Supplementary Information for
Optimal Hamiltonian recognition of unknown quantum dynamics

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In this Supplementary Information, we present detailed proofs of the theorems in the manuscript "Optimal Hamiltonian recognition of unknown quantum dynamics". In Section I, we review the tester formalism used for quantum channel discrimination and some useful results in quantum signal processing. In Section II, we present detailed proofs of Theorem 1 in the manuscript for binary Hamiltonian recognition. In Section III, we present detailed proofs of Theorem 3 in the manuscript for ternary Hamiltonian recognition. In Section IV, we give a detailed algorithm for the experiments on a superconducting computer. In Section V, we present numerical results on the recognition of general non-orthogonal Hamiltonians.

I. PRELIMINARIES

A. Tester formalism

We review the tester formalism for quantum channel discrimination based on the Choi-Jamiołkowski isomorphism [1]. A tester is defined as a set of positive semidefinite operators $T = \{T_0, T_1\}, T_i \in \mathcal{L}^\dagger(\mathcal{H}_I \otimes \mathcal{H}_O)$ where we denote by $\mathcal{L}^\dagger(\mathcal{H})$ be the set of Hermitian operators acting on a Hilbert space $\mathcal{H}$. By taking the trace with $J_{IO}^{\mathcal{N}}$ and $J_{IO}^{\mathcal{M}}$, it results in a valid probability distribution according to $p(\mathcal{N}_{I\to O}|J_{IO}^{\mathcal{N}}) = \mathrm{Tr}(T_0 J_{IO}^{\mathcal{N}})$ and $p(\mathcal{M}_{I\to O}|J_{IO}^{\mathcal{M}}) = \mathrm{Tr}(T_1 J_{IO}^{\mathcal{M}})$. Compared to how POVMs act on quantum states, these testers that act on quantum channels can be regarded as a 'measurement' of quantum channels. Supposing two channels $\mathcal{N}$ and $\mathcal{M}$ are given with prior probability p and $1-p$, respectively, we can donate the optimal success probability of discriminating $\mathcal{N}$ and $\mathcal{M}$ as

$$P = \max_{\{T_0,T_1\}} p\cdot \mathrm{Tr}\left(T_0 J_{IO}^{\mathcal{N}}\right) + (1-p)\cdot \mathrm{Tr}\left(T_1 J_{IO}^{\mathcal{M}}\right). \tag{I.1}$$

For simplicity of notations, the trace-and-replace operation in $\mathcal{H}_X$ is denoted as

$${}_X(\cdot) \coloneqq \mathrm{Tr}_X(\cdot)\otimes\frac{\mathbb{1}_X}{d_X}, \tag{I.2}$$

where $\mathbb{1}_X$ denotes the identity operator on $\mathcal{H}_X$ and d_X is the dimension of $\mathcal{H}_X$.

a. Parallel strategy. This strategy involves sending each component of a multipartite state through independent copies of an unknown channel. In this approach, the outputs from these channels do not interact with each other's inputs. These strategies are characterized by parallel k-slot testers $T^{\text{PAR}} = \{T_0^{\text{PAR}}, T_1^{\text{PAR}}\}$, $T_i^{\text{PAR}} \in \mathcal{L}^\dagger(\mathcal{H}_I\otimes\mathcal{H}_O)$. We set $W^{\text{PAR}} \coloneqq \sum_{i=0}^1 T_i^{\text{PAR}}$ and parallel k-slot testers are defined as

$$T_i^{\text{PAR}} \geq 0,\ \forall i, \tag{I.3}$$
$$\mathrm{Tr}\, W^{\text{PAR}} = d_O, \tag{I.4}$$
$$W^{\text{PAR}} = {}_O W^{\text{PAR}}, \tag{I.5}$$

where $O \coloneqq O_1 O_2\cdots O_k$ is a composite of k subsystems.

b. Sequential strategy. This strategy is also sometimes called adaptive strategy which involves sending a quantum system through a series of channels in sequence. In this approach, the output from each channel can be used as input for the next one. These strategies are characterized by sequential k-slot testers $T^{\text{SEQ}} = \{T_0^{\text{SEQ}}, T_1^{\text{SEQ}}\}$, $T_i^{\text{SEQ}} \in \mathcal{L}^\dagger(\mathcal{H}_I\otimes\mathcal{H}_O)$. We set $W^{\text{SEQ}} \coloneqq \sum_{i=0}^1 T_i^{\text{SEQ}}$ and sequential k-slot testers are defined as

$$T_i^{\text{SEQ}} \geq 0,\ \forall i, \tag{I.6}$$
$$\mathrm{Tr}\, W^{\text{SEQ}} = d_O, \tag{I.7}$$
$$W^{\text{SEQ}} = {}_{O_k} W^{\text{SEQ}}, \tag{I.8}$$
$${}_{I_kO_k}W^{\text{SEQ}} = {}_{O_{k-1}I_kO_k} W^{\text{SEQ}}, \tag{I.9}$$
$$\cdots$$
$${}_{I_2O_2\ldots I_kO_k}W^{\text{SEQ}} = {}_{O_1I_2O_2\ldots I_kO_k} W^{\text{SEQ}}. \tag{I.10}$$

c. General strategy. This strategy involves the most general types of operations that transform multiple quantum channels into a joint probability distribution. In this approach, general strategies do not impose any specific order on the channels, allowing for the most flexible approach. These strategies are characterized by general k-slot testers $T^{\text{GEN}} = \{T_0^{\text{GEN}}, T_1^{\text{GEN}}\}$, $T_i^{\text{GEN}} \in \mathcal{L}^\dagger(\mathcal{H}_I \otimes \mathcal{H}_O)$, which satisfy $p(i|J_{IO}^{\mathcal{N}}, J_{IO}^{\mathcal{M}}) = \operatorname{Tr}\left[T_i^{\text{GEN}}(J_{IO}^{\mathcal{N}} \otimes J_{IO}^{\mathcal{M}})\right]$. We set $W^{\text{GEN}} := \sum_{i=0}^{1} T_0^{\text{GEN}}$ and general k-slot testers are defined as

$$T_i^{\text{GEN}} \geq 0, \ \forall i, \tag{I.11}$$

$$\operatorname{Tr}\left[W^{\text{GEN}}(J_{IO}^{\mathcal{N}} \otimes J_{IO}^{\mathcal{M}})\right] = 1. \tag{I.12}$$

For any strategies mentioned above, we denote $\mathcal{S} \in \{\texttt{PAR}, \texttt{SEQ}, \texttt{GEN}\}$. By Eq. (I.1), the optimal success probability of discrimination can be expressed as

$$P^{\mathcal{S}} = \max_{\{T_0,T_1\}\in\mathcal{T}^{\mathcal{S}}} p \cdot \operatorname{Tr}\left[T_0(J_{IO}^{\mathcal{N}})^{\otimes k}\right] + (1-p) \cdot \operatorname{Tr}\left[T_1(J_{IO}^{\mathcal{M}})^{\otimes k}\right]. \tag{I.13}$$

B. Quantum signal processing

Quantum signal processing (QSP) is a technique that extends the concepts of composite pulse sequences proposed by Low, Yoder, and Chuang [2, 3]. A common QSP structure consists of four key components: (i) the signal unitary W, (ii) the QSP phase sequence $\vec{\phi} := (\phi_0, \phi_1, \cdots, \phi_k)$, (iii) the signal processing operators $S(\phi_j)$, and (iv) the measurement basis M in which the desired polynomial is obtained. A QSP circuit is constructed by interleaving the signal unitary W with the signal processing operators $S(\phi_j)$, followed by a projective measurement in the basis M. The key feature of QSP is that the signal rotation W always rotates through a fixed angle θ, while the angles for the signal processing rotations S can be chosen to fit desired functions of θ. For a comprehensive review of QSP, we refer the reader to Ref. [4]. A widely studied and employed signal unitary is

$$W_x(a) := \begin{pmatrix} a & i\sqrt{1-a^2} \\ i\sqrt{1-a^2} & a \end{pmatrix} = e^{i\arccos(a)X}, \tag{I.14}$$

which is a rotation around x-axis by angle $\theta = 2\arccos(a)$. We will also use $W_x(\theta)$ to denote $W_x(a)$. The function-fitting capability of a simple QSP structure is characterized by the following theorem.

Theorem S1 ([5], Theorem 4) *There exists a QSP phase sequence $\vec{\phi} \in \mathbb{R}^{d+1}$ such that*

$$e^{iZ\phi_0} \prod_{k=1}^{d} W(a) e^{iZ\phi_k} = \begin{pmatrix} P(a) & iQ(a)\sqrt{1-a^2} \\ iQ^*(a)\sqrt{1-a^2} & P^*(a) \end{pmatrix} \tag{I.15}$$

for $a \in [-1,1]$, and a $\vec{\phi}$ exists for any polynomials P, Q in a such that:

(i) $\deg(P) \leq k, \ \deg(Q) \leq k-1$,

(ii) *P has parity k mod 2 and Q has parity $(d-1)$ mod 2,*

(iii) $|P|^2 + (1-a^2)|Q|^2 = 1$.

Another useful result is

Theorem S2 ([4], Theorem 9) *There exists a QSP phase sequence $\vec{\phi} \in \mathbb{R}^{d+1}$ such that*

$$\text{Poly}(a) = \langle 0| e^{iZ\phi_0} \prod_{j=1}^{k} W_x(a) e^{iZ\phi_j} |0\rangle \tag{I.16}$$

for $a \in [-1,1]$, and for any polynomial $\text{Poly} \in \mathbb{C}[a]$ if and only if the following conditions hold:

(i) $\deg(\text{Poly}) \leq k$,

(ii) Poly *has parity* k mod 2,

(iii) $\forall a \in [-1,1], |\text{Poly}(a)| \leq 1$,

(iv) $\forall a \in (-\infty,-1] \cup [1,\infty), |\text{Poly}(a)| \geq 1$,

(v) if k is even, then $\forall a \in \mathbb{R}, \text{Poly}(ia)\text{Poly}^*(ia) \geq 1$.

II. PROOF OF THEOREM 1

In order to prove Theorem 1, we first prove the following lemmas.

