Szegedy Walk Unitaries for Quantum Maps

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Abstract: Szegedy developed a generic method for quantizing classical algorithms based on random walks (Szegedy, in: 45th annual IEEE Symposium on Foundations of Computer Science, pp 32–41, 2004. https://doi.org/10.1109/FOCS.2004.53). A major contribution of his work was the construction of a walk unitary for any reversible random walk. Such unitary posses two crucial properties: its eigenvector with eigenphase 0 is a quantum sample of the limiting distribution of the random walk and its eigenphase gap is quadratically larger than the spectral gap of the random walk. It was an open question if it is possible to generalize Szegedy’s quantization method for stochastic maps to quantum maps. We answer this in the affirmative by presenting an explicit construction of a Szegedy walk unitary for detailed balanced Lindbladians—generators of quantum Markov semigroups—and detailed balanced quantum channels. We prove that our Szegedy walk unitary has a purification of the fixed point of the Lindbladian as eigenvector with eigenphase 0 and that its eigenphase gap is quadratically larger than the spectral gap of the Lindbladian. To construct the walk unitary we leverage a canonical form for detailed balanced Lindbladians showing that they are structurally related to Davies generators. We also explain how the quantization method for Lindbladians can be applied to quantum channels. We give an efficient quantum algorithm for quantizing Davies generators that describe many important dynamics of open quantum systems, for instance, the relaxation of a quantum system coupled to a bath. Our algorithm extends known techniques for simulating dynamics of quantum systems on a quantum computer.

Szegedy developed a generic method for quantizing algorithms based on random walks [1]. An important contribution of this work was the quantization of any reversible (also called detailed balanced) random walk in the following sense: Let \( P = (p_{yx})_{x,y \in \Omega} \) denote the (column) stochastic matrix representing the reversible random walk on state space \( \Omega \) with limiting distribution \( \pi = (\pi_x)_{x \in \Omega} \); Szegedy showed how to construct a

\footnote{We will use the terms random walk, Markov chain, stochastic matrix, and stochastic map synonymously throughout the manuscript.}
corresponding walk unitary \( W(P) \) so that its unique eigenvector with eigenvalue 1 (or equivalently with eigenphase 0) is the quantum sample\(^2\)

\[
|\pi\rangle = \sum_{x \in \Omega} \sqrt{\pi_x} |x\rangle,
\]

that is, a coherent encoding of the limiting distribution \( \pi \). The reason for the many quantum speed-ups is that the phase gap of the walk unitary \( W(P) \) is approximately \( \sqrt{\Delta} \), where \( \Delta \) denotes the spectral gap of the stochastic matrix \( P \). Szegedy’s construction can now be understood using the quantum singular value transformation [2,3] that provides a unifying approach to many quantum algorithms and methods.

The purpose of the present work is to study certain coherent versions of quantum maps. Let \( T \) denote any detailed balanced quantum map with fixed point \( \sigma \). We construct a unitary \( W(T) \) such that its eigenvector with eigenphase 0 is the purification

\[
|\sigma\rangle = (\sigma^{1/2} \otimes I)|\Omega\rangle
\]

of \( \sigma \), where \( |\Omega\rangle = \sum_x |x\rangle \otimes |x\rangle \) denotes the (unnormalized) maximally entangled state. We prove that the eigenphase gap of \( W(T) \) is quadratically amplified compared to the spectral gap of the quantum map \( T \). We also present quantum circuits that efficiently implement \( W(T) \). To accomplish these goals we proceed as follows.

First, we develop a generic framework for constructing coherent versions of continuous time purely irreversible detailed balanced quantum maps. More precisely, we show how to construct coherent versions of quantum Markov semigroups. Let \( \mathcal{L} \) denote the Lindbladian, that is, the generator of a quantum Markov semigroup with fixed point \( \sigma \). Assuming that \( \mathcal{L} \) satisfies the detailed balanced condition with respect to \( \sigma \), we show how to construct a unitary \( W(\mathcal{L}) \) such that its eigenvector with eigenphase 0 is a purification of \( \sigma \) having the above form. We leverage the fact that detailed balanced Lindbladians can be expressed in a certain canonical form showing that they essentially have the structure of Davies generators. We relate the unitary \( W(\mathcal{L}) \) to a quantum discriminate \( Q \), which arises from \( \mathcal{L} \) through a similarity transformation defined with respect to the fixed point \( \sigma \). Analogously to the classical setting the quantum discriminate \( Q \) is shown to be independent of the fixed point \( \sigma \) and even the particular form in which the detailed balance condition is stated (due to the non-commutative nature of quantum mechanics, there are several natural notions of detailed balanced). Centrally, we prove that the phase gap of \( W(\mathcal{L}) \) is quadratically amplified compared to the spectral gap of \( \mathcal{L} \). We also discuss how the problem of quantizing detailed balanced quantum channels reduces to the problem of quantizing detailed balanced Lindbladians.

Second, we examine for which quantum maps the above method can be realized efficiently on a quantum computer. We focus on the special case of Davies generators that have thermal Gibbs states \( e^{-\beta H}/\text{Tr}(e^{-\beta H}) \) as fixed points for Hamiltonian \( H \) and inverse temperature \( \beta \). We show how to efficiently quantize Davies generators provided that the energies of the Hamiltonian \( H \) can be resolved, for instance, when we have access to a block encoding of the Hamiltonian \( H \) whose energies satisfy a rounding promise and we use the energy estimation method in [4].

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\(^2\) More precisely, the walk unitary \( W(P) \) acts on the Hilbert space \( \mathbb{C}^{|\Omega|} \otimes \mathbb{C}^{|\Omega|} \) and the corresponding eigenvector with eigenvalue 1 is the state \( |\pi\rangle = \sum_{x \in \Omega} \sqrt{\pi_x} |x\rangle \otimes \sum_{y \in \Omega} \sqrt{\pi_y} |y\rangle \).
The quadratic gap amplification is at the heart of the quantum speed-ups of many classical random walk based algorithms [5–8]. This polynomial speed-up is measured relative to the mixing time of the classical walk. For quantum maps, recent work [9–14] has investigated the mixing behavior of the corresponding Markov process. Tools have been developed to bound the mixing time and to analyze the spectral gaps of detailed balanced quantum maps. For several explicit examples [15–21] spectral gap bounds could be obtained.

A special case of a detailed balanced quantum map was introduced in the context of the quantum Metropolis algorithm [22] to prepare the Gibbs state of a quantum Hamiltonian with a time evolution that can be simulated efficiently. The Gibbs state can be prepared efficiently if the corresponding quantum map is rapidly mixing. A Szegedy walk unitary has been constructed for the classical Metropolis-Hastings algorithm [5]. The Metropolis-Hastings random walk prepares the Gibbs state for a Hamiltonian that is diagonal in the computational basis. An extension of this walk algorithm to non-diagonal quantum Hamiltonians subject to specific assumptions has been proposed in [23]. This proposal asks for access to some projective measurement that would enable one to distinguish between some arbitrary but fixed eigenvector basis of the system Hamiltonian. This assumption essentially makes it possible to reduce the problem to a classical Metropolis random walk on said fixed eigenbasis. We emphasize that when the system Hamiltonian has a degenerate spectrum such an eigenbasis measurement cannot be realized by a phase estimation routine for the Hamiltonian—even if one could perfectly resolve the energies. This is because one cannot distinguish between some arbitrary vectors within a degenerate eigenspace without any additional assumptions as discussed in more detail in “Appendix A”. Furthermore, in the generic situation of energy estimation with finite resources, any quantum Hamiltonian on an exponentially large Hilbert space with polynomial bounded operator norm will exhibit degeneracies. In contrast, the present work enables the direct “quantization” of thermalizing quantum maps such as Davies generators and therefore does not need to make any assumptions on the identifiability of some eigenbases.

Finally, we point out that our Szegedy walk unitaries could be used to obtain new quantum algorithms. For instance, the improved quantum algorithm for estimating partition functions of classical Hamiltonians [8] could be generalized to quantum Hamiltonians. We leave the question how to use our Szegedy walk unitaries for new quantum algorithms for future research.

The manuscript is organized as follows. In Sect. 1, we give an introduction to detailed balanced Lindbladians and present a canonical form for them. In Sect. 2, we present a quantum algorithm for implementing Szegedy walk unitaries for Davies generators whose coupling operators are reflections. To better explain the intuition behind our quantum algorithm, we assume that ideal energy estimation of the system Hamiltonian is possible. In Sect. 3, we remove the unphysical assumption of ideal energy estimation. We present an efficient quantum algorithm for implementing Davies generators whose coupling operators are reflection using the method for approximate energy estimation in [4]. In Sect. 4, we consider general detailed balanced Lindbladians and establish the existence of Szegedy walk unitaries for them. To achieve this, we show how to represent detailed balanced Lindbladian as Davies generators on a larger Hilbert space having reflections as coupling operators. This representation builds upon the canonical form of detailed balanced Lindbladians.
1. Canonical Form and Quantum Discriminate for Detailed Balanced Quantum Maps

We describe detailed balanced Lindbladians, present a canonical form, and also define the quantum discriminate for them. We also explain later how any detailed balanced quantum channel can be related to a detailed balanced Lindbladian.

