, \mathcal{D}_{\pi_\theta}} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \right\|_F^2 &= \text{Tr} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \left(\Phi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \Phi_{:, \mathcal{D}_{\pi_\theta}} \left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \right) \\
&\geq \lambda_{\min} \left(\left(\Phi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \Phi_{:, \mathcal{D}_{\pi_\theta}} \right) \text{Tr} \left(\left(\Psi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \Psi_{:, \mathcal{D}_{\pi_\theta}} \right) \\
&= \lambda_{\min} \left(\left(\Phi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \Phi_{:, \mathcal{D}_{\pi_\theta}} \right) \left(\sum_{i \in \mathcal{D}_{\pi_\theta}} \sum_{k=1}^R |\Psi_{k,i}|^2 \right) \\
&\geq \left(\frac{1}{1+\chi} \right)^2 \frac{1}{|\mathcal{D}_{\pi_\theta}|} \text{Tr} \left(\left(\Phi_{:, \mathcal{D}_{\pi_\theta}} \right)^\dagger \Phi_{:, \mathcal{D}_{\pi_\theta}} \right) \left(\sum_{i \in \mathcal{D}_{\pi_\theta}} \sum_{k=1}^R |\Psi_{k,i}|^2 \right) \\
&= \left(\frac{1}{1+\chi} \right)^2 \frac{1}{|\mathcal{D}_{\pi_\theta}|} \left(\sum_{j \in \mathcal{D}_{\pi_\theta}} \sum_{k=1}^L |\Phi_{k,j}|^2 \right) \left(\sum_{i \in \mathcal{D}_{\pi_\theta}} \sum_{k=1}^R |\Psi_{k,i}|^2 \right) \\
&\geq \left(\frac{1}{1+\chi} \right)^2 \frac{1}{|\mathcal{D}_{\pi_\theta}|} \left(\sum_{i \in \mathcal{D}_{\pi_\theta}} \left(\sum_{k=1}^L |\Phi_{k,i}|^2 \right) \left(\sum_{k=1}^R |\Psi_{k,i}|^2 \right) \right) \\
&\geq \left(\frac{1}{1+\chi} \right)^2 p_{\min}^2.
\end{aligned} \tag{D25}$$

The second inequality comes from Assumption C1. Plugging this bound into the above inequality, we have

$$|\theta_1^* - \lambda_{\pi_1}^*| < \sqrt{\log \left(\frac{1}{\frac{1+\chi}{2+\chi} - 3(1+\chi)p_{\text{tail}}/p_{\min}} \right)} \frac{1}{T} \leq \sqrt{\log \left(\frac{2(1+2\chi)}{1+\chi} \right)} \frac{1}{T}, \tag{D26}$$

where we use $3p_{\text{tail}}/p_{\min} \leq 1/2(1+2\chi)$ [Eq. (D4)] in the last step.

Furthermore, since $\text{dist}(\mathcal{I}_i, \mathcal{I}_j) > \Delta$, $T = \Omega((1+\alpha+q)/\Delta)$ and $\delta \ll \Delta$, we have

$$\left[\theta_1^* - \frac{\alpha}{T}, \theta_1^* + \frac{\alpha}{T} \right] \cap \left(\cup_{i \neq \pi_1} \left[\lambda_i^* - \frac{q}{2T}, \lambda_i^* + \frac{q}{2T} \right] \right) = \emptyset. \tag{D27}$$

This implies that the first block interval does not overlap with $\cup_{i \neq \pi_1} [\lambda_i^* - q/2T, \lambda_i^* + q/2T]$. In addition, $\alpha = \Omega \left(\max \left\{ \sqrt{\log(2(1+2\chi)/(1+\chi))}, \delta \cdot T \right\} \right)$, we have $\pi_2 \neq \pi_1$, meaning θ_2^* is not close to $\lambda_{\pi_1}^*$. More specifically, by Eq. (D27), we can repeat the above argument for θ_2^* and obtain

$$|\theta_2^* - \lambda_{\pi_2}^*| \leq \sqrt{\log \left(\frac{2(1+2\chi)}{1+\chi} \right)} \frac{1}{T} = \mathcal{O} \left(\frac{\alpha}{T} \right). \tag{D28}$$

If $\pi_2 = \pi_1$, then by Eq. (D26) and triangle inequality, we have

$$|\theta_2^* - \theta_1^*| \leq |\theta_2^* - \lambda_{\pi_1}^*| + |\theta_1^* - \lambda_{\pi_1}^*| < \frac{\alpha}{T}, \tag{D29}$$

which is impossible since the grid points that are α/T -close to θ_1^* have been blocked.

Repeating this argument for all $1 \leq j \leq I$, we can show

$$|\theta_j^* - \lambda_{\pi_j}^*| \leq \sqrt{\log \left(\frac{2(1+2\chi)}{1+\chi} \right)} \frac{1}{T} \tag{D30}$$

for all $1 \leq j \leq I$.

Step 2: Using the result obtained in Step 1, we can impose stronger bounds on $\mathcal{W}(\theta)$ to refine the error estimation. We will show

$$\sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi_j}^*| = \mathcal{O} \left((1 + \sigma) \frac{p_{\text{tail}}}{p_{\min}} \frac{1}{T} \right) \quad (\text{D31})$$

when Eq. (D12) holds true.