Lemma S3 *For any odd k, there exists a QSP phase sequence $\vec{\phi} \in \mathbb{R}^{k+1}$ such that*

$$\left| \langle 0| e^{iZ\phi_0} \prod_{j=1}^{k} W_x(\theta) e^{iZ\phi_j} |0\rangle \right|^2 = \sum_{l=-k}^{k} \frac{k-|l|+1}{(k+1)^2} e^{il\theta}. \tag{II.1}$$

Proof Denoting $f_k(\theta) = \sum_{l=-k}^{k} \frac{k-|l|+1}{(k+1)^2} e^{il\theta}$, we first note that the following polynomial $P_k(\theta)$

$$P_k(\theta) \coloneqq \frac{1}{k+1} \sum_{l=-k,\, l \text{ odd}}^{k} e^{il\theta/2} \tag{II.2}$$

satisfies $P_k(\theta)P_k^*(\theta) = f_k(\theta)$ because

$$P_k(\theta)P_k^*(\theta) = \frac{1}{(k+1)^2} \sum_{\substack{l=-k,\\ l \text{ odd}}}^{k} \sum_{\substack{m=-k,\\ m \text{ odd}}}^{k} e^{i(l+m)\theta/2} = \frac{1}{(k+1)^2} \sum_{j=-k}^{k} \sum_{2j=l+m} e^{ij\theta}. \tag{II.3}$$

By checking how many pairs (l, m) such that $2j = l + m$ where $-k \le j \le k$, we have that $P_k(\theta)P_k^*(\theta) = P_k(\theta)$. It is easy to see that $P_k(\theta) \in \mathbb{C}[e^{-i\theta/2}, e^{i\theta/2}]$ and has parity 1 because k is odd. Further, note that

$$P_k(\theta) = \frac{2}{k+1} \sum_{l=1,\, l \text{ odd}}^{k} \cos(l\theta/2) = \frac{2}{k+1} \sum_{l=1,\, l \text{ odd}}^{k} T_l\left(\cos(\theta/2)\right), \tag{II.4}$$

where T_l is the Chebyshev polynomial of the first kind with degree l. Denoting $a \coloneqq \cos(\theta/2)$, P_k can be rewritten as

$$P_k(a) = \frac{2}{k+1} \sum_{l=1,\, l \text{ odd}}^{k} T_l(a). \tag{II.5}$$

Such reconstruction gives

- $P_k(a) \in \mathbb{C}[a]$ with degree k,
- P_k has parity 1, since T_l has parity l mod 2,
- For all $a \in [-1, 1]$, $|P_k(a)| \le \frac{2}{k+1} \sum_l |T_l(a)| \le 1$,
- For all $a \in [1, +\infty)$, $|P_k(a)| \ge 1$ by Lemma S4.

Therefore, P_k satisfies all conditions in Theorem S2, and hence there exists a QSP phase sequence $\vec{\phi}$ such that

$$P_k(a) = \langle 0| e^{iZ\phi_0} \prod_{j=1}^{k} W_x(a) e^{iZ\phi_j} |0\rangle \implies f_k(\theta) = \left| \langle 0| e^{iZ\phi_0} \prod_{j=1}^{k} W_x(\theta) e^{iZ\phi_j} |0\rangle \right|^2, \tag{II.6}$$

which completes the proof. ■

Lemma S4 *For $a \in \mathbb{R}$ such that $|a| \ge 1$ and an odd k, P_k in Eq. (II.5) satisfies $|P_k(a)| \ge 1$.*

Proof Since P_k is an odd function, it suffices to prove the positive case. In the rest of the proof, we assume $a \ge 1$. By definition of the Chebyshev polynomials, in such case $T_l(a) = \cosh\left(l \cosh^{-1}(a)\right)$. One can denote $\phi = \cosh(a)$ such that $T_l(a) = \cosh(l\phi)$ and hence

$$P_k(a) = \frac{2}{k+1} \sum_{l=1,\, l \text{ odd}}^{k} \cosh(l\phi) = \frac{2}{k+1} \sum_{j=0}^{(k-1)/2} \cosh\left((2j+1)\phi\right) \tag{II.7}$$

$$= \frac{2}{k+1} \frac{\sinh\left((k+1)\phi\right)}{2\sinh(\phi)} = \frac{\sinh\left((k+1)\phi\right)}{(k+1)\sinh(\phi)}. \tag{II.8}$$

To show that the RHS of the equation is no less than 1, we further define $f_\phi(k) = \sinh\left((k+1)\phi\right) / \left((k+1)\sinh(\phi)\right)$. Since $f'_\phi(k) \ge 0$ and $f(0) = 1$, we conclude that $f(k) \ge 1$ for $k \ge 0$, and the statement follows. ■

Lemma S5 *Let $k \in \mathbb{N}^+$, and*

$$\Omega_H^{(k)}(\pi) = \frac{1}{2\pi}\int_0^{2\pi} \left[\left(e^{-iH\theta/2} \otimes \mathbb{1}\right) |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}| \left(e^{iH\theta/2} \otimes \mathbb{1}\right) \right]^{\otimes k} \mathrm{d}\theta, \tag{II.9}$$

where $H \in \{X, Y, Z\}$. It satisfies

$$\Omega_H^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0. \tag{II.10}$$

Proof Consider

$$\left(e^{-iZ\theta/2} \otimes \mathbb{1}\right) |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}| \left(e^{iZ\theta/2} \otimes \mathbb{1}\right) = \sum_{j,l=0,1} e^{i\theta(j-l)}|jj\rangle\langle ll|. \tag{II.11}$$

Taking the k-fold tensor product, we get

$$\left[\left(e^{-iZ\theta/2} \otimes \mathbb{1}\right) |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}| \left(e^{iZ\theta/2} \otimes \mathbb{1}\right) \right]^{\otimes k} = \sum_{j_1,l_1,\ldots,j_k,l_k=0,1} e^{i\theta\sum_{\ell=1}^k (j_\ell - l_\ell)}|j_1 j_1 \cdots j_k j_k\rangle\langle l_1 l_1 \cdots l_k l_k|. \tag{II.12}$$

Taking integral over θ from 0 to 2π, we see that

$$\frac{1}{2\pi}\int_0^{2\pi} e^{im\theta} d\theta = \delta_{m,0}. \tag{II.13}$$

Thus, only terms with $\sum_{\ell=1}^k (j_\ell - l_\ell) = 0$ survive and we can rewrite

$$\Omega_Z^{(k)}(\pi) = \sum_{\lambda\in\text{irrep}} \sum_{\mathbf{j}_\lambda\in\mathcal{B}_k(\lambda)} \sum_{\mathbf{k}_\lambda\in\mathcal{B}_k(\lambda)} |\mathbf{j}_\lambda\mathbf{j}_\lambda\rangle\langle\mathbf{k}_\lambda\mathbf{k}_\lambda|, \tag{II.14}$$

where λ runs over the irreducible representations of $\mathrm{U}(1)$: $\lambda(e^{i\theta}) = e^{i\lambda\theta}$ and

$$\mathcal{B}_k(\lambda) \coloneqq \left\{ \mathbf{j}_\lambda \;\middle|\; \mathbf{j}_\lambda \in \{0,1\}^k,\; R_z(\theta)^{\otimes k}|\mathbf{j}_\lambda\rangle = e^{i\lambda\theta}|\mathbf{j}_\lambda\rangle \right\}. \tag{II.15}$$

Here we consider the group action $\mathrm{U}(1) \to \mathrm{GL}((\mathbb{C}^2)^{\otimes 2k})$, $e^{i\theta} \mapsto R_z(\theta)^{\otimes k} \otimes \mathbb{1}^{\otimes k}$. Notably, by direct calculation, there are $k+1$ irreducible representations for k-fold tensor product. Meanwhile, we can also express $|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}$ as

$$|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} = \sum_{\lambda\in\text{irrep}} \sum_{\lambda'\in\text{irrep}} \sum_{\mathbf{j}_\lambda\in\mathcal{B}_k(\lambda)} \sum_{\mathbf{k}_{\lambda'}\in\mathcal{B}_k(\lambda')} |\mathbf{j}_\lambda\mathbf{j}_\lambda\rangle\langle\mathbf{k}_{\lambda'}\mathbf{k}_{\lambda'}|. \tag{II.16}$$

Consider $\max\{t \mid \Omega_Z^{(k)}(\pi) - t \cdot |\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0\}$. We have

$$t = \max_{|v\rangle} \frac{\langle v|\Omega_Z^{(k)}(\pi)|v\rangle}{\langle v|(|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k})|v\rangle}. \tag{II.17}$$

Choose a pure state

$$|v\rangle = \sum_{\lambda\in\text{irrep}} p_\lambda \sum_{\mathbf{j}_\lambda\in\mathcal{B}_k(\lambda)} |\mathbf{j}_\lambda\mathbf{j}_\lambda\rangle, \tag{II.18}$$

where $\sum_\lambda |p_\lambda|^2 = 1$. It follows that

$$\begin{aligned}\langle v|\Omega_Z^{(k)}(\pi)|v\rangle &= \sum_{\lambda\in\text{irrep}} p_\lambda^* d_\lambda \sum_{\mathbf{k}_\lambda\in\mathcal{B}_k(\lambda)} \langle\mathbf{k}_\lambda\mathbf{k}_\lambda| \left(\sum_{\lambda\in\text{irrep}} p_\lambda \sum_{\mathbf{j}_\lambda\in\mathcal{B}_k(\lambda)} |\mathbf{j}_\lambda\mathbf{j}_\lambda\rangle \right) \\ &= \sum_{\lambda\in\text{irrep}} p_\lambda^* p_\lambda d_\lambda^2,\end{aligned} \tag{II.19}$$

where $d_\lambda = |\mathcal{B}_k(\lambda)|$ and

$$\begin{aligned}\langle v|(|\mathbb{1}\rangle\!\rangle\langle\!\langle \mathbb{1}|^{\otimes k})|v\rangle &= \sum_{\lambda\in\text{irrep}} p_\lambda^* d_\lambda \sum_{\lambda'\in\text{irrep}} \sum_{\mathbf{k}_{\lambda'}\in\mathcal{B}_k(\lambda')} \langle \mathbf{k}_{\lambda'}\mathbf{k}_{\lambda'}| \left(\sum_{\lambda\in\text{irrep}} p_\lambda \sum_{\mathbf{j}_\lambda\in\mathcal{B}_k(\lambda)} |\mathbf{j}_\lambda\mathbf{j}_\lambda\rangle\right) \\ &= \sum_{\lambda\in\text{irrep}} p_\lambda^* d_\lambda \sum_{\lambda\in\text{irrep}} p_\lambda d_\lambda.\end{aligned} \tag{II.20}$$