1.1. Detailed balanced Lindbladians. Let $\mathcal{L}$ denote the generator of a quantum Markov semigroup. Throughout the entire manuscript, we consider purely irreversible Lindbladians, that is, their Hamiltonian part is equal to zero.\(^3\) We choose the Schrödinger picture so the Lindbladian $\mathcal{L}$ describes the evolution of quantum states $\rho$ according to

$$\dot{\rho} = \mathcal{L}(\rho).$$

Any (purely irreversible) Lindbladian $\mathcal{L}$ can be written in the form

$$\mathcal{L}(\rho) = \sum_i L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\},$$

where $L_i$ are the so-called Lindblad operators or jump operators. We require for the remainder of the manuscript that the operator norm of $\mathcal{L}$ satisfies $\|\mathcal{L}\| \leq 1$. Here the operator norm is the norm induced by the Hilbert Schmidt inner product, which is defined in the next paragraph. The normalization condition can always be achieved by suitably renormalizing the jump operators.

The Lindbladian $\mathcal{L}^*$ in the Heisenberg picture has the form

$$\mathcal{L}^*(O) = \sum_i L_i^\dagger O L_i - \frac{1}{2}\{L_i^\dagger L_i, O\},$$

where $O$ denotes an arbitrary observable. We point out that the Lindbladian $\mathcal{L}^*$ in the Heisenberg picture is the adjoint of the Lindbladian $\mathcal{L}$ in the Schrödinger picture with respect to the Hilbert Schmidt (HS) inner product, which is defined by $\langle X, Y \rangle = \text{Tr}(X^\dagger Y)$ for all matrices $X, Y$. This elementary observation will become important later.

There are no restrictions on the jump operators $L_i$ for a general Lindbladian (except for the normalization condition). However, it turns out that the jump operators of detailed balanced Lindbladians have very special and useful properties that enable us to construct a corresponding walk unitary with all the desired properties. We proceed by defining detailed balanced Lindbladians and discuss a canonical form that is the starting point for our quantization method.

In the manuscript [10] a certain notion of quantum detailed balance condition had been defined for every operator monotone function that obeys rather simple symmetry conditions. It had also been argued that this and other notions of quantum detailed balance are not equivalent. However, it was subsequently shown [24] that a stronger detailed balance condition—referred to as DBC—actually makes almost all notions of detailed balance collapse to a single notion and also enforces that a quantum map satisfying DBC always has a particular form.

Before introducing the quantum setting, we review the classical setting to explain the analogies and differences between the two. If $P = (P_{yx})$ denotes the transition matrix

\(^3\) It is not possible to obtain a coherent version of the Hamiltonian part, just as it is impossible to quantize a permutation matrix in the classical setting.
of a Markov chain on a finite state space \( \Omega \) with limiting distribution (probability vector) \( \pi \), we say that the detailed balanced condition holds if \( P_{x\pi} \pi_x = P_{y\pi} \pi_y \) for all \( x, y \in \Omega \).

An analytic way to formulate this condition is that \( P^T \) is Hermitian with respect to the weighted inner product on \( \mathbb{C}^{[\Omega]} \) defined by \( \langle v, w \rangle_1 = \sum_{x \in \Omega} \pi_x \bar{v}_x w_x \). Note that we use the subscript 1 to denote the weighted inner product to distinguish it from the standard inner product, but also to explain the analogy to the so-called GNS inner product that is introduced in the quantum setting below. Hermiticity of \( P^T \) with respect to this inner product means that \( \langle P^T v, w \rangle_1 = \langle v, P^T w \rangle_1 \) holds for all vectors \( v, w \in \mathbb{C}^{[\Omega]} \). Setting \( v \) and \( w \) to be the two standard basis vectors \( |x \rangle \) and \( |y \rangle \), allows us to recover the original definition of the detailed balanced condition. We can also state this condition in matrix form as \( D P^T = P D \), where \( D \) is the diagonal matrix whose entries are the \( \pi_x \) entries of the limiting distribution. Equivalently, we have \( D^{1/2} P^T D^{-1/2} = D^{-1/2} P D^{1/2} \).

Observe that the RHS of this equality is the discriminate matrix of the reversible Markov chain. We see that this discriminate matrix is Hermitian with respect to the standard inner product.

In the quantum setting, with reference density matrix \( \sigma \) of full rank that is not a multiple of the identity matrix, there are many candidates for such a weighted inner product. Let

\[
\sigma = \sum_{k=1}^{m} p_k P_k \tag{6}
\]

be the spectral decomposition of \( \sigma \), where \( p_k \in (0, 1) \) are the \( m \geq 2 \) different eigenvalues with \( \sum_{k=1}^{m} p_k = 1 \), and the orthogonal projectors form a resolution of the identity \( \sum_{k=1}^{m} P_k = I \).

For instance, given a density matrix \( \sigma \) as above and a real number \( s \in [0, 1] \), one can define a weighted inner product by

\[
\langle A, B \rangle_s = \langle A, \sigma^{1-s} B \sigma^s \rangle, \tag{7}
\]

where \( \langle X, Y \rangle = \text{Tr}(X^\dagger Y) \) denotes the Hilbert-Schmidt (HS) inner product. There are two important special cases. For \( s = 1 \), the inner product is called the Gelfand-Naimark-Segal (GNS) inner product, and for \( s = 1/2 \) it is called the Kubo-Martin-Schwinger (KMS) inner product.

The weighted inner product in (7) can also be written as

\[
\langle A, B \rangle_s = \langle A, \Delta_{\sigma}^{1-s} B \sigma \rangle, \tag{8}
\]

where \( \Delta_{\sigma} \) denotes the modular operator defined by \( \Delta_{\sigma} X = \sigma X \sigma^{-1} \). Here the power \( \Delta_{\sigma}^{1-s} \) of the modular operator \( \Delta_{\sigma} \) acts on \( B \) alone and not on the product of \( B \) and \( \sigma \).

More generally, given any function \( f : (0, \infty) \to (0, \infty) \), one can define a weighted inner product by

\[
\langle A, B \rangle_f = \langle A, f(\Delta_{\sigma}) B \sigma \rangle. \tag{9}
\]

Above we used again the convention that the superoperator \( f(\Delta_{\sigma}) \) acts on \( B \) alone and not on the product of \( B \) and \( \sigma \). Note that \( \langle \cdot, \cdot \rangle_1 \) is the GNS inner product whether \( 1 \) is interpreted as a number, as in (7), or as the constant function \( f(t) = 1 \), as in (9).

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4 We need that the matrix \( \sigma \) has full rank because otherwise the corresponding weighted inner product would not satisfy positive-definiteness. If \( \sigma \) were a multiple of the identity matrix, then the corresponding weighted inner product would reduce to the usual HS inner product.
Define the superoperator \( \Omega_\sigma^f = R_\sigma \circ f(\Delta_\sigma) \), where \( R_X \) denotes right multiplication by \( X \). Then, another way to write the weighted inner product in (9) is
\[
\langle A, B \rangle_f = \langle A, \Omega_\sigma^f B \rangle. \tag{10}
\]

It will be useful to establish some properties of \( \Omega_\sigma^f \) in the lemma below. We assume that \( f : (0, \infty) \to (0, \infty) \).

**Lemma 1** (Properties of \( \Omega_\sigma^f \)). We have

(i) \( \Omega_\sigma^f \) acts as follows
\[
\Omega_\sigma^f A = \sum_{k,\ell} f(p_k p_{\ell}^{-1}) \cdot p_{\ell} \cdot P_k AP_{\ell}. \tag{11}
\]

(ii) \( [\Omega_\sigma^f]^{-1} \) is \((1/f)(\Delta_\sigma) \circ R_\sigma^{-1} \), where the function \((1/f)\) is defined by \((1/f)(x) = 1/f(x)\) for all \( x \in (0, \infty) \), and acts as follows
\[
[\Omega_\sigma^f]^{-1} A = \sum_{k,\ell} (1/f)(p_k p_{\ell}^{-1}) \cdot p_{\ell}^{-1} \cdot P_k AP_{\ell}. \tag{12}
\]

(iii) \( \Omega_\sigma^f \) is positive definite with respect to the HS inner product.