Without loss of generality, we only consider $j = 1$. The other cases can be improved similarly. Let us pick $\tilde{\theta}_1^* \in [\lambda_{\pi_1}^* - q/2T, \lambda_{\pi_1}^* + q/2T] \cap \{\theta_j\}_{j=1}^J$, which is the closest energy grid point to the desired cluster center $\lambda_{\pi_1}^*$. It can vary from our computed estimate θ_1^* due to the errors arising from noise, contributions of nondominant eigenvectors, and of dominant eigenvectors in distant clusters, and it holds that $\mathcal{W}(\theta_1^*) \geq \mathcal{W}(\tilde{\theta}_1^*)$. We will bound the distance between θ_1^* and $\tilde{\theta}_1^*$, and thus between θ_1^* and $\lambda_{\pi_1}^*$.

We first define

$$\begin{aligned} G(\theta) &= \underbrace{\Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger}_{:=A(\theta)} \\ &+ \underbrace{\Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}^c} \right) \cdot (\Psi_{:, \mathcal{D}^c})^\dagger}_{:=B(\theta)} \\ &+ \underbrace{\sum_{i \neq \pi_1} \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right) \cdot (\Psi_{:, \mathcal{D}_i})^\dagger}_{:=C(\theta)} + \mathcal{E}(\theta). \end{aligned} \quad (\text{D32})$$

According to Eqs. (D22), (D12), and (D16), we have

$$\begin{aligned} \|A(\theta_1^*)\|_F &\leq \exp \left(-(\theta_1^* - \lambda_{\pi_1}^*)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F + \frac{1}{4} p_{\text{tail}} \leq \frac{5}{4} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F, \\ \|A(\tilde{\theta}_1^*)\|_F &\leq \exp \left(-(\tilde{\theta}_1^* - \lambda_{\pi_1}^*)^2 T^2 \right) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F + \frac{1}{4} p_{\text{tail}} \leq \frac{5}{4} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F, \end{aligned} \quad (\text{D33})$$

where we use $p_{\text{tail}} < p_{\min}/(1 + \chi) \leq \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F$ according to Eq. (D25) in the second inequalities, and

$$\|B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*)\|_F \leq \frac{5p_{\text{tail}}}{4}, \quad \|B(\tilde{\theta}_1^*) + C(\tilde{\theta}_1^*) + \mathcal{E}(\tilde{\theta}_1^*)\|_F \leq \frac{5p_{\text{tail}}}{4}. \quad (\text{D34})$$

Then, we get that

$$\begin{aligned} \mathcal{W}^2(\theta) &= \text{Tr}(G^\dagger(\theta)G(\theta)) \\ &= \text{Tr}(A^\dagger(\theta)A(\theta)) + 2\text{Re} \left(\text{Tr}(A^\dagger(\theta)(B(\theta) + C(\theta) + \mathcal{E}(\theta))) \right) \\ &\quad + \text{Tr}((B^\dagger(\theta) + C^\dagger(\theta) + \mathcal{E}^\dagger(\theta))(B(\theta) + C(\theta) + \mathcal{E}(\theta))). \end{aligned} \quad (\text{D35})$$

We first deal with the first term, the last term, and then the second term:

(1) For the first term, we have

$$\begin{aligned} A(\theta) &= \Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_{\pi_1}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \\ &+ \Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) - \exp(-(\theta - \lambda_{\pi_1}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right) \cdot (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger. \end{aligned} \quad (\text{D36})$$

Noticing $|\lambda_m - \lambda_{\pi_1}^*| \leq \delta$ when $m \in \mathcal{D}_{\pi_1}$, we have

$$\left\| \Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_m)^2 T^2) - \exp(-(\theta - \lambda_{\pi_1}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right) \cdot \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F \leq \sqrt{KLR} \delta \cdot T \quad (\text{D37})$$

according to Lemma D2 Eq. (D65). Thus, we obtain that

$$\left| \|A(\theta)\|_F - \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta - \lambda_{\pi_1}^*)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right) \cdot \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F \right| \leq \sqrt{KLR} \delta \cdot T, \quad (\text{D38})$$

where we use $\delta \cdot T < 1$.

(2) For the last term, by Eq. (D34), we have

$$\begin{aligned} \text{Tr}((B^\dagger(\theta_1^*) + C^\dagger(\theta_1^*) + \mathcal{E}^\dagger(\theta_1^*))(B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*))) &\leq \frac{9}{4} p_{\text{tail}}^2, \\ \text{Tr}((B^\dagger(\tilde{\theta}_1^*) + C^\dagger(\tilde{\theta}_1^*) + \mathcal{E}^\dagger(\tilde{\theta}_1^*))(B(\tilde{\theta}_1^*) + C(\tilde{\theta}_1^*) + \mathcal{E}(\tilde{\theta}_1^*))) &\leq \frac{9}{4} p_{\text{tail}}^2. \end{aligned} \quad (\text{D39})$$

(3) For the second term, we have

$$\begin{aligned} &2\text{Re} \left(\text{Tr}(A^\dagger(\theta_1^*)(B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*))) - 2\text{Re} \left(\text{Tr}(A^\dagger(\tilde{\theta}_1^*)(B(\tilde{\theta}_1^*) + C(\tilde{\theta}_1^*) + \mathcal{E}(\tilde{\theta}_1^*))) \right) \right) \\ &\leq 2 \|A(\theta_1^*) - A(\tilde{\theta}_1^*)\|_F \| (B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*)) \|_F \\ &\quad + 2 \|A(\tilde{\theta}_1^*)\|_F \| (B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*)) - (B(\tilde{\theta}_1^*) + C(\tilde{\theta}_1^*) + \mathcal{E}(\tilde{\theta}_1^*)) \|_F. \end{aligned} \quad (\text{D40})$$