Since $|v\rangle$ is feasible pure state, it follows that

$$t \geq \frac{\sum_\lambda p_\lambda^* p_\lambda d_\lambda^2}{|\sum_\lambda p_\lambda d_\lambda|^2} \geq \frac{\sum_\lambda |p_\lambda|^2 d_\lambda^2}{\sum_\lambda 1\cdot\sum_\lambda |p_\lambda d_\lambda|^2} = \frac{1}{k+1}, \tag{II.21}$$

where we used the Cauchy inequality for the second inequality. Therefore, we have $t \geq \frac{1}{k+1}$ and thus,

$$\Omega_Z^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0. \tag{II.22}$$

Followed by Eq. (II.22), we have for any unitary operator U,

$$(U\otimes\overline{U})^{\otimes k}\Omega_Z^{(k)}(\pi)(U^\dagger\otimes U^T)^{\otimes k} - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0, \tag{II.23}$$

where we used the fact that $|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|$ is invariant under $U\otimes\overline{U}$. Notice that

$$\begin{aligned}&(U\otimes\overline{U})\left(e^{-iZ\theta/2}\otimes\mathbb{1}\right)|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|\left(e^{iZ\theta/2}\otimes\mathbb{1}\right)(U^\dagger\otimes U^T)\\ &= (U\otimes\overline{U})\left(e^{-iZ\theta/2}\otimes\mathbb{1}\right)(U^\dagger\otimes U^T)|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|(U\otimes\overline{U})\left(e^{iZ\theta/2}\otimes\mathbb{1}\right)(U^\dagger\otimes U^T)\\ &= \left(Ue^{-iZ\theta/2}U^\dagger\otimes\mathbb{1}\right)|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|\left(Ue^{iZ\theta/2}U^\dagger\otimes\mathbb{1}\right).\end{aligned} \tag{II.24}$$

By choosing specific U, we can conclude that $\Omega_X^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0$ and $\Omega_Y^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \geq 0$ as well. ■

Lemma S6 *For any even number $k \geq 2$, there exist real Laurent polynomials $F, G \in \mathbb{R}[\omega^{-1}, \omega]$ where $\omega = e^{i\theta/2}$ such that*

1. *$F(1) = G(1) = \frac{1}{\sqrt{2}}$,*
2. *$F(\omega)F(\omega^{-1}) + G(\omega)G(\omega^{-1}) = 1$,*
3. *$F(\omega)G(\omega^{-1}) + F(\omega^{-1})G(\omega) = \frac{1}{k+1}\sum_{l=-k,\, l\text{ even}}^{k}\omega^l$.*

Proof Denote $P(\omega) := F(\omega) + G(\omega)$ and $Q(\omega) := F(\omega) - G(\omega)$. It follows that the above conditions can be equivalently written as

1. $P(1) = \sqrt{2},\ Q(1) = 0$,
2. $P(\omega)P(\omega^{-1}) = 1 + \frac{1}{k+1}\sum_{l=-k,\, l\text{ even}}^{k}\omega^l$,
3. $Q(\omega)Q(\omega^{-1}) = 1 - \frac{1}{k+1}\sum_{l=-k,\, l\text{ even}}^{k}\omega^l$.

Denote

$$\begin{aligned}H(z) &:= 1 + \frac{1}{k+1}\sum_{l=-k,\, l\text{ even}}^{k} z^l = \frac{1}{(k+1)z^k}\prod_{H(\zeta)=0}(z-\zeta),\\ L(z) &:= 1 - \frac{1}{k+1}\sum_{l=-k,\, l\text{ even}}^{k} z^l = -\frac{1}{(k+1)z^k}\prod_{L(\zeta)=0}(z-\zeta).\end{aligned} \tag{II.25}$$

In the following, we will prove the lemma by constructing Laurent polynomials $P, Q \in \mathbb{R}[\omega^{-1}, \omega]$ that satisfy the above three conditions.

First, notice that $\forall z \in \mathbb{C},\ H(z) = H(z^{-1}),\ H(\zeta) = 0 \implies H(\overline{\zeta}) = 0$, and $|z| = 1$ or $z \in \mathbb{R} \implies H(z) \neq 0$. We have

$$H(z) = \frac{1}{(k+1)z^k} \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta})(z-\zeta^{-1})(z-\overline{\zeta}^{-1}). \tag{II.26}$$

Let

$$P(z) = a \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta}) \tag{II.27}$$

$$= a \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z^2 - (\zeta+\overline{\zeta})z + \zeta\overline{\zeta}) \in \mathbb{R}[z, a]. \tag{II.28}$$

It follows that

$$P(z)P(z^{-1}) = a^2 \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta})(z^{-1}-\zeta)(z^{-1}-\overline{\zeta}) \tag{II.29}$$

$$= a^2 \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta})\frac{\zeta\overline{\zeta}}{z^2}(\zeta^{-1}-z)(\overline{\zeta}^{-1}-z) \tag{II.30}$$

$$= \frac{a^2}{z^k} \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} \zeta\overline{\zeta}(z-\zeta)(z-\overline{\zeta})(\zeta^{-1}-z)(\overline{\zeta}^{-1}-z) \tag{II.31}$$

$$= a^2(k+1)H(z) \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} \zeta\overline{\zeta}. \tag{II.32}$$

Then by choosing

$$a = \Big[(k+1) \prod_{H(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} \zeta\overline{\zeta}\Big]^{-1/2} \in \mathbb{R}, \tag{II.33}$$

we have

$$P(z)P(z^{-1}) = H(z) \text{ and } P(z) \in \mathbb{R}[z], \tag{II.34}$$

$H(1) = 2$ and $P(z) = \sqrt{2}$. Second, by calculating

$$\frac{d}{dz}L(z)|_{z=\pm1} = \frac{1}{k+1}\frac{d}{dz}\sum_{l=-k,\, l \text{ even}}^{k} z^l\Big|_{z=\pm1} = \frac{1}{k+1}\sum_{l=-k,\, l \text{ even}}^{k} lz^{l-1}\Big|_{z=\pm1} = \frac{1}{k+1}\sum_{l=-k,\, l \text{ even}}^{k} lz\Big|_{z=\pm1} = 0, \tag{II.35}$$

and

$$\frac{d^2}{dz^2}L(z)|_{z=\pm1} = \frac{1}{k+1}\frac{d^2}{dz^2}\sum_{l=-k,\, l \text{ even}}^{k} z^l|_{z=\pm1} = \frac{1}{k+1}\sum_{l=-k,\, l \text{ even}}^{k} l(l-1)z^{l-2}\Big|_{z=\pm1} = \frac{1}{k+1}\sum_{l=-k,\, l \text{ even}}^{k} l(l-1) > 0, \tag{II.36}$$

we know the zero multiplicity of the polynomial $L(z)$ at $z = \pm1$ is 2. Noticing that $\forall z \in \mathbb{C},\ L(z) = L(z^{-1}),\ L(\zeta) = 0 \implies L(\overline{\zeta}) = 0$, and $(|z| = 1$ or $z \in \mathbb{R}) \implies (L(z) \neq 0$ or $z = \pm1)$, we can rewrite

$$L(z) = -\frac{(z^2-1)^2}{(k+1)z^k} \prod_{L(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta})(z-\zeta^{-1})(z-\overline{\zeta}^{-1}). \tag{II.37}$$

Let

$$\begin{aligned} Q(z) &= b(z^2-1) \prod_{L(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z-\zeta)(z-\overline{\zeta}) \\ &= b(z^2-1) \prod_{L(\zeta)=0, |\zeta|>1, \operatorname{Im}\zeta>0} (z^2 - (\zeta+\overline{\zeta})z + \zeta\overline{\zeta}) \in \mathbb{R}[z, b]. \end{aligned} \tag{II.38}$$

It follows that

$$Q(z)Q(z^{-1}) = b^2(z^2-1)(z^{-2}-1)\prod_{L(\zeta)=0,|\zeta|>1,\operatorname{Im}\zeta>0}(z-\zeta)(z-\overline{\zeta})(z^{-1}-\zeta)(z^{-1}-\overline{\zeta}) \tag{II.39}$$

$$= -\frac{b^2(z^2-1)^2}{z^2}\prod_{L(\zeta)=0,|\zeta|>1,\operatorname{Im}\zeta>0}(z-\zeta)(z-\overline{\zeta})\frac{\zeta\overline{\zeta}}{z^2}(\zeta^{-1}-z)(\overline{\zeta}^{-1}-z) \tag{II.40}$$

$$= -\frac{b^2(z^2-1)^2}{z^k}\prod_{L(\zeta)=0,|\zeta|>1,\operatorname{Im}\zeta>0}\zeta\overline{\zeta}(z-\zeta)(z-\overline{\zeta})(\zeta^{-1}-z)(\overline{\zeta}^{-1}-z) \tag{II.41}$$

$$= b^2(k+1)L(z)\prod_{L(\zeta)=0,|\zeta|>1,\operatorname{Im}\zeta>0}\zeta\overline{\zeta}. \tag{II.42}$$

By choosing

$$b = \pm\Big[(k+1)\prod_{L(\zeta)=0,|\zeta|>1,\operatorname{Im}\zeta>0}\zeta\overline{\zeta}\Big]^{-1/2}\in\mathbb{R}, \tag{II.43}$$

we have

$$Q(z)Q(z^{-1}) = L(z) \text{ and } Q(z)\in\mathbb{R}[z], \tag{II.44}$$

and $Q(1)=0$. Hence, we complete the proof. ■

Now, we are ready to prove Theorem 1.

Theorem 1 (Binary Hamiltonian recognition) *For $H_0 = \vec{n}_0\cdot\vec{\sigma}$ and $H_1 = \vec{n}_1\cdot\vec{\sigma}$ with prior probabilities p and $1-p$, respectively, if $\vec{n}_0\perp\vec{n}_1$, the optimal average success probability of recognizing $\{H_0,H_1\}$ using k queries is given by*

$$\mathrm{Suc}_k^{GEN}(\{H_0,H_1\},\{p,1-p\},\pi) = \frac{k+\max\{p,1-p\}}{k+1}.$$

This limit is globally optimal, holding for all k-query strategies, and is saturated by a sequential protocol without entanglement.