*Proof.* Recall that \( \sigma = \sum_{k=1}^m p_k P_k \) is the spectral resolution of \( \sigma \). The eigenprojectors \( P_k \) of \( \sigma \) form a resolution of the identity so we can write \( A = \sum_{k,\ell} P_k AP_{\ell} \).

We have \( \Delta_\sigma (P_k AP_{\ell}) = p_k p_{\ell}^{-1} P_k AP_{\ell} \). Thus, \( f(\Delta_\sigma)(P_k AP_{\ell}) = f(p_k p_{\ell}^{-1}) P_k AP_{\ell} \). We have \( R_\sigma (P_k AP_{\ell}) = p_{\ell} P_k AP_{\ell} \). The two superoperators \( f(\Delta_\sigma) \) and \( R_\sigma \) commute. These observations establish the first statement. The second statement follows from \((1/f)(\Delta_\sigma) \circ f(\Delta_\sigma) = I\) and \( R_\sigma^{-1} \circ R_\sigma = I \). The third statement follows from
\[
\langle A, \Omega_\sigma^f A \rangle = \sum_{k,\ell} f(p_k p_{\ell}^{-1}) \cdot p_{\ell} \cdot \langle P_k AP_{\ell}, P_k AP_{\ell} \rangle > 0 \tag{13}
\]
for all non-zero \( A \), which is seen as follows. First, observe that the scalars \( f(p_k p_{\ell}^{-1}) \) and \( p_{\ell} \) are positive. Second, observe that the inner product \( \langle P_k AP_{\ell}, P_k AP_{\ell} \rangle \) must be positive for at least one pair of \( k \) and \( \ell \) since the HS inner product is positive definite and \( A \) is non-zero. \( \square \)

\( \Omega_\sigma^f \) is Hermitian with respect to HS inner product since it is positive definite as shown the lemma above in (iii). Therefore, we can equivalently apply \( \Omega_\sigma^f \) to the left argument of the HS inner product in (10).

Let \( \mathcal{M} \) be an arbitrary linear operator and \( \mathcal{M}^* \) its adjoint with respect to the HS inner product. Then, we have
\[
\langle A, \mathcal{M} B \rangle_f = \langle \Omega_\sigma^f A, \mathcal{M} B \rangle \tag{14}
\]
\[
= \langle \mathcal{M}^*(\Omega_\sigma^f A), B \rangle \tag{15}
\]
\[
= \langle [\Omega_\sigma^f]^{-1}(\mathcal{M}^*(\Omega_\sigma^f A)), B \rangle_f. \tag{16}
\]

This means that \( \mathcal{M} \) is Hermitian with respect to the weighted inner product \( \langle \cdot, \cdot \rangle_f \) if and only if
\[
\Omega_\sigma^f \circ \mathcal{M} = \mathcal{M}^* \circ \Omega_\sigma^f \tag{17}
\]
holds.
**Definition 1.** \((f\text{-DBC})\) The Lindbladian \(L\) in the Schrödinger picture is \(f\)-detailed balanced with respect to \(\sigma\) if and only if the Lindbladian \(L^*\) in the Heisenberg picture is Hermitian with respect to the weighted inner product \((\cdot, \cdot)\) in (9).

We say that the Lindbladian is detailed balanced with respect to \(\sigma\) when the weighted inner product is the GNS inner product, that is, the weighted inner product in (7) for \(s = 1\).

In the following we often omit “with respect to \(\sigma\)” when talking about \(f\)-detailed balance.

**Lemma 2** \((f\text{-detailed balanced implies fixed point}).\) Let \(L\) be \(f\)-detailed balanced. Then, \(\sigma\) is a fixed point of \(L\), that is, \(L(\sigma) = 0\).

**Proof.** Using that \(L^* (I) = 0\), \(L^*\) is Hermitian \((\cdot, \cdot)\), \(\Omega^f_\sigma (I) = \sigma\), and \(L^*\) is the adjoint of \(L\) with respect to the HS inner product, we obtain

\[
0 = \langle L^* (I), A \rangle^f \\
= \langle I, L^* (A) \rangle^f \\
= \langle \Omega^f_\sigma (I), L^* (A) \rangle_{\text{HS}} \\
= \langle \sigma, L^* (A) \rangle_{\text{HS}} \\
= \text{Tr}(\sigma L^* (A)) \\
= \text{Tr}(L(\sigma) A)
\]

for an arbitrary observable \(A\). The condition \(\text{Tr}(L(\sigma) A) = 0\) for all \(A\) implies that \(L(\sigma) = 0\). \(\square\)

If \(L\) is \(f\)-detailed balanced, then it holds that

\[
\Omega^f_\sigma \circ L^* = L \circ \Omega^f_\sigma.
\]

This follows from the characterization in (17) with \(M = L^*\) and \(L^{**} = L\). The condition in (24) can also be expressed as

\[
[\Omega^f_\sigma]^{1/2} \circ L^* \circ [\Omega^f_\sigma]^{-1/2} = [\Omega^f_\sigma]^{-1/2} \circ L \circ [\Omega^f_\sigma]^{1/2}.
\]

We are now ready to define the \(f\)-quantum discriminate \(Q^f\).

**Definition 2** \((f\text{-quantum discriminate } Q^f)\). Assume the Lindbladian \(L\) is \(f\)-detailed balanced with respect to the state \(\sigma\). We define the corresponding \(f\)-quantum discriminate \(Q^f\) to be

\[
Q^f = I + \mathcal{K}^f,
\]

where \(\mathcal{K}^f\) is the operator defined to be the LHS or equivalently the RHS of (25), that is,

\[
\mathcal{K}^f = [\Omega^f_\sigma]^{1/2} \circ L^* \circ [\Omega^f_\sigma]^{-1/2} = [\Omega^f_\sigma]^{-1/2} \circ L \circ [\Omega^f_\sigma]^{1/2}.
\]

When the weighted inner product is the GNS inner product, we simply say the quantum discriminate \(Q\).
Lemma 3 (f-quantum discriminate is Hermitian). Assume that $\mathcal{L}$ is $f$-detailed balanced with respect to the state $\sigma$, where $f$ is any function $f : (0, \infty) \rightarrow (0, \infty)$. Then, we have: (i) the $f$-quantum discriminate $Q^f$ is Hermitian with respect to the Hilbert-Schmidt inner product; (ii) it is has $\tau = \sigma^{1/2}$ as a fixed point, that is, $Q^f(\tau) = \tau$; (iii) the spectral gap of $\mathcal{L}$ and the spectral gap of the $f$-quantum discriminate $Q^f$ are equal.

Proof. The superoperator $\Omega_\sigma^f$ is Hermitian with respect to the HS inner product. Thus, $[\Omega_\sigma^f]^{\pm 1/2}$ are also Hermitian. We now see that both sides of (25) are adjoints of each other (observe that the adjoint operation reverses the order of the superoperators) and, thus, $\mathcal{K}^f$ is Hermitian.

Using property (i) in Lemma 1, we obtain that $[\Omega_\sigma^f]^{1/2}(\tau)$ is proportional to $\sigma$ so that $\mathcal{K}^f(\tau) = 0$. The proportionality factor is $\sqrt{f}(1)$. Finally, $Q^f$ and $\mathcal{L}$ have the same spectral gap because $\mathcal{K}^f$ and $\mathcal{L}$ are related by a similarity transformation. ⊓⊔

We now see that the $f$-detailed balanced condition ensures that the Lindbladian $\mathcal{L}$ has real spectrum since it is similar to the Hermitian operator $\mathcal{K}^f$. Moreover, its spectrum of $\mathcal{L}$ is contained in the interval $[-1, 0]$; we have $-1$ as the left end of the interval because we assume that the operator norm of $\mathcal{L}$ satisfies $\|\mathcal{L}\| \leq 1$. The fixed point $\sigma$ of $\mathcal{L}$ is the eigenvector with eigenvalue 0.

We now discuss the independence of the definitions of $f$-detailed balance and $f$-quantum discriminate $Q^f$ of the particular weighted inner product $\langle \cdot, \cdot \rangle_f$.

The equivalence of Hermiticity with respect to the different weighted inner products described in the remark below essentially enables us to restrict ourselves to the GNS inner product.

Remark 1. It was shown in [24] that if a linear operator $\mathcal{M}$ is Hermitian with respect to $\langle \cdot, \cdot \rangle_s$ for some $s \in I = [0, \frac{1}{2}) \cup (\frac{1}{2}, 1]$, then it is automatically Hermitian with respect $\langle \cdot, \cdot \rangle_s$ for all $s \in [0, 1]$, including $s = \frac{1}{2}$. Moreover, it is also Hermitian with respect to $\langle \cdot, \cdot \rangle_f$ for any function $f : (0, \infty) \rightarrow (0, \infty)$.