Similar to the calculation in Eq. (D19), we obtain from Eq. (D38) that

$$\begin{aligned} \|A(\theta_1^*) - A(\tilde{\theta}_1^*)\|_F &\leq T |\theta_1^* - \tilde{\theta}_1^*| \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F + 2\sqrt{KLR} \delta \cdot T \\ &\leq T |\theta_1^* - \tilde{\theta}_1^*| \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F + \frac{p_{\text{tail}}}{2}, \end{aligned} \quad (\text{D41})$$

where we use $\delta \cdot T = \mathcal{O}(p_{\text{tail}}/\sqrt{KLR})$ in the last inequality. According to Lemma D2, Eq. (D65) and Lemma D1, Eq. (D58), we have

$$\|B(\theta) - B(\theta')\|_F \leq p_{\text{tail}} \sigma T |\theta - \theta'|/2, \quad \Pr[\forall \theta \neq \theta' \in \Theta : \|\mathcal{E}(\theta) - \mathcal{E}(\theta')\|_F \leq p_{\text{tail}} \sigma T |\theta - \theta'|/2] \geq 1 - \frac{\eta}{2}. \quad (\text{D42})$$

And we have

$$\begin{aligned}
& \|C(\theta_1^*) - C(\tilde{\theta}_1^*)\|_F \\
& \leq \sum_{i \neq \pi_1} \left\| \Phi_{:, \mathcal{D}_i} (\exp(-(\theta_1^* - \lambda_i^*)^2 T^2) - \exp(-(\tilde{\theta}_1^* - \lambda_i^*)^2 T^2)) \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F \\
& \quad + \sum_{i \neq \pi_1} \left\| \Phi_{:, \mathcal{D}_i} \text{diag} \left(\left\{ \exp(-(\theta_1^* - \lambda_m)^2 T^2) - \exp(-(\theta_1^* - \lambda_i^*)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right) \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F \\
& \quad + \sum_{i \neq \pi_1} \left\| \Phi_{:, \mathcal{D}_i} \text{diag} \left(\left\{ \exp(-(\tilde{\theta}_1^* - \lambda_m)^2 T^2) - \exp(-(\tilde{\theta}_1^* - \lambda_i^*)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right) \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F \\
& \leq \sum_{i \neq \pi_1} \left\| \Phi_{:, \mathcal{D}_i} (\exp(-(\theta_1^* - \lambda_i^*)^2 T^2) - \exp(-(\tilde{\theta}_1^* - \lambda_i^*)^2 T^2)) \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F \\
& \quad + 2\delta \cdot T\sqrt{KLR} \\
& \leq \sum_{i \neq \pi_1} |\exp(-(\theta_1^* - \lambda_i^*)^2 T^2) - \exp(-(\tilde{\theta}_1^* - \lambda_i^*)^2 T^2)| \left\| \Phi_{:, \mathcal{D}_i} \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F + \frac{p_{\text{tail}}^2}{4\sqrt{KLR}} \\
& \leq \frac{p_{\text{tail}}^2}{4\sqrt{KLR}} + o(p_{\text{tail}} T |\theta - \theta'|), \tag{D43}
\end{aligned}$$

where we use a similar calculation as Eq. (D19) and $\delta \cdot T = \mathcal{O}(p_{\text{tail}}^2/KLR)$ in the second step. And the third step follows from

$$\begin{aligned}
(\exp(-(\theta_1^* - \lambda_i^*)^2 T^2) - \exp(-(\tilde{\theta}_1^* - \lambda_i^*)^2 T^2)) & \leq T|\theta_1^* - \tilde{\theta}_1^*| \left(\sup_{|x| \geq \min\{|\theta_1^* - \lambda_i^*|T, |\tilde{\theta}_1^* - \lambda_i^*|T\}} 2x \exp(-x^2) \right) \\
& = o\left(\frac{p_{\text{tail}} T |\theta_1^* - \tilde{\theta}_1^*|}{K \left\| \Phi_{:, \mathcal{D}_i} \Psi_{:, \mathcal{D}_i}^\dagger \right\|_F} \right),
\end{aligned}$$

where the last inequality comes from $\min\{|\theta_1^* - \lambda_i^*|T, |\tilde{\theta}_1^* - \lambda_i^*|T\} \geq T\Delta/4$ and $T = \Omega((1/\Delta) \log(KLR/p_{\text{tail}}))$.