We will first prove the result for $\vec{n}_0 = [1,0,0]$ and $\vec{n}_1 = [0,0,1]$ and reduce the general cases to this one. For $H_0 = X$ and $H_1 = Z$, we are going to show that $\mathrm{Suc}_k^{\mathrm{SEQ}}(\{H_0,H_1\},\{p,1-p\},\pi)\geq(k+\max\{p,1-p\})/(k+1)$ by utilizing the framework of quantum signal processing to construct a protocol for the recognition explicitly; and then prove $\mathrm{Suc}_k^{\mathrm{SEQ}}(\{H_0,H_1\},\{p,1-p\},\pi)\leq(k+\max\{p,1-p\})/(k+1)$ by using the SDP dual formalism of the problem. In the following, the proof is presented for the range $\frac{1}{2}\leq p<1$, with the rationale to be detailed later.

A. Achievability

a. When k is odd. We construct a protocol for recognizing $\{X,Z\}$ as follows. First, we explicitly chose $k+1$ angles $\phi_j, j=0,1,...,k$. Given an unknown unitary $e^{-iH\theta}$, we sequentially apply $e^{iZ\phi_k}e^{iH\theta}e^{iZ\phi_{k-1}}e^{iH\theta}\cdots e^{iZ\phi_1}e^{iH\theta}e^{iZ\phi_0}$ to the zero state. Then we measure the state on a computational basis. If outcome is 0, we decide H is Z; if outcome is 1, we decide H is X. We will explain later how we chose $\vec{\phi}$. It can be seen that the composed unitary is reminiscent of the QSP framework, where U_H is the signal unitary and one has control over the angles $\vec{\phi}$, which are called QSP phase sequences. Therefore, we denote the composed unitary as

$$\mathrm{QSP}_{H,k}(\theta) := R_z(\phi_0)\prod_{j=1}^{k}U_H(\theta)R_z(\phi_j). \tag{II.45}$$

If the unknown unitary is $U_Z(\theta)=e^{-iZ\theta}$, we have

$$\mathrm{QSP}_{Z,k}(\theta/2) = R_z(\phi_0)\prod_{j=1}^{k}R_z(\theta)R_z(\phi_j) = R_z(n\theta+\phi_{:k}), \tag{II.46}$$

where $\phi_{:k} \coloneqq \sum_{j=1}^{k} \phi_j$. It follows that for any chosen parameters $\vec{\phi}$, it always holds that

$$\left|\langle 1|\mathrm{QSP}_{Z,k}(\theta)|0\rangle\right| = 0 \text{ and } \left|\langle 0|\mathrm{QSP}_{Z,k}(\theta)|0\rangle\right| = 1,\ \forall\theta \in [0,\pi]. \tag{II.47}$$

If the unknown unitary is $U_X(\theta) = e^{-iX\theta}$, we have

$$\mathrm{QSP}_{X,k}(\theta/2) = R_z(\phi_0)\prod_{j=1}^{k} R_x(\theta)R_z(\phi_j). \tag{II.48}$$

According to Lemma S3, we can choose a specific $\vec{\phi}$ for our protocol such that

$$\left|\langle 0|\mathrm{QSP}_{X,k}(\theta/2)|0\rangle\right|^2 = \sum_{l=-k}^{k} \frac{k-|l|+1}{(k+1)^2} e^{il\theta}. \tag{II.49}$$

Combining Eq. (II.49) and Eq. (II.47), the average success probability is lower bounded by

$$\begin{aligned}
\mathrm{Suc}_k^{\texttt{SEQ}}(\{X,Z\},\{p,1-p\},\pi) &\geq \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} p\left|\langle 0|\mathrm{QSP}_{Z,k}(\theta_0/2)|0\rangle\right|^2 + (1-p)\left|\langle 1|\mathrm{QSP}_{X,k}(\theta_1/2)|0\rangle\right|^2 \mathrm{d}\theta_0\mathrm{d}\theta_1 \\
&= \frac{1}{2\pi}\int_0^{2\pi} p + (1-p)\Big[\frac{k}{k+1} - \frac{2}{(k+1)^2}\sum_{l=1}^{k}(k-l+1)\cos(l\theta_1)\mathrm{d}\theta_1\Big] \\
&= \frac{k+p}{k+1} - \frac{1}{2\pi}\frac{2(1-p)}{(k+1)^2}\sum_{l=1}^{k}(k-l+1)\int_0^{2\pi}\cos(l\theta_1)\mathrm{d}\theta_1 \\
&= \frac{k+p}{k+1},
\end{aligned} \tag{II.50}$$

where in the second line we used the fact that $\left(e^{il\theta}+e^{-il\theta}\right) = 2\cos(l\theta)$ and

$$1 - \sum_{l=-k}^{k}\frac{k-|l|+1}{(k+1)^2}e^{il\theta} = \frac{k}{k+1} - \frac{2}{(k+1)^2}\sum_{l=1}^{k}(k-l+1)\cos(l\theta). \tag{II.51}$$

Remark 1 For $\frac{1}{2} \leq p < 1$, the average success probability is given by $(k+p)/(k+1)$. In the case where $0 < p < \frac{1}{2}$, the recognition problem exhibits a symmetry under the interchange of X and Z via the Hadamard transformation H, since $HXH = Z$ and $HZH = X$. Consequently, the scenario is equivalent to one with parameter $1-p$, and the average success probability becomes $(k+1-p)/(k+1)$. Subsequent proofs follow from an analogous reasoning.

b. When k is even. Let $k = 2n$, and we construct a similar protocol with a quantum circuit read as

$$\mathrm{QSP}_{H,k}(\theta/2) \coloneqq R_x(\phi_0)\left(\prod_{j=1}^{n} R_H(\theta)R_x(\phi_j)\right) R_z(\pi)R_x(-\phi_n)\left(\prod_{j=n-1}^{0} R_H(\theta)R_x(-\phi_j)\right), \tag{II.52}$$

where we set $\sum_{j=0}^{n}\phi_j = -\pi/2$. Let the input state be the zero state, and measure the output state on a computational basis. If outcome is 0, we decide H is Z; if outcome is 1, we decide H is X.

If the unknown unitary is $U_Z(\theta) = e^{-iZ\theta}$, we have

$$\mathrm{QSP}_{Z,k}(\theta/2) = R_x(\phi_0)\left(\prod_{j=1}^{n} R_z(\theta)R_x(\phi_j)\right) R_z(\pi)R_x(-\phi_n)\left(\prod_{j=n-1}^{0} R_z(\theta)R_x(-\phi_j)\right). \tag{II.53}$$

Noticing the relationship between different types of QSP, we have

$$R_x(\phi_0)\left(\prod_{j=1}^{n} R_z(\theta)R_x(\phi_j)\right) = HR_z(\phi_0)\left(\prod_{j=1}^{n} R_x(\theta)R_x(\phi_j)\right)H = \begin{pmatrix} F(\omega) & iG(\omega) \\ iG(\omega^{-1}) & F(\omega^{-1}) \end{pmatrix}, \tag{II.54}$$

where F, G are real Laurent polynomials $F, G \in R[\omega, \omega^{-1}]$ with parity n mod 2, and $\omega = e^{i\theta/2}$ [4]. Notice that

$$
\begin{aligned}
R_x(-\phi_n)\left(\prod_{j=n-1}^{0} R_z(\theta)R_x(-\phi_j)\right) &= XR_x(-\phi_n)\left(\prod_{j=n-1}^{0} R_z(-\theta)R_x(-\phi_j)\right)X \\
&= X\begin{pmatrix} F(\omega^{-1}) & -iG(\omega) \\ -iG(\omega^{-1}) & F(\omega) \end{pmatrix}X \\
&= \begin{pmatrix} F(\omega) & -iG(\omega^{-1}) \\ -iG(\omega) & F(\omega^{-1}) \end{pmatrix}.
\end{aligned} \tag{II.55}
$$

It follows that

$$
\begin{aligned}
\mathrm{QSP}_{Z,k}(\theta/2) &= \begin{pmatrix} F(\omega) & iG(\omega) \\ iG(\omega^{-1}) & F(\omega^{-1}) \end{pmatrix}\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} F(\omega) & -iG(\omega^{-1}) \\ -iG(\omega) & F(\omega^{-1}) \end{pmatrix} \\
&= -i\begin{pmatrix} F^2(\omega) - G^2(\omega) & -i\Big[F(\omega)G(\omega^{-1}) + F(\omega^{-1})G(\omega)\Big] \\ i\Big[F(\omega)G(\omega^{-1}) + F(\omega^{-1})G(\omega)\Big] & -F^2(\omega^{-1}) + G^2(\omega^{-1}) \end{pmatrix}.
\end{aligned} \tag{II.56}
$$

By Lemma S6, we can construct a QSP phase sequence $\vec{\phi}$ such that

$$
\langle 1|\mathrm{QSP}_{Z,k}(\theta/2)|0\rangle = \frac{1}{k+1}\sum_{l=-k,\, l \text{ even}}^{k} e^{il\theta/2} \tag{II.57}
$$

and thus

$$
\left|\langle 1|\mathrm{QSP}_{Z,k}(\theta/2)|0\rangle\right|^2 = \sum_{l=-k}^{k} \frac{k-|l|+1}{(k+1)^2}e^{il\theta}. \tag{II.58}
$$

If the unknown unitary is $U_X(\theta) = e^{-iX\theta}$, we have

$$
\mathrm{QSP}_{X,k}(\theta/2) \coloneqq R_x(\phi_0)\left(\prod_{j=1}^{n} R_x(\theta)R_x(\phi_j)\right)R_z(\pi)R_x(-\phi_n)\left(\prod_{j=n-1}^{0} R_x(\theta)R_x(-\phi_j)\right). \tag{II.59}
$$

Since we choose $\phi_{:n} \coloneqq \sum_{j=0}^{n}\phi_j = -\pi/2$, we further have

$$
\mathrm{QSP}_{X,k}(\theta/2) = R_x(n\theta + \phi_{:n})R_z(\pi)R_x(n\theta - \phi_{:n}) = \begin{pmatrix} -i\cos\phi_{:n} & \sin\phi_{:n} \\ -\sin\phi_{:n} & i\cos\phi_{:n} \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{II.60}
$$

It follows that $\left|\langle 0|\mathrm{QSP}_{X,k}(\theta/2)|0\rangle\right|^2 = 1$. Combining this with Eq. (II.58), we have

$$
\begin{aligned}
&\mathrm{Suc}_k^{\mathtt{SEQ}}(\{X,Z\},\{p,1-p\},\pi) \\
\geq\, &\frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} p\left|\langle 0|\mathrm{QSP}_{Z,k}(\theta_0/2)|0\rangle\right|^2 + (1-p)\left|\langle 0|\mathrm{QSP}_{X,k}(\theta_1/2)|1\rangle\right|^2 \mathrm{d}\theta_0\mathrm{d}\theta_1 = \frac{k+p}{k+1}.
\end{aligned} \tag{II.61}
$$

Hence, we complete the achievability part.