In the next subsection, we leverage the canonical form for detailed balanced Lindbladians to establish that the $f$-quantum discriminate $Q^f$ is independent of $f$.

1.2. Canonical form for detailed balanced Lindbladians. To analyze the present case of a detailed balanced Lindbladian $\mathcal{L}$ with respect to $\sigma$ and later the more special case of a Davies generator, whose fixed point is always a thermal Gibbs state, in a unifying approach, we define the corresponding “Hamiltonian” $h$ for $\sigma$ by setting $h = -\ln \sigma$. Its spectral decomposition is

$$h = \sum_{k=1}^{m} \varepsilon_k P_k$$

(28)

where the “energies” are simply given by $\varepsilon_k = -\ln p_k$. We can now formally express the state $\sigma$ as a Gibbs state for the Hamiltonian $h$ at inverse temperature $\beta = 1$, that is,

$$\sigma = e^{-h}$$

(29)

Note that the corresponding partition function is $Z = \sum_k e^{-\varepsilon_k} = \sum_k p_k = 1$. We call the differences of the form $\omega_{k\ell} = \varepsilon_k - \varepsilon_\ell$ the Bohr frequencies of $h$, where $k, \ell = 1, \ldots, m$. 

We now introduce a canonical form for detailed balanced Lindbladians. We leverage this canonical form to construct walk unitaries for all detailed balanced Lindbladians.

**Definition 3** *(Canonical form for detailed balanced Lindbladians)*. Let $L$ be a (purely irreversible) Lindbladian that is detailed balanced with respect to $\sigma$. We say the Lindbladian $L$ is in canonical form if it is given as a convex combination

$$L(\rho) = \sum_\alpha w_\alpha L^\alpha(\rho)$$

and each term $L^\alpha$ has the following form

$$L^\alpha(\rho) = \sum_\omega G^\alpha(\omega) \left( X^\alpha(\omega) \rho X^{\alpha\dagger}(\omega) - \frac{1}{2} \{ X^{\alpha\dagger}(\omega) X^\alpha(\omega), \rho \} \right),$$

where we use $X^{\alpha\dagger}(\omega)$ to denote the Hermitian conjugate of $X^\alpha(\omega)$. For each $\alpha$, the summation index $\omega$ in (31) runs over all different Bohr frequencies of the Hamiltonian $h = -\ln \sigma$. The operators $X^\alpha(\omega)$ and scalars $G^\alpha(\omega)$ satisfy the following conditions:

$$X^\alpha(\omega) = X^{\alpha\dagger}(-\omega)$$

$$\Delta_\sigma X^\alpha(\omega) = e^{-\omega} X^\alpha(\omega)$$

$$G^\alpha(\omega) \geq 0$$

$$G^\alpha(-\omega) = e^{\omega} G^\alpha(\omega).$$

We will also assume that $1 \geq G^\alpha(\omega)$ for all $\alpha$ and $\omega$.

It is of paramount importance that any detailed balanced Lindbladian $L$ can written in the canonical form. We have formulated this key result in the lemma below.

**Lemma 4.** A detailed balanced Lindbladian $L$ can always be written in the canonical form presented in the definition above, which shows that detailed balanced Lindbladians essentially have the structure of Davies generators.

**Proof.** This follows directly from the results in [25, Theorem 2], [26, Remark on page 101], and [24, Theorem 2.4].

We now establish some elementary results that we will use for showing that the $f$-quantum discriminate $Q^f$ is independent of $f$. For each Bohr frequency $\omega$, define the set

$$J_\omega = \{(k, \ell) : \varepsilon_k - \varepsilon_\ell = \omega\}. $$

$B$ is an eigenvector of the modular operator $\Delta_\sigma$ with eigenvalue $e^{-\omega}$ iff

$$B = \sum_{(k, \ell) \in J_\omega} P_k B P_{\ell}. $$

This is because the RHS of the equation above is precisely the projection of $B$ onto the eigensubspace of $\Delta_\sigma$ with eigenvalue $e^{-\omega}$. We will apply this characterization to

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5 The property for $G^\alpha(\omega)$ in (35) is a statement about the ratio of $G^\alpha(\pm \omega)$. It is clear that all bounded functions $G^\alpha(\omega)$ can be rescaled to ensure that $1 \geq G^\alpha(\omega)$ holds. We point out that the widely used Metropolis-Hastings filter $\min\{1, e^{-\omega}\}$ and Glauber filter $e^{-\omega}/(1 + e^{-\omega})$ are both bounded from above by 1.
$X_\alpha(\omega)$, $X_\alpha^\dagger(\omega)$, and $X_\alpha^\dagger(\omega)X_\alpha(\omega)$. Recall that $X_\alpha(\omega)$ is an eigenvector of $\Delta_\sigma$ with eigenvalue $e^{-\omega}$ and that $X_\alpha^\dagger(\omega) = X_\alpha(-\omega)$; these are the first two properties in the canonical form. It is elementary to verify that $X_\alpha^\dagger(\omega)X_\alpha(\omega)$ is an eigenvector of $\Delta_\sigma$ with eigenvalue 1, that is, the corresponding Bohr frequency is 0.

Property (35) is equivalent to

$$G_\alpha(\omega)e^{\omega/2} = \sqrt{G_\alpha(\omega)}G_\alpha(-\omega).$$

Lemma 5 (Quantum discriminate). Let $\mathcal{L}$ be a detailed balanced Lindbladian with respect to $\sigma$. Then, the $f$-quantum discriminate $\mathcal{Q}^f$ is independent of $f$. It acts as $\mathcal{Q} = I + \mathcal{K}$, where

$$\mathcal{K}(A) = \sum_\alpha \sum_\omega \sqrt{G_\alpha(\omega)G_\alpha(-\omega)}X_\alpha(\omega)AX_\alpha^\dagger(\omega) - \frac{G_\alpha(\omega)}{2}\{X_\alpha^\dagger(\omega)X_\alpha(\omega), A\}.$$  

Proof. To abbreviate, we set $\Omega = \Omega_{\sigma}^f$. We consider arbitrary but fixed $\alpha$ and $\omega$. We drop the subscript $\alpha$ when writing $X_\alpha(\omega)$.

First, we analyze how the similarity transformation acts on the first term in (31). Using properties (i) and (ii) in Lemma 1, we obtain

$$\Omega^{-1/2}(X(\omega)\Omega^{1/2}(A)X^\dagger(\omega))$$

$$= \sum_{k,\ell} \sum_{m, n} [(1/f)(e^{-(\varepsilon_k-\varepsilon_\ell)}) e^{\varepsilon_\ell}]^{1/2}[f(e^{-(\varepsilon_m-\varepsilon_n)})e^{-(\varepsilon_n)}]^{1/2} P_k X(\omega)P_m A P_n X^\dagger(\omega)P_\ell$$

$$= \sum_{(k,m) \in J_\omega}(\ell,n) \in J_\omega \sum [(1/f)(e^{-(\varepsilon_k-\varepsilon_\ell)}) f(e^{-(\varepsilon_m-\varepsilon_n)})]^{1/2} e^{\omega/2} P_k X(\omega)P_m A P_n X^\dagger(\omega)P_\ell$$

$$= \sum_{(k,m) \in J_\omega}(\ell,n) \in J_\omega e^{\omega/2} P_k X(\omega)P_m A P_n X^\dagger(\omega)P_\ell$$

$$= e^{\omega/2} X(\omega)AX^\dagger(\omega).$$

We have used that $\varepsilon_k - \varepsilon_m = \omega$ and $\varepsilon_\ell - \varepsilon_n = \omega$ must hold or otherwise the term is zero. But in this case we have $\varepsilon_k - \varepsilon_\ell = \varepsilon_m - \varepsilon_n$. This shows that the arguments for $(1/f)$ and $f$ are the same so that the value of the product inside the square brackets simplifies to 1. To get the first term of (39), we now use that $G(\omega)e^{\omega/2} = \sqrt{G(\omega)}G(-\omega)$.