Plugging these three inequalities into the second term and using Eqs. (D33) and (D34), we have probability at least $1 - \eta$ such that

$$\begin{aligned}
& 2\text{Re}(\text{Tr}(A^\dagger(\theta_1^*)(B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*))) - 2\text{Re}(\text{Tr}(A^\dagger(\tilde{\theta}_1^*)(B(\tilde{\theta}_1^*) + C(\tilde{\theta}_1^*) + \mathcal{E}(\tilde{\theta}_1^*)))) \\
& \leq 2 \left(T|\theta_1^* - \tilde{\theta}_1^*| \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F + \frac{p_{\text{tail}}}{2} \right) \cdot \frac{5}{4} p_{\text{tail}} \\
& \quad + 2 \cdot \frac{5}{4} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F \cdot \left(2p_{\text{tail}} \sigma T |\theta_1^* - \tilde{\theta}_1^*| + \frac{p_{\text{tail}}^2}{4\sqrt{KLR}} \right) \\
& \leq (3 + 5\sigma) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F T |\theta_1^* - \tilde{\theta}_1^*| p_{\text{tail}} + \frac{15}{8} p_{\text{tail}}^2 \\
& \leq (3 + 5\sigma) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F T \left(|\theta_1^* - \lambda_{\pi_1}^*| + \frac{q}{T} + \delta \right) p_{\text{tail}} + \frac{15}{8} p_{\text{tail}}^2 \\
& \leq (3 + 5\sigma) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F T |\theta_1^* - \lambda_{\pi_1}^*| p_{\text{tail}} + \frac{23}{8} p_{\text{tail}}^2, \tag{D44}
\end{aligned}$$

where we use $\left\| \Phi_{:, \mathcal{D}_{\pi_1}} (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \right\|_F \leq \sqrt{KLR}$ [according to similar calculation as Eq. (D16)] in the second inequality and $q = \mathcal{O}(p_{\text{tail}}/((1 + \sigma)\sqrt{KLR}))$ and $\delta = \mathcal{O}(p_{\text{tail}}/(T(1 + \sigma)\sqrt{KLR}))$ in the last inequality.

Now, plugging $\theta = \theta_1^*$ and $\theta = \tilde{\theta}_1^*$ into $\mathcal{W}^2(\theta)$ and using Eqs. (D25) and (D38), we have

$$\begin{aligned}
0 &\leq \mathcal{W}^2(\theta_1^*) - \mathcal{W}^2(\tilde{\theta}_1^*) \\
&\leq \underbrace{\left(\exp\left(-2\left(\theta_1^* - \lambda_{\pi_1}^*\right)^2 T^2\right) - \exp\left(-2\left(\tilde{\theta}_1^* - \lambda_{\pi_1}^*\right)^2 T^2\right) \right)}_{\leq 0 \text{ by the definition of } \tilde{\theta}_1^*} \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F^2 \\
&\quad + \underbrace{6KLR\delta \cdot T}_{\leq p_{\text{tail}}^2} + (3 + 5\sigma) \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F T \left| \theta_1^* - \lambda_{\pi_1}^* \right| p_{\text{tail}} + \frac{23}{8} p_{\text{tail}}^2 + \underbrace{\frac{9}{2} p_{\text{tail}}^2}_{\text{last term}}, \tag{D45}
\end{aligned}$$

where we use the condition that $\delta \cdot T = \mathcal{O}(p_{\text{tail}}^2/KLR)$. Because we have already shown $\left| \theta_1^* - \lambda_{\pi_1}^* \right| = \mathcal{O}(1/T)$ (noticing $\chi = \mathcal{O}(1)$) in the first step, let $\delta_\theta = T \left| \theta_1^* - \lambda_{\pi_1}^* \right|$, the above inequality implies that

$$-C\delta_\theta^2 + \left((3 + 5\sigma)p_{\text{tail}} / \left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F \right) \delta_\theta + \frac{67}{8} \frac{p_{\text{tail}}^2}{\left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F^2} \geq 0, \tag{D46}$$

where C is a uniform constant. Thus, we have that

$$\left| \theta_1^* - \lambda_{\pi_1}^* \right| = \mathcal{O} \left((1 + \sigma) \frac{p_{\text{tail}}}{\left\| \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right\|_F} \frac{1}{T} \right) = \mathcal{O} \left((1 + \sigma) \frac{p_{\text{tail}}}{p_{\min}} \frac{1}{T} \right), \tag{D47}$$

where we use Eq. (D25) and $\chi = \mathcal{O}(1)$ for the last equality. This concludes the first part of the proof.

Step 3: We show that $m_j = |\mathcal{D}_{\pi_j}|$ when $1 \leq j \leq I$.

Without loss of generality, we only consider $i = 1$. The other cases can also be shown similarly. Define $s_k(A)$ as the k th singular value of A . Recall

$$\begin{aligned}
G(\theta_1^*) &= \underbrace{\Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\left\{ \exp(-(\theta_1^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_{\pi_1}} \right)}_{:=A(\theta_1^*)} \cdot \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \\
&\quad + \underbrace{\Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\left\{ \exp(-(\theta_1^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}^c} \right)}_{:=B(\theta_1^*)} \cdot \left(\Psi_{:, \mathcal{D}^c} \right)^\dagger \\
&\quad + \underbrace{\sum_{i \neq \pi_1} \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\left\{ \exp(-(\theta_1^* - \lambda_m)^2 T^2) \right\}_{m \in \mathcal{D}_i} \right)}_{:=C(\theta_1^*)} \cdot \left(\Psi_{:, \mathcal{D}_i} \right)^\dagger + \mathcal{E}(\theta_1^*). \tag{D48}
\end{aligned}$$

With probability at least $1 - \eta$, we have

$$\|B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*)\|_2 \leq \|B(\theta_1^*) + C(\theta_1^*) + \mathcal{E}(\theta_1^*)\|_F \leq 2p_{\text{tail}}. \tag{D49}$$