Remark 2 We remark on the robustness of our QSP-based protocol under depolarizing noise. Suppose in practice, every quantum gate is concatenated with a depolarizing noise $\mathcal{D}_\lambda(\cdot) = (1-\lambda)(\cdot) + \lambda\mathbb{1}/2$. Since the depolarizing channel commutes with unitary gates, which means that applying a unitary gate followed by a depolarizing channel is equivalent to applying the depolarizing channel first. By calculating the average success probability, we have

$$
\mathrm{Suc}_{k,\text{depo}}^{\mathtt{SEQ}}(\{X,Z\},\{p,1-p\},\pi) = \begin{cases} \frac{1}{2} + \frac{1}{2}(1-\lambda)^{2k+1}\cdot\frac{k}{k+1} & \text{when } k \text{ is odd} \\ \frac{1}{2} + \frac{1}{2}(1-\lambda)^{2k+3}\cdot\frac{k}{k+1} & \text{when } k \text{ is even.} \end{cases} \tag{II.62}
$$

B. Optimality

The primal problem for calculating the optimal average success probability of discriminating X and Z over time can be written as

$$\mathrm{Suc}_k^{\text{SEQ}}(\{X,Z\},\{p,1-p\},\pi) = \max_{\{T_0,T_1\}\in\mathcal{T}^{\text{SEQ}}} \operatorname{Tr}\left(pT_0\Omega_X^{(k)}(\pi) + (1-p)T_1\Omega_Z^{(k)}(\pi)\right). \tag{II.63}$$

Recall that Ref. [6] presented a method to obtain a dual problem of the primal problem in Eq. (II.63) based on the characterization of dual affine spaces. The dual problem of Eq. (II.63) can be written as follows, and Slater's condition holds.

$$\begin{aligned} \mathrm{Suc}_k^{\text{SEQ}}(\{X,Z\},\{p,1-p\},\pi) = \min\ & \lambda \\ \text{s.t. }\ & \Omega_X^{(k)}(\pi) \le \frac{1}{p}\lambda\overline{W}, \\ & \Omega_Z^{(k)}(\pi) \le \frac{1}{1-p}\lambda\overline{W}, \\ & \overline{W} \in \overline{\mathcal{W}}^{\text{SEQ}}. \end{aligned} \tag{II.64}$$

For k-slot sequential strategies, the dual affine space $\overline{\mathcal{W}}^{\text{SEQ}}$ is given by the set of Choi operators of $k-1$-slot quantum combs [6]. In the following, we will construct a feasible solution to the above optimization problem as $\lambda_k = \frac{k+p}{k+1}$ and

$$\overline{W}_k = \frac{p(k+1)}{k+p}\Omega_X^{(k)}(\pi) + \frac{(1-p)(k+1)}{k+p}\Omega_Z^{(k)}(\pi) - \frac{(1-p)}{k+p}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}. \tag{II.65}$$

First, by Lemma S5, we have

$$\Omega_X^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \ge 0, \quad \text{and} \quad \Omega_Z^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \ge 0. \tag{II.66}$$

It follows that $\overline{W}_k \ge 0$. Moreover, it is easy to see that $\Omega_X^{(k)}(\pi)$, $\Omega_Z^{(k)}(\pi)$, and $|\Phi\rangle\langle\Phi|^{\otimes k}$ are Choi operators of $k-1$-slot quantum combs. It is then easy to see that $\overline{W}_k$ is the Choi operator of a $k-1$-slot quantum comb and thus, $\overline{W} \in \overline{\mathcal{W}}^{\text{SEQ}}$. Second, since $\frac{1}{2} \le p < 1$, it can be verified that

$$\begin{aligned} &\frac{1}{p}\lambda_k\overline{W}_k - \Omega_X^{(k)}(\pi) = \frac{1-p}{p}\left(\Omega_Z^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}\right) \ge 0, \\ &\frac{1}{1-p}\lambda_k\overline{W}_k - \Omega_Z^{(k)}(\pi) = \frac{p}{1-p}\left(\Omega_X^{(k)}(\pi) - \frac{1}{k+1}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}\right) + \frac{2p-1}{1-p}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k} \ge 0. \end{aligned} \tag{II.67}$$

Therefore, $\{\lambda_0, \overline{W}_k\}$ satisfies all constraints in the SDP (II.64) and is a feasible solution to it. As the SDP (II.64) is a minimization problem, it follows that

$$\mathrm{Suc}_k^{\text{SEQ}}(\{X,Z\},\{p,1-p\},\pi) \le \frac{k+p}{k+1}. \tag{II.68}$$

Combining Eq. (II.50), Eq. (II.61) and Eq. (II.68), we arrive at

$$\mathrm{Suc}_k^{\text{SEQ}}(\{X,Z\},\{p,1-p\},\pi) = \frac{k+p}{k+1}. \tag{II.69}$$

Moreover, we show that general strategies do not offer any advantage for recognizing X, Z. This is because the dual affine space $\overline{\mathcal{W}}^{\text{GEN}}$ of $\mathcal{W}^{\text{GEN}}$, the set of all general strategies that encompasses indefinite causal orders, is given by the set of Choi operators of k-partite non-signaling channels without the positivity constraint [6]:

$$\begin{aligned} {}_{O_1}\overline{W}^{\text{GEN}} &= {}_{I_1O_1}\overline{W}^{\text{GEN}}, \\ {}_{O_2}\overline{W}^{\text{GEN}} &= {}_{I_2O_2}\overline{W}^{\text{GEN}}, \\ &\cdots \\ {}_{O_k}\overline{W}^{\text{GEN}} &= {}_{I_kO_k}\overline{W}^{\text{GEN}}, \\ \operatorname{Tr}\overline{W}^{\text{GEN}} &= d_{I_1}d_{I_2}\cdots d_{I_k}. \end{aligned} \tag{II.70}$$

It can be checked that $\Omega_X^{(k)}(\pi), \Omega_Z^{(k)}(\pi)$ and $|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}$ all satisfy the above conditions, implying that $\overline{W}_k$ also satisfies these conditions. Consequently, $\overline{W}_k$ is a feasible solution for the following SDP for recognizing $\{X, Z\}$ with general strategies.

$$\begin{aligned} \mathrm{Suc}_k^{\mathrm{GEN}}\left(\{X,Z\},\{p,1-p\},\pi\right) = \min\ & \lambda \\ \text{s.t. }\ & \Omega_X^{(k)}(\pi) \leq \frac{1}{p}\lambda\overline{W}, \\ & \Omega_Z^{(k)}(\pi) \leq \frac{1}{1-p}\lambda\overline{W}, \\ & \overline{W} \in \overline{\mathcal{W}}^{\mathrm{GEN}}. \end{aligned} \tag{II.71}$$

It follows $\mathrm{Suc}_k^{\mathrm{GEN}}\left(\{X,Z\},\{p,1-p\},\pi\right) \leq \frac{k+p}{k+1}$. Since $\mathrm{Suc}_k^{\mathrm{GEN}}\left(\{X,Z\},\{p,1-p\},\pi\right) \geq \mathrm{Suc}_k^{\mathrm{SEQ}}\left(\{X,Z\},\{p,1-p\},\pi\right)$ by definition, we conclude that $\mathrm{Suc}_k^{\mathrm{GEN}}\left(\{X,Z\},\{p,1-p\},\pi\right) = \frac{k+p}{k+1}$.

Now we consider the case for general $\vec{n}_0$ and $\vec{n}_1$. Since $\vec{n}_0 \cdot \vec{n}_1 = 0$, we can construct a third orthonormal real vector $\vec{n}_2$ that is orthogonal to $\vec{n}_0$ and $\vec{n}_1$. Consider a rotation matrix $R \in \mathrm{SO}(3)$

$$R = \begin{pmatrix} h_{0x} & h_{2x} & h_{1x} \\ h_{0y} & h_{2y} & h_{1y} \\ h_{0z} & h_{2z} & h_{1z} \end{pmatrix}. \tag{II.72}$$

Note there is a correspondence between rotation matrices in $\mathrm{SO}(3)$ and unitary operators in $\mathrm{SU}(2)$. Specifically, for every rotation matrix R, there exists a unitary operator U such that

$$U(\vec{n}\cdot\vec{\sigma})U^\dagger = (R\vec{n})\cdot\vec{\sigma},\ \forall \vec{n}\in\mathbb{R}^3. \tag{II.73}$$

Therefore, we have $UH_0U^\dagger = U(\vec{n}_0\cdot\vec{\sigma})U^\dagger = [1,0,0]\cdot\vec{\sigma} = X$, and $UH_1U^\dagger = U(\vec{n}_1\cdot\vec{\sigma})U^\dagger = [0,0,1]\cdot\vec{\sigma} = Z$. It follows that

$$\widetilde{U}_0 = Ue^{-i\theta(\vec{n}_0\cdot\vec{\sigma})}U^\dagger = e^{-i\theta U(\vec{n}_0\cdot\vec{\sigma})U^\dagger} = e^{-i\theta X}, \tag{II.74}$$

and

$$\widetilde{U}_1 = Ue^{-i\theta(\vec{n}_2\cdot\vec{\sigma})}U^\dagger = e^{-i\theta U(\vec{n}_1\cdot\vec{\sigma})U^\dagger} = e^{-i\theta Z}. \tag{II.75}$$

After pre-processing the unknown evolution and applying the protocol for $\{X, Z\}$, we complete the proof.