Second, we analyze how the similarity transformation acts on the two terms arising from the anticommutator. For the first term, we have

$$\Omega^{-1/2}(X(\omega)X^\dagger(\omega)\Omega^{1/2}(A))$$

$$= \sum_{k,\ell} \sum_{m} [(1/f)(e^{-(\varepsilon_k-\varepsilon_\ell)}) e^{\varepsilon_\ell}]^{1/2}[f(e^{-(\varepsilon_m-\varepsilon_n)})e^{-(\varepsilon_n)}]^{1/2} P_k X(\omega)X^\dagger(\omega)P_m A P_n P_\ell$$

$$= \sum_{k,\ell} \sum_{m} [(1/f)(e^{-(\varepsilon_k-\varepsilon_\ell)})]^{1/2}[f(e^{-(\varepsilon_m-\varepsilon_n)})]^{1/2} P_k X(\omega)X^\dagger(\omega)P_m A P_\ell$$
\[
\sum_{k,\ell} \left[ \frac{1}{f} e^{-(\varepsilon_k - \varepsilon_\ell)} \right] \frac{1}{2} \left[ f e^{-(\varepsilon_k - \varepsilon_\ell)} \right]^{1/2} P_k X(\omega) X^\dagger(\omega) P_\ell A P_\ell \tag{48}
\]

\[
= \sum_{k,\ell} P_k X(\omega) X^\dagger(\omega) P_\ell A P_\ell \tag{49}
\]

\[
= \sum_k P_k X(\omega) X^\dagger(\omega) P_k A \tag{50}
\]

\[
= X(\omega) X^\dagger(\omega) A. \tag{51}
\]

We used that we must have \( n = \ell \) and then \( m = k \) or otherwise the term is zero since the corresponding projectors are orthogonal. We used that the projectors \( P_\ell \) add up to the identity. Finally, we have used the operator \( X(\omega) X^\dagger(\omega) \) is block diagonal, where the blocks correspond to the projectors \( P_k \). The second term is analyzed analogously.  

1.3. Detailed balanced quantum channels. We now briefly explain that our theoretical results and our quantum algorithm also apply to (discrete-time) quantum channels.

Let \( T \) be a quantum channel in the Schrödinger picture. Using the Kraus representation, we can write it as

\[
T(\rho) = \sum_i A_i \rho A_i^\dagger
\]

where the Kraus operators \( A_i \) satisfy the condition

\[
\sum_i A_i^\dagger A_i = I
\]

The quantum channel \( T^* \) in the Heisenberg picture is simply

\[
T^*(O) = \sum_i A_i^\dagger O A_i
\]

**Definition 4 (Detailed balanced quantum channel).** Let \( T \) be a quantum channel. We call \( T \) detailed balanced with respect to the state \( \sigma \) if the quantum channel \( T^* \) in the Heisenberg picture is Hermitian with respect to the GNS inner product.

**Lemma 6** (Detailed balanced implies fixed point). If \( T \) is detailed balanced with respect to \( \sigma \), then \( \sigma \) is a fixed point.

**Proof.** We have

\[
\text{Tr}(\sigma A) = \langle I, A \rangle_1 = \langle T^*(I), A \rangle_1 = \langle I, T^*(A) \rangle_1 = \text{Tr}(\sigma T^*(A)) = \text{Tr}(T(\sigma) A)
\]

for all \( A \) so that \( T(\sigma) = \sigma \) holds.  

**Remark 2.** We can associate a Lindbladian \( L \) to the quantum channel \( T \) by setting

\[
L(\rho) = \sum_i A_i \rho A_i^\dagger - \frac{1}{2} \{ A_i^\dagger A_i, \rho \}
\]

Note that \( L = T - I \) because of condition (53). It is now clear that \( T \) is detailed balanced iff the corresponding Lindbladian \( L \) is detailed balanced. The canonical form for the Lindbladians also carries over for the quantum channels.
2. Quantum Algorithm for Szegedy Walk Unitaries for Davies Generators with Ideal Energy Estimation

The goal of this section is to present a quantum algorithm for implementing Szegedy walk unitaries for Davies generators whose coupling operators are restricted to be reflections. Davies generators are Lindbladians that satisfy the detailed balanced condition as in Definition 1. Our algorithmic implementation exploits how these operators are specified. Therefore, some comments are in order that highlight the differences of this particular setting from the case of the most general form of detailed balanced Lindbladians.

The Davies generator $L$ is specified by a system Hamiltonian $H$, coupling operators $S^\alpha$ to an environment, filter functions $G^\alpha(\omega)$, and an inverse temperature $\beta$. It is detailed balanced with respect to the thermal Gibbs state $\sigma = e^{-\beta H}/\text{Tr}(e^{-\beta H})$. This specification directly yields a detailed balanced Lindbladian in canonical form as in Definition 3, and we can use $H$, $S^\alpha$, $G^\alpha$, and $\beta$ in our quantum algorithm. In contrast, a general detailed balanced Lindbladian could be specified by some arbitrary collection of jump operators and the relationship between the latter and the operators appearing in the canonical form could be highly complicated. For instance, if we have some Lindbladian that is detailed balanced with respect to some state $\sigma$, then the corresponding Hamiltonian $h = -\ln \sigma$ arising in the canonical form could be very costly to represent on a quantum computer.

The section is organized as follows. First, we introduce Davies generators. Second, we give an expression for the quantum discriminate in the vectorized representation. Third, we show how to efficiently obtain a block encoding of the vectorized quantum discriminate provided that we can perfectly resolve the energies of $H$. Fourth, we discuss how spectral gap amplification techniques applied to the vectorized quantum discriminate enable us to obtain the desired walk unitary for $W(L)$ so that the purification $|\sigma\rangle = (\sigma^{1/2} \otimes I) |\Omega\rangle$ is its unique eigenvector with eigenphase 0 and its eigenphase gap is quadratically larger than the spectral gap of $L$.

2.1. Davies generators. A particular class of Liouvillians [27,28], which describes the thermalization of a quantum mechanical system subject to thermal noise, is known as Davies generators [29,30]. This class of Liouvillians describes the dissipative dynamics resulting as the weak (or singular) coupling limit from a joint Hamiltonian evolution of a system coupled to a large heat bath. The weak coupling limit permits to consider only the reduced dissipative dynamics, which gives rise to a Markovian semi-group generated by the aforementioned Davies Liouvillian. This generator retains the information of the bath temperature $\beta$ and converges to the Gibbs distribution of the system, constructed from the system Hamiltonian $H$. We assume that the system is coupled to a bath through the Hermitian operators $S^\alpha$ that drive the dissipative dynamics. If a sufficiently large set of such operators is given, then the Gibbs state is the unique fixed point of the map. We discuss the properties of this generator directly, and are not concerned with the actual derivation.

We write the system Hamiltonian $H$ as

$$H = \sum_{k=1}^{m} \varepsilon_k P_k,$$

where $\varepsilon_k \in [0, 1]$ denote the $m$ different eigenvalues and $P_k$ are the projectors onto the corresponding eigenspaces. We choose the Schrödinger picture as a convention so that the Davies generator $L$ describes the evolution of states.
The Davies generator $\mathcal{L}$ is given by

$$\mathcal{L}(\rho) = \sum_{\alpha} w_{\alpha} \mathcal{L}^\alpha(\rho)$$

$$= \sum_{\alpha} w_{\alpha} \sum_{\omega} G^\alpha(\omega) \left( S^\alpha(\omega) \rho S^\alpha(\omega) - \frac{1}{2} \left\{ S^\alpha(\omega) S^\alpha(\omega), \rho \right\} \right). \quad (58)$$

The index $\alpha$ enumerates the coupling operators $S^\alpha$ to the environment. Note that the weights $w_{\alpha}$ could be absorbed into the coupling operators $S^\alpha$, but it is more convenient for our purposes to write the Davies generator $\mathcal{L}$ as a convex sum of Lindbladians $\mathcal{L}^\alpha$. For a fixed $\alpha$, the variable $\omega$ runs over all different Bohr frequencies of the system Hamiltonian $H$, that is, the energy differences of the form $\omega = \varepsilon_k - \varepsilon_\ell$. The functions $G^\alpha(\omega)$ correspond to the Fourier transform of the two point correlation functions of the environment, and are bounded $[28,31]$. These functions depend on the bath operators as well as the thermal state of the bath and encode the equilibrium temperature. We may assume them to be simply given by the Metropolis filter rule or a similar filter as defined by the Glauber dynamics. The Lindblad operators $S^\alpha(\omega)$ are given by the Fourier components of the coupling operators $S^\alpha$ which evolve according to the system Hamiltonian

$$e^{iHt} S^\alpha e^{-iHt} = \sum_{\omega} S^\alpha(\omega) e^{i\omega t}. \quad (59)$$

The Lindblad operators $S^\alpha(\omega)$ induce transitions between the eigenvectors of $H$ with energy $E$ to eigenvectors of $H$ with energy $E + \omega$, and hence act as quantum jump operators, which transfer energy $\omega$ from the system to the bath. A direct evaluation shows that the jump operators $S^\alpha(\omega)$ are of the form

$$S^\alpha(\omega) = \sum_{(k,\ell) \in J_\omega} P_k S^\alpha P_\ell. \quad (60)$$

The jump operators $S^\alpha(\omega)$ and filter functions $G^\alpha(\omega)$ satisfy the properties $33 - 35$ in Definition 3. Therefore, the Davies generator $\mathcal{L}$ is detailed balanced with respect to $\sigma$.