Furthermore, for $1 \leq k \leq |\mathcal{D}_{\pi_1}|$, Eq. (D5) implies that

$$\begin{aligned}
s_k(A(\theta_1^*)) &= \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\lambda_k \left(\Psi_{:, \mathcal{D}_{\pi_1}} \Phi_{:, \mathcal{D}_{\pi_1}}^\dagger \Phi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right) \right)^{1/2} \\
&\geq \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\lambda_{\min} \left(\Phi_{:, \mathcal{D}_{\pi_1}}^\dagger \Phi_{:, \mathcal{D}_{\pi_1}} \right) \right)^{1/2} \left(\lambda_k \left(\Psi_{:, \mathcal{D}_{\pi_1}} \left(\Psi_{:, \mathcal{D}_{\pi_1}} \right)^\dagger \right) \right)^{1/2} \\
&\geq \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\lambda_{\min} \left(\Phi_{:, \mathcal{D}_{\pi_1}}^\dagger \Phi_{:, \mathcal{D}_{\pi_1}} \right) \right)^{1/2} \left(\lambda_{\min} \left(\Psi_{:, \mathcal{D}_{\pi_1}}^\dagger \Psi_{:, \mathcal{D}_{\pi_1}} \right) \right)^{1/2} \\
&\geq \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\frac{1}{1+\chi} \right)^2 \frac{\|\Phi_{:, \mathcal{D}_i}\|_F \|\Psi_{:, \mathcal{D}_i}\|_F}{|\mathcal{D}_i|} \\
&= \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\frac{1}{1+\chi} \right)^2 \frac{\sqrt{\sum_{m \in \mathcal{D}_i} \|\Phi_{:,m}\|^2} \sqrt{\sum_{m \in \mathcal{D}_i} \|\Psi_{:,m}\|^2}}{|\mathcal{D}_i|} \\
&\geq \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\frac{1}{1+\chi} \right)^2 \frac{\sum_{m \in \mathcal{D}_i} \|\Phi_{:,m}\| \|\Psi_{:,m}\|}{|\mathcal{D}_i|} \\
&\geq \exp(-\mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)) \left(\frac{1}{1+\chi} \right)^2 p_{\min} \\
&\geq \frac{1 - \mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)}{(1+\chi)^2} p_{\min},
\end{aligned} \tag{D50}$$

where we use $\delta = \mathcal{O}(1/T)$, Assumption C1, and the definition of $p_{\min}$.

Because

$$\frac{1 - \mathcal{O}((1+\sigma)(p_{\text{tail}}/p_{\min}) + \delta \cdot T^2)}{(1+\chi)^2} = \Omega\left(\frac{p_{\text{tail}}}{p_{\min}}\right), \tag{D51}$$

we have

$$\inf_{1 \leq k \leq |\mathcal{D}_1|} s_k(G(\theta_1^*)) \geq \inf_{1 \leq k \leq |\mathcal{D}_1|} s_k(A(\theta_1^*)) - 2p_{\text{tail}} > \tau \geq 2p_{\text{tail}} \geq \sup_{k > |\mathcal{D}_1|} s_k(G(\theta_1^*)). \tag{D52}$$

This guarantees that $m_1 = |\mathcal{D}_{\pi_1}|$.

Step 4: We show that $m_i = 0$ when $i > I$.

For $i > I$, because of the block intervals from $1 \leq i \leq I$, we first have

$$\inf_j \text{dist}(\theta_i^*, \mathcal{I}_j) \geq \frac{\alpha}{T} - \mathcal{O}\left((1+\sigma)\left(\frac{p_{\text{tail}}}{p_{\min}}\right)\frac{1}{T}\right) - \delta/2 \geq \frac{\alpha}{2T}, \tag{D53}$$

where we use $\alpha = \Omega(\chi^2 + (1+\sigma)^2(p_{\text{tail}}/p_{\min})^2)$ and $\alpha = \mathcal{O}(\Delta \cdot T)$ in the last inequality. Using Lemma D2, Eq. (D64), we have

$$\begin{aligned}
G(\theta_i^*) &= \underbrace{\Phi_{:, \mathcal{D}} \cdot \text{diag}\left(\left\{\exp(-(\theta_i^* - \lambda_m)^2 T^2)\right\}_{m \in \mathcal{D}}\right)}_{\|\cdot\|_2 \leq \sqrt{KLR} \exp(-\alpha^2/4)} \cdot (\Psi_{:, \mathcal{D}})^\dagger \\
&\quad + \underbrace{\Phi_{:, \mathcal{D}^c} \cdot \text{diag}\left(\left\{\exp(-(\theta_i^* - \lambda_m)^2 T^2)\right\}_{m \in \mathcal{D}^c}\right)}_{\|\cdot\|_2 \leq p_{\text{tail}}} \cdot (\Psi_{:, \mathcal{D}^c})^\dagger + \mathcal{E}(\theta_i^*).
\end{aligned} \tag{D54}$$

Because $\alpha = \Omega(\log(KLR/p_{\text{tail}}))$, we have

$$\|G(\theta_i^*)\|_2 \leq 2p_{\text{tail}} < \tau \tag{D55}$$

for $i > I$. This implies that $m_i = 0$ for $i > I$ and concludes the proof. ■

1. Useful lemmas

Lemma D1. Given $\beta > 0$. Let $\{t_n\}$ be i.i.d. sampled from the truncated Gaussian $a_T(t)$ defined as Eq. (16). Define

$$\mathcal{E}(\theta) := \frac{1}{N} \sum_{n=1}^N Z_n \exp(i\theta t_n) - \Phi \cdot \text{diag}(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in [M]}) \cdot \Psi^\dagger \in \mathbb{C}^{L \times R}. \quad (\text{D56})$$

Let $\Theta := \{\theta_j\}_{j=1}^J \cup \{\lambda_m\}_{m \in \mathcal{D}}$.