Remark 3 Second, we note that the variance of the recognition success probability can be calculated as

$$\begin{aligned} & \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi}\left[p\left|\langle 0|\mathrm{QSP}_{Z,k}(\theta_0/2)|0\rangle\right|^2 + (1-p)\left|\langle 1|\mathrm{QSP}_{X,k}(\theta_1/2)|1\rangle\right|^2 - \frac{k+p}{k+1}\right]^2 \mathrm{d}\theta_0\mathrm{d}\theta_1 \\ =\ & \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi}\left[p + \frac{(1-p)k}{k+1} - \frac{2(1-p)}{(k+1)^2}\sum_{l=1}^k (k-l+1)\cos(l\theta_1) - \frac{k+p}{k+1}\right]^2 \mathrm{d}\theta_0\mathrm{d}\theta_1 \\ =\ & \frac{1}{2\pi}\int_0^{2\pi}\left[-\frac{2(1-p)}{(k+1)^2}\sum_{l=1}^k (k-l+1)\cos(l\theta_1)\right]^2 \mathrm{d}\theta_1 \\ =\ & \frac{1}{2\pi}\frac{2(1-p)}{(k+1)^4}\sum_{i=1}^k\sum_{j=1}^k \frac{(k-i+1)(k-j+1)}{2}\int_0^{2\pi}\left[\cos\Big((i+j)\theta_1\Big) + \cos\Big((i-j)\theta_1\Big)\right]\mathrm{d}\theta_1 \\ =\ & \frac{k(2k+1)(1-p)}{6(k+1)^3}, \end{aligned} \tag{II.76}$$

where for $(\sum_{l=1}^k (k-l+1)\cos(l\theta_1))^2$, we have

$$\Big(\sum_{l=1}^k (k-l+1)\cos(l\theta_1)\Big)^2 = \sum_{i=1}^k\sum_{j=1}^k \frac{(k-i+1)(k-j+1)}{2}\left[\cos\Big((i+j)\theta_1\Big) + \cos\Big((i-j)\theta_1\Big)\right]. \tag{II.77}$$

We see that the variance of the recognition success probability vanishes very quickly with the increasing number of queries to the unknown unitary.

III. PROOF OF THEOREM 3

Theorem 3 (Ternary Hamiltonian recognition) *For $H_0 = \vec{n}_0 \cdot \vec{\sigma}$, $H_1 = \vec{n}_1 \cdot \vec{\sigma}$ and $H_2 = \vec{n}_2 \cdot \vec{\sigma}$ with prior probabilities p_0, p_1, p_2, respectively, where $p_0 + p_1 + p_2 = 1$, if $\vec{n}_0 \perp \vec{n}_1 \perp \vec{n}_2$, the optimal average success probability of recognizing $\{H_0, H_1, H_2\}$ via a k-slot sequential strategy, where k is odd, is given by*

$$\mathrm{Suc}_k^{SEQ}\left(\{H_i\}_{i=0}^2, \{p_i\}_{i=0}^2, \pi\right) = \frac{k + \max\{p_0, p_1, p_2\}}{k+1}. \tag{III.1}$$

In the following, the proof is presented for the range $p_2 \geq p_1 \geq p_0$ as well.

A. Achievability

We will first prove the case $H_0 = X, H_1 = Y, H_2 = Z$. The main idea is to coherently use the protocols given in Theorem 1 for recognizing $\{X, Y\}$ and $\{Y, Z\}$. Recall that by Theorem 1, there exists a QSP phase sequence $\vec{\phi}_x = (\phi_{x,0}, \phi_{x,1}, \cdots, \phi_{x,k})$ such that one can use the following QSP circuit to recognize $\{X, Z\}$

$$\mathrm{QSP}_{H,k}^{\{X,Z\}}(\theta) = R_z(\phi_{x,0}) \prod_{j=1}^{k} U_H(\theta) R_z(\phi_{x,j}), \tag{III.2}$$

where $U_H(\theta) = e^{-iH\theta/2}$ is an unknown unitary operation with $H \in \{X, Z\}$. After applying $\mathrm{QSP}_{H,k}^{\{X,Z\}}(\theta)$ on $|0\rangle$ and measuring the output state in the computational basis, we decide $H = X$ if the outcome is '1'. Theorem 1 ensures that this protocol has a success probability $\frac{2k+1}{2k+2}$ by querying the unknown unitary k times. In specific, by Theorem 1, we have

$$\mathrm{QSP}_{X,k}^{\{X,Z\}}(\theta/2) = \begin{pmatrix} P_{x,k}(\theta) & -Q_{x,k}^*(\theta) \\ Q_{x,k}(\theta) & P_{x,k}^*(\theta) \end{pmatrix}, \tag{III.3}$$

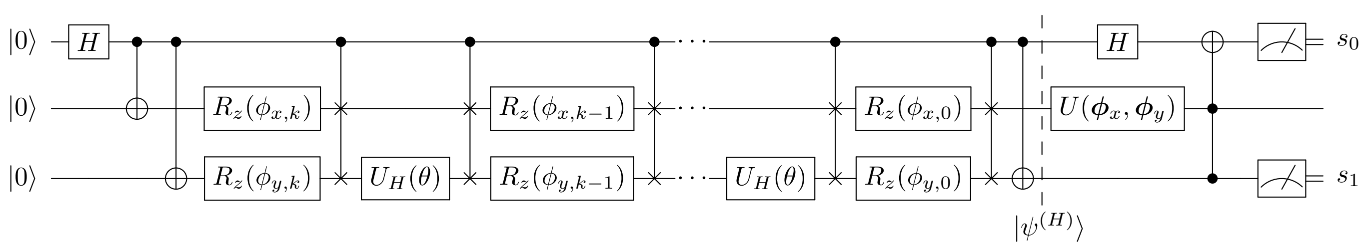
with

$$\int_0^{2\pi} |Q_{x,k}(\theta)|^2 \mathrm{d}\theta = \frac{k}{k+1} \tag{III.4}$$

as the average success probability of recognizing X. Similarly, there exists a QSP phase sequence $\vec{\phi}_y = (\phi_{y,0}, \phi_{y,1}, \cdots, \phi_{y,k})$ such that

$$\mathrm{QSP}_{H,k}^{\{Y,Z\}}(\theta) = R_z(\phi_{y,0}) \prod_{j=1}^{k} U_H(\theta) R_z(\phi_{y,j}). \tag{III.5}$$

This QSP circuit can be used to optimally sense Y and Z, and we have $\mathrm{QSP}_{Y,k}^{\{Y,Z\}}(\theta)|0\rangle = P_{y,k}(\theta)|0\rangle + Q_{y,k}(\theta)|1\rangle$. In particular, we could set $Q_{y,k}(\theta) = iQ_{x,k}^*(\theta)$. Based on the above, we construct a protocol for recognizing $\{X, Y, Z\}$. The quantum circuit of the protocol is given as follows.



Here the angles for rotation gates in the second qubit are $\vec{\phi}_x = (\phi_{x,0}, \phi_{x,1}, \cdots, \phi_{x,k})$ and the angles for rotation gates in the third qubit are $\vec{\phi}_y = (\phi_{y,0}, \phi_{y,1}, \cdots, \phi_{y,k})$. Denote $\boldsymbol{\phi}_l = \sum_j \phi_{l,j}$, $l \in \{x, y\}$. The gate $U(\boldsymbol{\phi}_x, \boldsymbol{\phi}_y)$ has a matrix form

$$U(\boldsymbol{\phi}_x, \boldsymbol{\phi}_y) = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{i\boldsymbol{\phi}_y/2} & \frac{1}{\sqrt{2}} e^{-i\boldsymbol{\phi}_x/2} \\ \frac{1}{\sqrt{2}} e^{i\boldsymbol{\phi}_x/2} & -\frac{1}{\sqrt{2}} e^{-i\boldsymbol{\phi}_y/2} \end{pmatrix}. \tag{III.6}$$

Then the protocol is as follows.

1. Input a zero state $|000\rangle$ and apply the unitary operations.
2. Measure the first and third qubits to obtain a measurement outcome $s = s_0 s_1$.
   - If $s = 00$ or 10, decide the Hamiltonian is Z;
   - If $s = 01$, decide the Hamiltonian is Y;
   - If $s = 11$, decide the Hamiltonian is X.

In the following, we analyze the specific average success probability of recognizing different unknown Hamiltonians using this protocol. For convenience, we denote the state after the CNOT gate as

$$
\begin{aligned}
|\psi^{(H)}\rangle &= \frac{1}{\sqrt{2}}\left(|0\rangle \otimes R_z(\phi_x)|0\rangle \otimes \mathrm{QSP}_{H,k}^{\{Y,Z\}}(\theta)|0\rangle + |1\rangle \otimes R_z(\phi_y)|1\rangle \otimes X \cdot \mathrm{QSP}_{H,k}^{\{X,Z\}}(\theta)|1\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left(e^{-i\phi_x/2}|00\rangle \otimes \mathrm{QSP}_{H,k}^{\{Y,Z\}}(\theta)|0\rangle + e^{i\phi_y/2}|11\rangle \otimes X \cdot \mathrm{QSP}_{H,k}^{\{X,Z\}}(\theta)|1\rangle\right),
\end{aligned}
\tag{III.7}
$$

and notice that all gates after the CNOT gate will not affect the third qubit.

<u>If $U_H(\theta) = e^{-iZ\theta}$</u>, we have

$$
|\psi^{(H)}\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\phi_x/2}|00\rangle \otimes R_z(\phi_y+\theta)|0\rangle + e^{i\phi_y/2}|11\rangle \otimes R_z(\phi_x+\theta)|0\rangle\right). \tag{III.8}
$$

Measuring the third qubit at the end will obtain the outcome '0' regardless of what θ is. Thus, the average success probability in this case is given by $\Pr(s_1 = 0|H = Z) = 1$.