We already know that the Gibbs state $\sigma$ is a fixed point of the Davies generator $\mathcal{L}$. This follows from Lemma 2 since $\mathcal{L}$ is detailed balanced with respect to $\sigma$. The next lemma provides a sufficient condition for the Gibbs state $\sigma$ to be the unique fixed point. This result was proved in [31].

**Lemma 7** (Uniqueness of fixed point). If the coupling algebra

$6$ It is important that a small number of generators will suffice to generate the entire matrix algebra and, thus, guarantee that the fixed point $\sigma$ is unique.

5 It is important that a small number of generators will suffice to generate the entire matrix algebra and, thus, guarantee that the fixed point $\sigma$ is unique.
Then, there exists a corresponding walk unitary $W(L)$ such that its unique eigenvector with eigenphase $0$ is the purification $|\sigma\rangle = (\sigma^{1/2} \otimes I) |\Omega\rangle$ of the Gibbs state $\sigma$ and its phase gap is quadratically larger than the spectral gap of the Davies generator $L$. It can be obtained by standard methods for spectral gap amplification applied to the block encoding of the vectorized quantum discriminate matrix. The block encoding of the quantum discriminate can be implemented exactly provided that we can exactly determine the energies of the Hamiltonian $H$.

We prove this theorem in the next three subsections.

2.2. Quantum discriminate in the vectorized representation. For the sake of simplicity, we consider the case that there is only one coupling operator $S$, that is, we can drop the index $\alpha$. The general case of multiple coupling operators can be handled easily.

In Sect. 1, we showed that a detailed balanced Lindbladian $L$ is similar to an operator $K$ that has the following form

$$K(A) = \sum_\omega \sqrt{G(\omega) G(-\omega)} S(\omega) A S^\dagger(\omega) - \frac{G(\omega)}{2} \{ S^\dagger(\omega) S(\omega), A \}. \quad (61)$$

Let us recall the key properties of $K$:

(a) $K(\sqrt{\sigma}) = 0$,

(b) $K$ is Hermitian with respect to the HS inner product, and

(c) $K$ does not depend explicitly on the fixed point $\sigma$ (although the similarity transformation was defined using $\sigma$).

We will now use the vectorization operation to map the superoperator $K$ acting on $\mathbb{C}^d \times \mathbb{C}^d$ to the matrix $\hat{K}$ acting $\mathbb{C}^d \otimes \mathbb{C}^d$. Recall that the vectorization operation is defined by

$$\text{vec}(i \langle j |) = |i \rangle \otimes |j \rangle \quad (62)$$

and satisfies the useful identity

$$\text{vec}(ABC) = (A \otimes C^T) \text{vec}(B) \quad (63)$$

for all matrices $A$, $B$, and $C$. The vectorized representation $\hat{K}$ of $K$ is the unique matrix so that

$$\text{vec}(K(A)) = \hat{K}\text{vec}(A). \quad (64)$$

Using the above identity we obtain

$$\hat{K} = \sum_\omega \sqrt{G(\omega) G(-\omega)} S(\omega) \otimes \tilde{S}(\omega) - \frac{G(\omega)}{2} \left( S^\dagger(\omega) S(\omega) \otimes I + I \otimes \tilde{S}^\dagger(\omega) \tilde{S}(\omega) \right). \quad (65)$$

The properties (a) and (b) manifest themselves in the vectorized representation as follows:
(a) The fixed point $\sqrt{\sigma}$ of $K$ becomes the fixed point $|\sigma\rangle = (\sqrt{\sigma} \otimes I) |\Omega\rangle$ of $\hat{K}$, where $|\Omega\rangle$ denotes the unnormalized maximally entangled state. Note that $|\sigma\rangle$ is a purification of $\sigma$.

(b) Hermiticity of $K$ with respect to the HS trace inner product on $\mathbb{C}^{d \times d}$ becomes Hermiticity of $\hat{K}$ with respect to the standard inner product on $\mathbb{C}^{d} \otimes \mathbb{C}^{d}$.

(c) This is evident by inspecting the form of $K$ in (61).

The vectorized quantum discriminate is simply given by $\hat{Q} = I + \hat{K}$, where $\hat{K}$ is as in (65). To simplify the notation, we will use $Q$ to also denote the quantum discriminate in the vectorization representation.

2.3. Block encoding of quantum discriminate. We construct a block encoding of the vectorized quantum discriminate $Q$ assuming ideal energy estimation. We assume as before that there is only one coupling operator $S$ so we may drop the index $\alpha$ when writing the jump operators $S(\omega)$. We define an isometry $T$ and a reflection $R$ to embed the quantum discriminate $Q = I + \hat{K}$ as follows

$$Q = T^\dagger R T.$$  

(66)

Let us explain why we seek to embed $Q = I + \hat{K}$ instead of $\hat{K}$. The “fixed point” of $\hat{K}$ is $|\sigma\rangle$ with $\hat{K}|\sigma\rangle = 0$. However, for the Szegedy walk unitary we want to quantize a discriminate matrix satisfying $Q|\sigma\rangle = |\sigma\rangle$. This is accomplished by working with $Q = I + \hat{K}$. We will also see that $Q$ can be embedded in a very natural and elegant way.

To construct the isometry $T$ and the reflection $R$, we need to define the following building blocks.

- **Ideal energy estimation unitaries:**
  
  $$\Phi = \sum_p \sum_k P_k \otimes |p - \varepsilon_k\rangle \langle p|$$  
  
  (67)

  $$\bar{\Phi} = \sum_p \sum_k \bar{P}_k \otimes |p - \varepsilon_k\rangle \langle p|$$  
  
  (68)

  Here $\Phi$ denotes phase estimation of the unitary $e^{-iH}$ where $H = \sum_k \varepsilon_k P_k$, while $\bar{\Phi}$ denotes phase estimation of the unitary $e^{-i\bar{H}}$, where $\bar{H} = \sum_k \varepsilon_k \bar{P}_k$. Here the bar over $P_k$ means entry-wise conjugation. The variable $p$ runs over all possible values of the energy pointer register.

  Note that both $\Phi$ and $\bar{\Phi}$ constitute idealized energy estimation procedures making it possible to resolve the energies perfectly.

- **The coupling/kick operator:**
  
  We consider a coupling/kick operator that serves both as observable and as unitary that can be implemented. We require that it is a reflection so that $S = S^\dagger$ as well as $S^\dagger S = SS^\dagger = I$. We also assume that we can implement $\bar{S}$ (by complex conjugating the elementary gates used in the decomposition of $S$).

- **The controlled filter rotation:**
  
  $$W = \sum_\omega |\omega\rangle \langle \omega| \otimes \hat{G}(\omega),$$  
  
  (69)
Fig. 1. Circuits for the subisometries $T_0$ and $T_1$

\[
\hat{G}(w) = \begin{pmatrix}
\sqrt{1 - G(\omega)} & -\sqrt{G(\omega)} \\
\sqrt{G(\omega)} & \sqrt{1 - G(\omega)}
\end{pmatrix}. \tag{70}
\]

- **The sign flip reflection:**
  We define a reflection on a single register that maps computational basis states from $|\omega\rangle$ to $|-\omega\rangle$ by setting

\[
F = \sum_\omega | -\omega \rangle \langle \omega |. \tag{71}
\]

This map is a reflection since it squares to the identity.

Let us now implement the isometry $T$. It is composed of the two sub-isometries $T_0$ and $T_1$ that are defined in the circuits below (Fig. 1).

There are four registers. The registers $sys1$ and $sys2$ correspond to a “doubled” physical register that can encode purifications of quantum states. The register $freq$ encodes the Bohr frequencies of the Hamiltonian. It is prepared in $|0\rangle$. The register $filter$ is a single qubit register on which we perform the controlled rotation $\hat{G}(\omega)$. It is prepared in $|0\rangle$. The sub-isometry $T_0$ has the kick operator $S$ act on the register $sys2$, whereas the sub-isometry $T_1$ has the complex-conjugate kick operator $\bar{S}$ act on the register $sys1$.

The full isometry $T$ is obtained by coherently adding $T_0$ and $T_1$. To this end, we introduce a single qubit register $add$ that is prepared in $|+\rangle$ and apply controlled versions of these two respective isometries as shown in the circuit below (Fig. 2).