If $\sigma = \Omega\left(\log^{1/2}\left(\sqrt{LR}/\beta\right)\right)$ as in Eq. (16) and $N = \Omega\left((LR/\beta^2) \log((J + |\mathcal{D}|)(LR/\eta))\right)$, we have

$$\Pr\left[\max_{\theta \in \Theta} \|\mathcal{E}(\theta)\|_F \leq \beta\right] \geq 1 - \eta \quad (\text{D57})$$

and

$$\Pr\left[\bigcap_{\theta, \theta' \in \Theta} \|\mathcal{E}(\theta) - \mathcal{E}(\theta')\|_F \leq \beta \sigma T |\theta - \theta'|\right] \geq 1 - \eta. \quad (\text{D58})$$

Proof. For each $1 \leq i \leq L$ and $1 \leq j \leq R$, by Lemma D3 with $\tilde{\beta} = \beta/\sqrt{LR}$ and $\tilde{\eta} = \eta/LR$, we have

$$\Pr\left[\max_{\theta \in \Theta} |\mathcal{E}_{ij}(\theta)| \leq \frac{\beta}{\sqrt{LR}}\right] \geq 1 - \frac{\eta}{LR} \quad (\text{D59})$$

and

$$\Pr\left[\bigcap_{\theta, \theta' \in \Theta} \left\{|\mathcal{E}_{ij}(\theta) - \mathcal{E}_{ij}(\theta')| \leq \frac{\beta}{\sqrt{LR}} \sigma T |\theta - \theta'|\right\}\right] \geq 1 - \frac{\eta}{LR}. \quad (\text{D60})$$

By union bound, the first equation implies that

$$\Pr\left[\max_{\theta \in \Theta} \|\mathcal{E}(\theta)\|_F = \max_{\theta \in \Theta} \sqrt{\sum_{i,j} |\mathcal{E}_{ij}(\theta)|^2} \leq \beta\right] \geq \Pr\left[\bigcap_{i,j} \left\{\max_{\theta \in \Theta} |\mathcal{E}_{ij}(\theta)| \leq \frac{\beta}{\sqrt{LR}}\right\}\right] \geq 1 - \eta. \quad (\text{D61})$$

And the second equation implies

$$\begin{aligned} & \Pr\left[\bigcap_{\theta, \theta' \in \Theta} \|\mathcal{E}(\theta) - \mathcal{E}(\theta')\|_F = \sqrt{\sum_{i,j} |\mathcal{E}_{ij}(\theta) - \mathcal{E}_{ij}(\theta')|^2} \leq \beta \sigma T |\theta - \theta'|\right] \\ & \geq \Pr\left[\bigcap_{i,j} \left\{\bigcap_{\theta, \theta' \in \Theta} |\mathcal{E}_{ij}(\theta) - \mathcal{E}_{ij}(\theta')| \leq \frac{\beta}{\sqrt{LR}} \sigma T |\theta - \theta'|\right\}\right] \geq 1 - \eta. \end{aligned} \quad (\text{D62})$$

This completes the proof of the lemma. ■

Lemma D2. Given any matrix $\Phi \in \mathbb{C}^{L \times M}$, $\Psi \in \mathbb{C}^{R \times M}$, and $\{\lambda_m\}_{m \in [M]}$. Define

$$G(\theta) = \Phi \cdot \text{diag}(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in [M]}) \cdot \Psi^\dagger. \quad (\text{D63})$$

We have

$$\|G(\theta)\|_F \leq \left(\max_m \exp(-(\theta - \lambda_m)^2 T^2) \right) \sum_{m \in [M]} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)} \quad (\text{D64})$$

and

$$\begin{aligned} \|G(\theta) - G(\theta')\|_F &\leq T|\theta - \theta'| \sum_{m \in [M]} \|\Phi_{:,m} \Psi_{:,m}^\dagger\|_F \\ &\leq \sqrt{2/e} T |\theta - \theta'| \sum_{m \in [M]} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)}. \end{aligned} \quad (\text{D65})$$

Proof. First, we note that

$$\begin{aligned} \|G(\theta)\|_F &\leq \sum_{m \in [M]} \|\Phi_{:,m} \exp(-(\theta - \lambda_m)^2 T^2) \Psi_{:,m}^\dagger\|_F \\ &\leq \left(\max_m \exp(-(\theta - \lambda_m)^2 T^2) \right) \sum_{m \in [M]} \|\Phi_{:,m} \Psi_{:,m}^\dagger\|_F \\ &= \left(\max_m \exp(-(\theta - \lambda_m)^2 T^2) \right) \sum_{m \in [M]} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)}. \end{aligned} \quad (\text{D66})$$

This concludes the proof of Eq. (D64).