<u>If $U_H(\theta) = e^{-iX\theta}$</u>, we have

$$
\begin{aligned}
|\psi^{(X)}\rangle &= \frac{1}{\sqrt{2}}\left(e^{-i\phi_x/2}|00\rangle \otimes \mathrm{QSP}_{X,k}^{\{Y,Z\}}(\theta)|0\rangle + e^{i\phi_y/2}|11\rangle \otimes X \cdot \mathrm{QSP}_{X,k}^{\{X,Z\}}(\theta)|1\rangle\right) \\
&= \frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle \otimes \left(P_{y,k}(\theta)|0\rangle - iQ_{y,k}(\theta)|1\rangle\right) + \frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle \otimes \left(P_{x,k}^*(\theta)|0\rangle - Q_{x,k}^*(\theta)|1\rangle\right) \\
&= \left(P_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle + P_{x,k}^*(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |0\rangle \\
&\quad + \left(-iQ_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle - Q_{x,k}^*(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |1\rangle,
\end{aligned}
\tag{III.9}
$$

where in the second equality we used the fact that $R_x(\theta) = R_z(-\pi/2)R_y(\theta)R_z(\pi/2), \forall\theta \in [0, 2\pi]$, and thus

$$
\begin{aligned}
\mathrm{QSP}_{X,k}^{\{Y,Z\}}(\theta/2)|0\rangle &= R_z\left(-\frac{\pi}{2}\right)\mathrm{QSP}_{Y,k}^{\{Y,Z\}}(\theta/2)R_z\left(\frac{\pi}{2}\right)|0\rangle \\
&= P_{y,k}(\theta)|0\rangle + e^{-i\pi/2}Q_{y,k}(\theta)|1\rangle = P_{y,k}(\theta)|0\rangle - iQ_{y,k}(\theta)|1\rangle.
\end{aligned}
\tag{III.10}
$$

It can be seen that if a unitary $e^{-iX\theta}$ is inserted into a QSP circuit QSP_H^Y, compared with inserting a unitary $e^{-iY\theta}$, a relative phase $-i$ will be accumulated. Since we determine $H = X$ if the outcome on the first and third qubit is '11' and all gates after the CNOT gate will not affect the third qubit, now we could only consider the case where the third qubit outcome is in $|1\rangle$. Followed by Eq. (III.9), applying post-selection and the rest of gates gives

$$
\left(\mathbb{1}^{\otimes 2} \otimes |1\rangle\langle 1|\right)|\psi^{(X)}\rangle \tag{III.11}
$$

$$
= \left(-iQ_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle - Q_{x,k}^*(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |1\rangle \tag{III.12}
$$

$$
\xrightarrow{H} Q_{x,k}^*(\theta)\left[|0\rangle \otimes \left(\frac{e^{-i\phi_x/2}}{2}|0\rangle - \frac{e^{i\phi_y/2}}{2}|1\rangle\right) \otimes |1\rangle + |1\rangle \otimes \left(\frac{e^{-i\phi_x/2}}{2}|0\rangle + \frac{e^{i\phi_y/2}}{2}|1\rangle\right) \otimes |1\rangle\right] \tag{III.13}
$$

$$
\xrightarrow{U(\phi_x,\phi_y)} Q_{x,k}^*(\theta)\left(\frac{1}{\sqrt{2}}|011\rangle + \frac{e^{-i(\phi_x-\phi_y)/2}}{\sqrt{2}}|101\rangle\right) \tag{III.14}
$$

$$
\xrightarrow{\text{Toffoli}} Q_{x,k}^*(\theta)\left(|1\rangle \otimes \frac{1}{\sqrt{2}}\left(|1\rangle + e^{-i(\phi_x-\phi_y)/2}|0\rangle\right) \otimes |1\rangle\right), \tag{III.15}
$$

where in Eq. (III.13) we used $Q_{y,k}(\theta) = iQ^*_{x,k}(\theta)$, and in Eq. (III.14) we used

$$U(\phi_x, \phi_y)\left(\frac{e^{-i\phi_x/2}}{2}|0\rangle - \frac{e^{i\phi_y/2}}{2}|1\rangle\right) = \frac{1}{\sqrt{2}}|1\rangle, \tag{III.16}$$

and

$$U(\phi_x, \phi_y)\left(\frac{e^{-i\phi_x/2}}{2}|0\rangle + \frac{e^{i\phi_y/2}}{2}|1\rangle\right) = \frac{e^{-i(\phi_x-\phi_y)/2}}{\sqrt{2}}|0\rangle. \tag{III.17}$$

Therefore, the average probability of getting outcome '11' in the first and third qubits when asserting $e^{-iX\theta/2}$ is determined by

$$\Pr(s = 11|H = X) = \int_0^{2\pi} |Q^*_{x,k}(\theta)|^2 \mathrm{d}\theta = \frac{k}{k+1}. \tag{III.18}$$

When $U_H(\theta) = e^{-iY\theta}$, we have

$$\begin{aligned}
|\psi^{(Y)}\rangle &= \frac{1}{\sqrt{2}}\Big(e^{-i\phi_x/2}|00\rangle \otimes \mathrm{QSP}^{\{Y,Z\}}_{Y,k}(\theta/2)|0\rangle + e^{i\phi_y/2}|11\rangle \otimes X \cdot \mathrm{QSP}^{\{X,Z\}}_{Y,k}(\theta/2)|1\rangle\Big) \\
&= \frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle \otimes \big(P_{y,k}(\theta)|0\rangle + Q_{y,k}(\theta)|1\rangle\big) + \frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle \otimes \big(P^*_{x,k}(\theta)|0\rangle + iQ^*_{x,k}(\theta)|1\rangle\big) \\
&= \left(P_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle + P^*_{x,k}(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |0\rangle \\
&\quad + \left(Q_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle + iQ^*_{x,k}(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |1\rangle,
\end{aligned} \tag{III.19}$$

where in the second equality we used the fact that $R_y(\theta) = R_z(\pi/2)R_x(\theta)R_z(-\pi/2), \forall\theta \in [0, 2\pi]$, and thus

$$\begin{aligned}
\mathrm{QSP}^{\{X,Z\}}_{Y,k}(\theta/2)|1\rangle &= R_z\left(\frac{\pi}{2}\right)\mathrm{QSP}^{\{X,Z\}}_{X,k}(\theta/2)R_z\left(-\frac{\pi}{2}\right)|1\rangle \\
&= -e^{-i\pi/2}Q^*_{x,k}(\theta)|0\rangle + P^*_{x,k}(\theta)|1\rangle = iQ^*_{x,k}(\theta)|0\rangle + P^*_{x,k}(\theta)|1\rangle.
\end{aligned} \tag{III.20}$$

Similarly to the previous one, consider the case where the third qubit is in $|1\rangle$.

$$\big(\mathbb{1}^{\otimes 2} \otimes |1\rangle\langle 1|\big)\,|\psi^{(Y)}\rangle \tag{III.21}$$

$$= \left(Q_{y,k}(\theta)\frac{e^{-i\phi_x/2}}{\sqrt{2}}|00\rangle + iQ^*_{x,k}(\theta)\frac{e^{i\phi_y/2}}{\sqrt{2}}|11\rangle\right) \otimes |1\rangle \tag{III.22}$$

$$\xrightarrow{H} iQ^*_{x,k}(\theta)\left[|0\rangle \otimes \left(\frac{e^{-i\phi_x/2}}{2}|0\rangle + \frac{e^{i\phi_y/2}}{2}|1\rangle\right) \otimes |1\rangle + |1\rangle \otimes \left(\frac{e^{-i\phi_x/2}}{2}|0\rangle - \frac{e^{i\phi_y/2}}{2}|1\rangle\right) \otimes |1\rangle\right] \tag{III.23}$$

$$\xrightarrow{U(\phi_x,\phi_y)} iQ^*_{x,k}(\theta)\left(\frac{e^{-i(\phi_x-\phi_y)/2}}{\sqrt{2}}|001\rangle + \frac{1}{\sqrt{2}}|111\rangle\right) \tag{III.24}$$

$$\xrightarrow{\text{Toffoli}} iQ^*_{x,k}(\theta)\left(|0\rangle \otimes \frac{1}{\sqrt{2}}\left(e^{-i(\phi_x-\phi_y)/2}|0\rangle + |1\rangle\right) \otimes |1\rangle\right), \tag{III.25}$$

where we used $-iQ_{y,k}(\theta) = Q^*_{x,k}(\theta)$ in Eq. (III.13). Therefore, the average probability of getting outcome '01' in the first and third qubits when asserting $e^{-iY\theta}$ is given by

$$\Pr(s = 01|H = Y) = \int_0^{2\pi} |iQ^*_{x,k}(\theta)|^2 \mathrm{d}\theta = \frac{k}{k+1}. \tag{III.26}$$

Combining the above three cases, we have the overall average success probability that satisfies

$$\begin{aligned}
\mathrm{Suc}^{\mathtt{SEQ}}_k\big(\{H_0, H_1, H_2\}, \{p_0, p_1, p_2\}, \pi\big) &\geq p_2 \Pr(s_1 = 0|H = Z) + p_0 \Pr(s = 11|H = X) + p_1 \Pr(s = 01|H = Y) \\
&= p_2 + \frac{(p_0 + p_1)k}{k+1} = \frac{k + p_2}{k+1}.
\end{aligned} \tag{III.27}$$

B. Optimality

Similar to the case of binary Hamiltonian recognition, the optimal average success probability can be written as the following SDP problem.

$$\mathrm{Suc}_k^{\mathrm{SEQ}}\left(\{H_0,H_1,H_2\},\{p_0,p_1,p_2\},\pi\right)=\max_{\substack{\{T_0,T_1,T_2\}\in\mathcal{T}^{\mathrm{SEQ}}\\ p_2\geq p_1\geq p_0}}\operatorname{Tr}\left(p_0T_0\Omega_X^{(k)}(\pi)+p_1T_1\Omega_Y^{(k)}(\pi)+p_2T_2\Omega_Z^{(k)}(\pi)\right).\tag{III.28}$$

And the dual problem of Eq. (III.28) can be written as follows.

$$\begin{aligned}\mathrm{Suc}_k^{\mathrm{SEQ}}\left(\{H_0,H_1,H_2\},\{p_0,p_1,p_2\},\pi\right)=\min\ &\lambda\\ \text{s.t. }\ &\Omega_X^{(k)}(\pi)\leq\frac{1}{p_0}\lambda\overline{W},\\ &\Omega_Y^{(k)}(\pi)\leq\frac{1}{p_1}\lambda\overline{W},\\ &\Omega_Z^{(k)}(\pi)\leq\frac{1}{p_2}\lambda\overline{W},\\ &\overline{W}\in\overline{\mathcal{W}}^{\mathrm{SEQ}}.\end{aligned}\tag{III.29}$$