The full isometry $T$ is given by

\[
T = \frac{1}{\sqrt{2}} (T_0 \otimes |0\rangle + T_1 \otimes |1\rangle). \tag{72}
\]

Before we analyze $T$ in detail, let us first understand the action of the ideal energy estimation operations and kick operators. It suffices to focus on $T_0$ as $T_1$ behaves analogously. We only consider the action on the two “active” registers $sys2$ and $freq$ for notional simplicity.
The ideal energy estimation acts as
\[
\Phi^\dagger(S \otimes I)\Phi = \sum_p \sum_k \sum_q \sum_\ell P_k S P_\ell \otimes |q\rangle \langle q - \varepsilon_k| p - \varepsilon_\ell\rangle \langle p | \tag{73}
\]
\[
= \sum_p \sum_k \sum_\ell P_k S P_\ell \otimes |\varepsilon_k - \varepsilon_\ell + p\rangle \langle p | \tag{74}
\]
\[
= \sum_p \sum_\omega S(\omega) \otimes |\omega + p\rangle \langle p |, \tag{75}
\]
where we used the definition of the ideal phase estimation unitary \(\Phi\) as well as the definition of the jump operators \(S(\omega) = \sum_{(k,\ell) \in J_\omega} P_k S P_\ell\).

According to the circuits, these isometries are defined to be
\[
T_0 = W \Phi_1^\dagger(S \otimes I) \Phi_1 (I \otimes I \otimes |0\rangle \otimes |0\rangle) \tag{76}
\]
\[
T_1 = W \Phi_2^\dagger(I \otimes \bar{S}) \Phi_2 (I \otimes I \otimes |0\rangle \otimes |0\rangle). \tag{77}
\]

Using the expression for the ideal energy estimation, we obtain
\[
T_0 = \sum_\omega S(\omega) \otimes I \otimes |\omega\rangle \otimes \left(\sqrt{1 - G(\omega)}|0\rangle + \sqrt{G(\omega)}|1\rangle\right) \tag{78}
\]
\[
T_1 = \sum_\omega I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes \left(\sqrt{1 - G(\omega)}|0\rangle + \sqrt{G(\omega)}|1\rangle\right) \tag{79}
\]
for the isometries \(T_0\) and \(T_1\). Hence, we obtain
\[
T = \frac{1}{\sqrt{2}} \sum_\omega S(\omega) \otimes I \otimes |\omega\rangle \otimes \left(\sqrt{1 - G(\omega)}|0\rangle + \sqrt{G(\omega)}|1\rangle\right) \otimes |0\rangle \tag{80}
\]
\[
+ \frac{1}{\sqrt{2}} \sum_\omega I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes \left(\sqrt{1 - G(\omega)}|0\rangle + \sqrt{G(\omega)}|1\rangle\right) \otimes |1\rangle \tag{81}
\]
for the full isometry \(T\).

Before we define the reflection \(R\), we recall that the registers in the order from left to right are: \text{sys2}, \text{sys1}, \text{freq}, \text{filter}, and \text{add} in the above expression for the full isometry \(T\).

The reflection operator \(R\) is defined by the circuit (Fig. 3) \(R\) applies the sign flip \(\omega \leftrightarrow -\omega\) in \text{freq} and the bit flip \(0 \leftrightarrow 1\) in \text{add} iff the control qubit \text{filter} is in the state \(|1\rangle\). The expression for \(R\) is
\[ R = I \otimes I \otimes I \otimes |0\rangle \langle 0| \otimes I + I \otimes I \otimes F \otimes |1\rangle \langle 1| \otimes X, \]  
\[ (82) \]

where \( F \) and \( X \) denote the sign and bit flips, respectively.

The remainder of this section is devoted to proving that the desired vectorized quantum discriminant \( Q \) is given by the block encoding

\[ Q = T^\dagger R T. \]  
\[ (84) \]

We begin by computing the product \( RT \). To this end, it is convenient to rearrange the terms of \( T \) as follows

\[ T = \frac{1}{\sqrt{2}} \sum_\omega \sqrt{1-G(\omega)} \ S(\omega) \otimes I \otimes |\omega\rangle \otimes |0\rangle \otimes |0\rangle \]  
\[ (85) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{1-G(\omega)} \ I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes |0\rangle \otimes |1\rangle \]  
\[ (86) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{G(\omega)} \ S(\omega) \otimes I \otimes |\omega\rangle \otimes |1\rangle \otimes |0\rangle \]  
\[ (87) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{G(\omega)} \ I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes |1\rangle \otimes |1\rangle. \]  
\[ (88) \]

Using the above expression for \( T \), it is seen that the product \( RT \) is given by

\[ RT = \frac{1}{\sqrt{2}} \sum_\omega \sqrt{1-G(\omega)} \ S(\omega) \otimes I \otimes |\omega\rangle \otimes |0\rangle \otimes |0\rangle \]  
\[ (89) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{1-G(\omega)} \ I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes |0\rangle \otimes |1\rangle \]  
\[ (90) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{G(\omega)} \ S(\omega) \otimes I \otimes |\omega\rangle \otimes |1\rangle \otimes |0\rangle \]  
\[ (91) \]

\[ + \frac{1}{\sqrt{2}} \sum_\omega \sqrt{G(\omega)} \ I \otimes \bar{S}(\omega) \otimes |\omega\rangle \otimes |1\rangle \otimes |1\rangle. \]  
\[ (92) \]

Observe the sign flip \( |\omega\rangle \leftrightarrow | - \omega\rangle \) and the bit flip \( |0\rangle \leftrightarrow |1\rangle \) in the final two lines. Using the above expression for \( RT \), it is now seen that the quantum discriminate \( Q = T^\dagger(RT) \) is given by

\[ Q = \frac{1}{2} \sum_\omega \left(1 - G(\omega)\right) \ S^\dagger(\omega)S(\omega) \otimes I \]  
\[ (93) \]

\[ + \frac{1}{2} \sum_\omega \left(1 - G(\omega)\right) \ I \otimes \bar{S}^\dagger(\omega)\bar{S}(\omega) \]  
\[ (94) \]

\[ + \frac{1}{2} \sum_{\omega,\nu} \sqrt{G(\omega)} \ G(\nu) \ S(\omega) \otimes \bar{S}^\dagger(\nu) \delta_{-\omega,\nu} \]  
\[ (95) \]

\[ + \frac{1}{2} \sum_{\omega,\nu} \sqrt{G(\omega)} \ G(\nu) \ S^\dagger(\nu) \otimes \bar{S}(\omega) \delta_{-\omega,\nu}. \]  
\[ (96) \]
To further simplify the above expression for $Q$, we use the following two elementary properties of the jump operators $S(\omega)$: (i) $S^\dagger(-\omega) = S(\omega)$ and (ii) $\sum_\omega S^\dagger(\omega)S(\omega) = I$. Note that it is essential for (ii) that $S$ is a reflection. For the sake of completeness, we provide a proof for (ii). We have

$$\sum_\omega S^\dagger(\omega)S(\omega) = \sum_\omega \left( \sum_{(k,\ell) \in J_\omega} P_\ell S^\dagger P_k \right) \left( \sum_{(m,n) \in J_\omega} P_m S P_n \right)$$

(97)

$$= \sum_\omega \sum_{(k,\ell) \in J_\omega} P_\ell S^\dagger P_k S P_n$$

(98)

$$= \sum_\omega \sum_{(k,\ell) \in J_\omega} P_\ell S^\dagger P_k S P_\ell$$

(99)

$$= \sum_{k,\ell} P_\ell S^\dagger P_k S P_\ell = S^\dagger S = I.$$  

(100)

We now obtain the final desired expression for the vectorized quantum discriminate $Q$

$$Q = I \otimes I + \sum_\omega \sqrt{G(\omega)G(-\omega)} \ S(\omega) \otimes \tilde{S}(\omega)$$

$$- \frac{G(\omega)}{2} \left( S^\dagger(\omega)S(\omega) \otimes I + I \otimes \tilde{S}^\dagger(\omega)\tilde{S}(\omega) \right).$$

(101)

Using the expression of $\hat{K}$ in (65), we see that the definition of the vectorized quantum discriminate $Q = I + \hat{K}$ coincides with the constructed block encoding $Q = T^\dagger RT$.

2.4. Gap amplification of quantum discriminate. In the previous two subsections, we considered the case of a single coupling operator $S$. Let us now show how to handle the general case of multiple coupling operators $S^\alpha$. Let $w_\alpha$ denote the corresponding weights. Recall that in the canonical form of a detailed balanced Lindbladian and the definition of a Davies generator the weights $w_\alpha$ are assumed to be non-negative and to sum up to 1.