Second, we have

$$\begin{aligned} \|G(\theta) - G(\theta')\|_F &\leq \sum_{m \in [M]} \|\Phi_{:,m} (\exp(-(\theta - \lambda_m)^2 T^2) - \exp(-(\theta' - \lambda_m)^2 T^2)) \Psi_{:,m}^\dagger\|_F \\ &\leq \left(\max_m (\exp(-(\theta - \lambda_m)^2 T^2) - \exp(-(\theta' - \lambda_m)^2 T^2)) \right) \sum_{m \in [M]} \|\Phi_{:,m} \Psi_{:,m}^\dagger\|_F \\ &\leq \sqrt{2/e} T |\theta - \theta'| \sum_{m \in [M]} \|\Phi_{:,m} \Psi_{:,m}^\dagger\|_F \\ &= \sqrt{2/e} T |\theta - \theta'| \sum_{m \in [M]} \sqrt{\left(\sum_{l=1}^L |\Phi_{l,m}|^2 \right) \left(\sum_{r=1}^R |\Psi_{r,m}|^2 \right)}, \end{aligned} \quad (\text{D67})$$

where the last step follows from the Lipschitzness of $\exp(-x^2)$.

This concludes the proof of Eq. (D65). ■

Lemma D3 (Lemma A.1 of Ref. [64]). Given $\tilde{\beta} > 0$, $i \in [L]$, $j \in [R]$. Let $\{t_n\}$ to be i.i.d. sampled from the truncated Gaussian $a_T^{\text{trunc}}(t)$ defined as Eq. (16). Define

$$\mathcal{E}_{i,j}(\theta) := \frac{1}{N} \sum_{n=1}^N (Z_n)_{i,j} \exp(i\theta t_n) - \Phi_{i,:} \cdot \text{diag}(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in [M]}) \cdot (\Psi^\dagger)_{:,j} \in \mathbb{C}. \quad (\text{D68})$$

Let $\Theta := \{\theta_j\}_{j=1}^J \cup \{\lambda_m\}_{m \in \mathcal{D}}$. If $\sigma = \Omega(\log^{1/2}(1/\tilde{\beta}))$ and $N = \Omega((1/\tilde{\beta}^2) \log((J + |\mathcal{D}|)(1/\tilde{\eta})))$, we have

$$\Pr \left[\max_{\theta \in \Theta} |\mathcal{E}_{i,j}(\theta)| > \tilde{\beta} \right] \leq \tilde{\eta}, \quad (\text{D69})$$

and Ref. [143],

$$\Pr \left[\bigcap_{\theta, \theta' \in \Theta} |\mathcal{E}_{i,j}(\theta) - \mathcal{E}_{i,j}(\theta')| \leq \tilde{\beta} \sigma T |\theta - \theta'| \right] \geq 1 - \tilde{\eta}. \quad (\text{D70})$$

APPENDIX E: ANALYSIS OF THE OBSERVABLE ESTIMATION

In this Appendix, we give the proof of Proposition 1. In addition to the assumptions in Theorem D1, we assume $\delta = 0$, $p_{\text{tail}} = 0$, $p_{\min} = \Omega(1)$, and $K, L, R = \mathcal{O}(1)$. Following the proof of Theorem D1, when $T = \tilde{\Omega}(\Delta^{-1})$ and $N = \Omega(1)$, we first have

$$\sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi(j)}^*| \leq \Delta/4. \quad (\text{E1})$$

This implies θ_j^* is at least $\Delta/2$ away from λ_i^* when $i \neq \pi(j)$.

Now, we improve the above bound and aim to show

$$\sup_{1 \leq j \leq I} |\theta_j^* - \lambda_{\pi(j)}^*| = \mathcal{O} \left(\frac{1}{T} (\exp(-\Delta^2 T^2/32) + N^{-1/2}) \right). \quad (\text{E2})$$

Without loss of generality, we consider $j = 1$. Because $p_{\text{tail}} = 0$, we have

$$\begin{aligned} G(\theta) &= \underbrace{\Phi_{:, \mathcal{D}_{\pi_1}} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}_{\pi_1}} \right)}_{:=A(\theta)} \cdot (\Psi_{:, \mathcal{D}_{\pi_1}})^\dagger \\ &\quad + \underbrace{\Phi_{:, \mathcal{D}^c} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}^c} \right)}_{=0} \cdot (\Psi_{:, \mathcal{D}^c})^\dagger \\ &\quad + \underbrace{\sum_{i \neq \pi_1} \Phi_{:, \mathcal{D}_i} \cdot \text{diag} \left(\{\exp(-(\theta - \lambda_m)^2 T^2)\}_{m \in \mathcal{D}_i} \right)}_{:=C(\theta)} \cdot (\Psi_{:, \mathcal{D}_i})^\dagger + \mathcal{E}(\theta). \end{aligned} \quad (\text{E3})$$

Because $K, L, R = \mathcal{O}(1)$ and $|\theta_1^* - \lambda_j^*| \geq \Delta/2$ for $j \neq \pi_1$, we first have $|\theta_1^* - \lambda_m| \geq \Delta/4$ if the dominant index $m \notin \mathcal{D}_{\pi_1}$. This implies

$$\|C(\theta)\|_F = \mathcal{O}(\exp(-\Delta^2 T^2/16)) \quad (\text{E4})$$

and

$$\|G(\theta) - A(\theta) - \mathcal{E}(\theta)\|_F = \mathcal{O}(\exp(-\Delta^2 T^2/16)). \quad (\text{E5})$$

Using Lemma D3, with high probability, we also have

$$\|\mathcal{E}(\theta)\|_F = \tilde{\mathcal{O}}(N^{-1/2}), \quad \|\mathcal{E}(\theta) - \mathcal{E}(\theta')\|_F = \mathcal{O}(\sigma T |\theta - \theta'| N^{-1/2}). \quad (\text{E6})$$