In the following, we will construct a feasible solution to the above optimization problem as $\lambda_k=\frac{k+p_2}{k+1}$ and

$$\overline{W}_k=\frac{p_0(1+k)}{k+p_2}\Omega_X^{(k)}(\pi)+\frac{p_1(1+k)}{k+p_2}\Omega_Y^{(k)}(\pi)+\frac{p_2(1+k)}{k+p_2}\Omega_Z^{(k)}(\pi)-\frac{(p_0+p_1)}{k+p_2}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}.\tag{III.30}$$

By Lemma S5, we have $\overline{W}_k\geq 0$. It is easy to see that $\Omega_X^{(k)}(\pi)$, $\Omega_Z^{(k)}(\pi)$, and $|\mathbb{1}\rangle\!\langle\mathbb{1}|^{\otimes k}$ are Choi operators of $k-1$-slot quantum combs. Therefore, $\overline{W}_k$ is also the Choi operator of a $k-1$-slot quantum comb, thus $\overline{W}_k\in\overline{\mathcal{W}}^{\mathrm{SEQ}}$. Moreover, by Lemma S5, we have

$$\begin{aligned}\frac{1}{p_0}\lambda_k\overline{W}_k-\Omega_X^{(k)}(\pi)&=\frac{p_1}{p_0}\Omega_Y^{(k)}(\pi)+\frac{p_2}{p_0}\Omega_Z^{(k)}(\pi)-\frac{(p_0+p_1)}{p0(k+1)}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}\geq 0,\\ \frac{1}{p_1}\lambda_k\overline{W}_k-\Omega_Y^{(k)}(\pi)&=\frac{p_0}{p_1}\Omega_X^{(k)}(\pi)+\frac{p_2}{p_1}\Omega_Z^{(k)}(\pi)-\frac{(p_0+p_1)}{p1(k+1)}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}\geq 0,\\ \frac{1}{p_2}\lambda_k\overline{W}_k-\Omega_Z^{(k)}(\pi)&=\frac{p_0}{p_2}\Omega_X^{(k)}(\pi)+\frac{p_1}{p_2}\Omega_Y^{(k)}(\pi)-\frac{(p_0+p_1)}{p2(k+1)}|\mathbb{1}\rangle\!\rangle\langle\!\langle\mathbb{1}|^{\otimes k}\geq 0.\end{aligned}\tag{III.31}$$

It follows that $\{\lambda_k,\overline{W}_k\}$ satisfies all constraints in the SDP (III.29) and is a feasible solution to it. Therefore, we have

$$\mathrm{Suc}_k^{\mathrm{SEQ}}\left(\{H_0,H_1,H_2\},\{p_0,p_1,p_2\},\pi\right)\leq\frac{k+p_2}{k+1}.\tag{III.32}$$

Combining Eq. (III.27) and Eq. (III.32), we arrive at

$$\mathrm{Suc}_k^{\mathrm{SEQ}}\left(\{H_0,H_1,H_2\},\{p_0,p_1,p_2\},\pi\right)=\frac{k+p_2}{k+1}.\tag{III.33}$$

Using the same argument in Theorem 1, and considering a rotation matrix in Eq. (II.72), we know that the above result holds for any $H_0=\vec{n}_0\cdot\vec{\sigma},\ H_1=\vec{n}_1\cdot\vec{\sigma}$ and $H_2=\vec{n}_2\cdot\vec{\sigma}$ such that $\vec{n}_0\perp\vec{n}_1\perp\vec{n}_2$. Hence, we complete the proof.

Remark 4 We would like to emphasize that during the proof, we have constructed two QSP phase sequences for recognizing Hamiltonian pairs $\{X,Z\}$ and $\{Y,Z\}$, respectively. However, it is noteworthy that every QSP phase sequence that can sense $\{X,Z\}$ can also sense $\{Y,Z\}$, but we could not use the same QSP in our circuit structure. The reason is as follows: if $\mathrm{QSP}_{H,k}^{\{Y,Z\}}(\theta/2)=\mathrm{QSP}_{H,k}^{\{X,Z\}}(\theta/2)$, followed by Eq. (III.10), we have $P_{y,k}(\theta)=P_{x,k}(\theta),-iQ_{y,k}(\theta)=Q_{x,k}(\theta)$. Thus, the state in Eq. (III.13) can be written as

$$|0\rangle\otimes\left(Q_{x,k}(\theta)\frac{e^{-i\phi_x/2}}{2}|0\rangle-Q_{x,k}^*(\theta)\frac{e^{i\phi_y/2}}{2}|1\rangle\right)\otimes|1\rangle+|1\rangle\otimes\left(Q_{x,k}(\theta)\frac{e^{-i\phi_x/2}}{2}|0\rangle+Q_{x,k}^*(\theta)\frac{e^{i\phi_y/2}}{2}|1\rangle\right)\otimes|1\rangle.\tag{III.34}$$

Notice that we can not extract the same phase for the above state to allow the intermediate state to go to $|0\rangle$ or $|1\rangle$.

Remark 5 Similar to the binary case, general strategies do not offer any advantage in recognizing $\{X,Y,Z\}$.

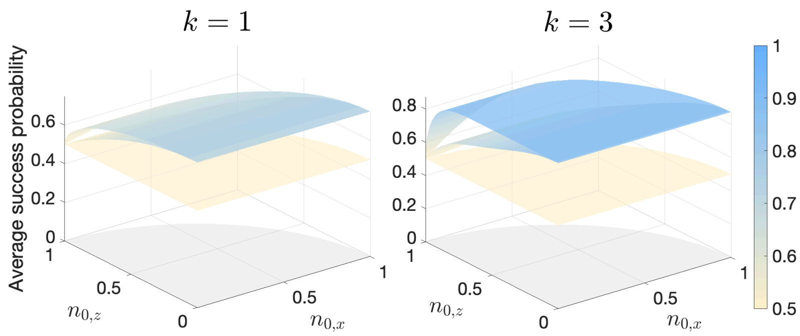


Fig S1. Average success probability of recognizing $\{H_0, Z\}$.

IV. EXPERIMENTS ON A SUPERCONDUCTING QUANTUM COMPUTER

The QPU device is a surface-13 tunable coupling superconducting quantum processor [7]. For the processor, the median single-qubit gate fidelity shows a tiny decrease from about 99.95% for the isolated Randomized Benchmarking to 99.94% for the simultaneous one. First, we uniformly sample 64 values of θ_j from $(0, \pi]$ to construct two sets of gates, $\{e^{-iX\theta_j}\}_{j=1}^k$ and $\{e^{-iZ\theta_j}\}_{j=1}^k$, corresponding to the Hamiltonians X and Z, respectively. For each gate, as a given unknown unitary, we repeat Algorithm 1 512 times and record our predictions.

Algorithm 1: Hamiltonian recognition for $\{X, Z\}$

Input : k copies of an evolution dynamic $U_H(\theta) = e^{-iH\theta}$, where k is odd, $t \in \mathbb{R}$ is unknown and H is an unknown Hamiltonian from a known set $\{X, Z\}$.

Output: a guess of H from $\{X, Z\}$.

1 Determine the vector of angles $\vec{\phi} = \phi_0, \ldots, \phi_k$ such that

$$\langle 0| R_z(\phi_0) \prod_{j=1}^{k} W_x(a) R_z(\phi_j) |0\rangle = \frac{2}{k+1} \sum_{l=1,\, l \text{ odd}}^{k} T_l(a). \tag{IV.1}$$

This can be achieved following the implementation of Theorem 3-5 in [5];

2 Construct the single-qubit circuit as follows:

$$\mathrm{QSP}_{H,k}(\theta) = R_z(\phi_0) \prod_{j=1}^{k} U_H(\theta) R_z(\phi_j). \tag{IV.2}$$

3 Input the zero state $|0\rangle$, run the circuit, and perform a computational basis measurement at the end;

4 If the measurement outcome is 0, return $H = Z$; Otherwise return $H = X$.

V. GENERAL AXIS DIRECTIONS

Now we consider a more general scenario where $\vec{n}_0$ and $\vec{n}_1$ are not orthogonal for $H_0 = \vec{n}_0 \cdot \vec{\sigma}$ and $H_1 = \vec{n}_1 \cdot \vec{\sigma}$. Without loss of generality, we set $H_1 = Z$. Since $\vec{n}_0 := (n_{0,x}, n_{0,y}, n_{0,z})$ is a unit vector, we can find a unitary U that diagonalize H_0 such that $UH_0U^\dagger = Z$. Therefore, for fixed k and $\vec{n}_0$, we could obtain $\Omega_{H_0}^{(k)}(\pi) = (U \otimes U^*) \Omega_Z^{(k)}(\pi) (U^\dagger \otimes U^T)$. Further, we numerically solve SDP

$$\begin{aligned} \mathrm{Suc}_k^{\mathrm{SEQ}}\big(\{H_0, Z\}, \pi\big) = \min\ & \lambda \\ \text{s.t.}\ & \Omega_{H_0}^{(k)}(\pi) \leq 2\lambda \overline{W}, \\ & \Omega_Z^{(k)}(\pi) \leq 2\lambda \overline{W}, \\ & \overline{W} \in \overline{\mathcal{W}}^{\mathrm{SEQ}}. \end{aligned} \tag{V.1}$$

to estimate $\mathrm{Suc}_k^{\mathrm{SEQ}}\left(\big\{H_0, Z\big\}, \pi\right)$ for varying $n_{0,x}$ and $n_{0,z}$.

We illustrate the average success probability of recognizing $\{H_0, Z\}$ in Fig. S1, for the cases of $k = 1$ and $k = 3$. In each subplot, the top layer represents the average success probability corresponding to the optimal protocol obtained by solving the SDP; the middle layer depicts the average success probability given by the protocol in Theorem 1 specifically designed for $\{X, Z\}$, and the bottom layer shows the performance of random guessing. It can be observed that within a certain range, the $\{X, Z\}$ protocol performs well. As the number of slots increases, the optimal protocol exhibits high accuracy over a larger range.

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