Let $\tilde{\theta}_1^*$ be the closest energy grid point to the desired cluster center $\lambda_{\pi_1}^*$. Similar to Eq. (D44) in the second step of the proof of Theorem D1, we have

$$\begin{aligned} & 2\text{Re}(\text{Tr}(A^\dagger(\theta_1^*)\mathcal{E}(\theta_1^*))) - 2\text{Re}(\text{Tr}(A^\dagger(\tilde{\theta}_1^*)\mathcal{E}(\tilde{\theta}_1^*))) \\ &= \mathcal{O}(T|\theta_1^* - \tilde{\theta}_1^*|N^{-1/2} + \sigma T|\theta_1^* - \tilde{\theta}_1^*|N^{-1/2}) \\ &= \mathcal{O}\left((1 + \sigma)T\left(|\theta_1^* - \lambda_{\pi_1}^*| + \frac{q}{T}\right)N^{-1/2}\right). \end{aligned} \quad (\text{E7})$$

Choosing $q = \tilde{\mathcal{O}}(N^{-1/2})$, similar to Eq. (D45), we have

$$\begin{aligned} & \underbrace{\left(\exp\left(-2\left(\tilde{\theta}_1^* - \lambda_{\pi_1}^*\right)^2 T^2\right) - \exp\left(-2\left(\theta_1^* - \lambda_{\pi_1}^*\right)^2 T^2\right)\right)}_{\leq 0} \\ &= \mathcal{O}\left(T|\theta_1^* - \lambda_{\pi_1}^*|N^{-1/2} + \frac{1}{N} + \exp(-\Delta^2 T^2/16)\right). \end{aligned} \quad (\text{E8})$$

Following a similar calculation as Eq. (D46), we have

$$T|\theta_1^* - \lambda_{\pi_1}^*| = \mathcal{O}\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/32)\right). \quad (\text{E9})$$

We conclude the proof of Eq. (E2).

Next, we consider the observation data matrix error. For a fixed i , we define the exact data matrix for the generalized eigenvalue problem:

$$G_{\text{exact}} = \Phi_{:, \mathcal{D}_i}(\Psi_{:, \mathcal{D}_i})^\dagger, \quad G_{\text{exact}}^O = \Phi_{:, \mathcal{D}_i} \cdot O_{\mathcal{D}_i} \cdot (\Psi_{:, \mathcal{D}_i})^\dagger, \quad (\text{E10})$$

where $O_{\mathcal{D}_i}$ is defined in Eq. (37). According to Eq. (E2), Lemma D1, and following a similar calculation as Eq. (67), we have

$$\begin{aligned} \|G(\theta_i^*) - G_{\text{exact}}\|_2 &= \mathcal{O}\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/16)\right), \\ \|G^O(\theta_i^*) - G_{\text{exact}}^O\|_2 &= \mathcal{O}\left(\|O\|\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/16)\right)\right), \end{aligned} \quad (\text{E11})$$

where $G(\theta_i^*)$ and $G^O(\theta_i^*)$ are defined in Eqs. (18) and (32), respectively.

According to Assumption C1, G_{exact} has rank m_i with smallest nonzero singular value lower bounded by $p_{\min}/(1 + \chi)$. Combining this and Eq. (E11), $|m_i|$ th singular value of $G(\theta_i^*)$ can be lower bound by $p_{\min}/(2(1 + \chi))$ when $T = \Omega(\Delta^{-1})$ and $N = \Omega(1)$. Furthermore, following the third step of the proof of Theorem D1, the $(m_i + 1)$ th singular value of $G(\theta_i^*)$ can be upper bound by $p_{\min}/(4(1 + \chi))$ when $T = \Omega(\Delta^{-1})$ and $N = \Omega(1)$. Using singular value perturbation theory, these imply that

$$\begin{aligned} \|\tilde{G}(\theta_i^*) - \tilde{G}_{\text{exact}}\|_2 &= \mathcal{O}\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/32)\right), \\ \|\tilde{G}^O(\theta_i^*) - \tilde{G}_{\text{exact}}^O\|_2 &= \mathcal{O}\left(\|O\|\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/32)\right)\right), \end{aligned} \quad (\text{E12})$$

where $\tilde{G}_{\text{exact}}$ and $\tilde{G}_{\text{exact}}^O$ are defined using the same forms as Eq. (34). Here, both $\tilde{G}(\theta_i^*)$ and $\tilde{G}_{\text{exact}}$ are full-rank matrices with smallest singular value lower bounded by $p_{\min}/(2(1 + \chi))$. According to generalized eigenvalue perturbation theory, we finally have

$$|\lambda_k^O - \lambda_{k, \text{exact}}| = \mathcal{O}\left(\|O\|\left(\frac{1}{\sqrt{N}} + \exp(-\Delta^2 T^2/32)\right)\right), \quad (\text{E13})$$

where $\lambda_{k, \text{exact}}$ is the k th generalized eigenvalue with respect to the matrix pencil $(\tilde{G}_{\text{exact}}^O, \tilde{G}_{\text{exact}})$. Therefore to achieve ϵ_O precision in λ_k^O , it is required that $N = \tilde{\Omega}(\epsilon_O^{-2})$ and $T = \tilde{\mathcal{O}}(\Delta^{-1})$. This concludes the proof.

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