The results in the previous two subsections show how to construct an isometry $T^\alpha$ for each $\alpha$ such that $Q^\alpha = T^{\alpha\dagger}RT^\alpha$, where $R$ is the reflection defined in (82) and (83). We define the isometry

$$T = \sum_\alpha T^\alpha \otimes \sqrt{w_\alpha}|\alpha\rangle.$$  

(102)

Let us use the abbreviation $R$ to denote the reflection $R \otimes I$, where $I$ acts on the register holding $|\alpha\rangle$. We now see that

$$Q = T^\dagger RT.$$  

(103)

The desired walk unitary is given by

$$W(\mathcal{L}) = R(2\Pi - I),$$  

(104)
where Π denotes the projector onto the image of the isometry T. This is a very well-known result in quantum algorithms. For the sake of completeness, we have included a proof of this result in “Appendix B”.

We point out that the quantum singular value transformation (QSVT) [2] enables us to directly construct the projector |σ⟩⟨σ| onto the eigenvector of Q with eigenvalue 1, that is, the purification |σ⟩, by invoking the block encoding O(1/√Δ) many times, where Δ is the spectral gap of Q (which is equal to the spectral gap of the Lindbladian). Being able to implement this projector (or the corresponding reflection) is what is really needed for quantum algorithms. Before the advent of QSVT, the usual approach to realize this projector was to perform quantum phase estimation of the walk unitary to distinguish the eigenphase 0 from the other eigenphases.

3. Quantum Algorithm for Szegedy Walk Unitaries for Davies Generators with Approximate Energy Estimation

In the preceding section, we assumed ideal energy estimation in our quantum algorithm for implementing Szegedy walk unitaries for Davies generators. We now remove this unphysical assumption and work with the method [4] for energy estimation. To state the performance of this energy estimation method, we need to first introduce the following rounding promise.

**Definition 5 (Rounding promise).** Let r be a positive integer and α ∈ (0, 1). A Hermitian matrix H with spectral decomposition

\[ H = \sum_k \varepsilon_k P_k \]  

is said to satisfy an \((r, \alpha)\)-rounding promise if for all its eigenvalues \(0 \leq \varepsilon_k < 1\) and for all \(x \in \{0, \ldots, 2^r\}\):

\[ |\varepsilon_k - \frac{x}{2^r}| \geq \frac{\alpha}{2^{r+1}} \]  

The rounding promise effectively disallows the eigenvalues \(\varepsilon_k\) of \(H\) from certain sub-intervals of \([0, 1)\). The definition above is chosen such that the total length of these disallowed subintervals is \(\alpha\), regardless of the value of \(r\). We acknowledge that guaranteeing a rounding-promise would demand a tremendous amount of knowledge about energies of Hamiltonians. It is not expected that many Hamiltonians in practice provably satisfy such a strong promise. But it seems likely that the energy estimation method still works sufficiently well even if the rounding promise is violated so it can be used a subroutine for quantizing Davies generators. As shown below, the rounding promise enables us to precisely analyze the method for quantizing Davies generators.

**Theorem 2 (Approximate energy estimation).** Assume that we are given access to a block encoding of a Hermitian matrix \(H = \sum_k \varepsilon_k P_k\) satisfying an \((r, \alpha)\)-rounding promise. Then, we can realize a quantum map \(\Phi\) that is \(\delta\)-close in \(\diamond\)-norm to the unitary energy estimation map \(U\) that acts on states\(^7\) \(|\psi\rangle \otimes |0^n\rangle\) as

\[ U(|\psi\rangle \otimes |0^n\rangle) = \sum_k P_k |\psi\rangle \otimes |\lfloor \varepsilon_k 2^r \rfloor\rangle. \]  

\(^7\) Note that action of \(U\) on states \(|\psi\rangle \otimes |z\rangle\) with \(z \neq 0^n\) can be arbitrary.
The query complexity with respect to the block encoding of \( H \) is bounded by

\[
O\left( \alpha^{-1} \log(\delta^{-1})(2^r + \log(\alpha^{-1})) \right).
\]  

(108)

The above result is proved in [4, Corollary 16. Improved Energy Estimation]. We emphasize that without any rounding promise any method for energy estimation will necessarily produce states close to

\[
\sum_k P_k \otimes \sum_x c_{k,x} |x\rangle.
\]  

(109)

where the magnitude of \( c_{k,x} \) depends on the distance between \( \varepsilon_k 2^r \) and \( x \). In words, instead of obtaining a single estimate for each \( k \), we would obtain a superposition of estimates. This is unavoidable as discussed in [4, 1 Preliminaries]. Roughly speaking, the reason is as follows: there are only a finite number of possible pointer values for the energies, whereas the energies can be arbitrary values in the interval \([0, 1)\).

It should not be possible to improve the scaling with \( 2^r \). It is known that highly precise energy estimation would make it possible to solve \( \text{PSPACE} \)-hard problems [32].

Using the above method for energy estimation, we can approximately determine the Bohr frequencies and also approximately realize the jump operators.

**Lemma 8** (Bohr frequency estimation and approximate jump operators). Given a reflection \( S \) and access to a block encoding of a Hermitian matrix \( H = \sum k \varepsilon_k P_k \) satisfying an \((r, \alpha)\)-rounding promise we can implement a quantum map \( \Psi \) that is \( \delta \)-close in \( \diamond \)-norm to the unitary \( V \) that acts on states \( |\psi\rangle \otimes |0^r\rangle \otimes |0^r\rangle \) as

\[
V(|\psi\rangle \otimes |0^r\rangle \otimes |0^r\rangle) = \sum_{k,\ell} P_k S P_\ell |\psi\rangle \otimes |[\varepsilon_k 2^r] - [\varepsilon_\ell 2^r] \rangle \otimes |0^r\rangle.
\]

(110)

The query complexity with respect to the block encoding of \( H \) is three times the query complexity of the method for energy estimation in (108).

**Proof.** The unitary \( V \) can be implemented using the unitary \( U \) in Theorem 2 twice and \( U^\dagger \) once and a unitary that performs integer subtraction. The circuit is composed of the following sub-circuits:

- apply \( U \) to compute \( [\varepsilon_k 2^r] \) into the energy register \( A \)
- apply the reflection \( S \)
- apply \( U \) to compute \( [\varepsilon_\ell 2^r] \) into the energy register \( B \)
- apply a unitary that subtracts the value stored in \( B \) from the value stored \( A \)
- apply \( U^\dagger \) to uncompute \( [\varepsilon_\ell 2^r] \) in \( B \)

\[ \square \]

**Theorem 3** (Quantizing Davies generators with approximate energy estimation). Given access to a block encoding of a Hermitian matrix \( H = \sum k \varepsilon_k P_k \) satisfying an \((r, \alpha)\)-rounding promise, we can realize a quantum map that is \( \delta \)-close in \( \diamond \)-norm to a block encoding of the quantum discriminate matrix \( \tilde{Q} \) corresponding to the Davies generator \( \tilde{L} \) for the approximate Hamiltonian

\[
\tilde{H} = \sum_k \frac{[\varepsilon_k 2^r]}{2^r} P_k.
\]

(111)
The query complexity with respect to the block encoding of $H$ is bounded by

$$O\left(\alpha^{-1} \log(\delta^{-1})(2^r + \log(\alpha^{-1}))\right).$$

(112)

**Proof.** The following observation is simple yet it greatly improves the analysis. Observe that the unitary $V$ in (110) can be interpreted as performing *ideal* Bohr frequency estimation for the *approximate* Hamiltonian $\tilde{H}$. We can write its action\(^8\) as

$$V(|\psi\rangle \otimes |0^r\rangle) = \sum_{\tilde{\omega}} S(\tilde{\omega}) |\psi\rangle \otimes |\tilde{\omega}\rangle,$$

(113)

where $\tilde{\omega}$ runs over the Bohr frequencies of the approximate Hamiltonian $\tilde{H}$ and $S(\tilde{\omega})$ denote the corresponding jump operators for $\tilde{H}$. Now everything can be analyzed exactly as in the previous section by replacing $H$ with $\tilde{H}$, $\omega$ with $\tilde{\omega}$, $S(\omega)$ with $S(\tilde{\omega})$, etc. Of course, we also have to take into account that $V$ (or its complex conjugate version) cannot be realized exactly, but is only approximated by a quantum map that is $\delta$-close in $\cdash$-norm to the unitary map $V$. The query complexity in (112) follows from the discussion in the lemma. \(\square\)

**Remark 3.** To summarize, we accomplish the following. Given a block encoding of a Hamiltonian $H$ with an $(r, \alpha)$ rounding promise, we can quantize a Davies generator $\tilde{L}$ for the approximate Hamiltonian $\tilde{H}$. Note that the eigenvector of the corresponding approximate walk unitary $\tilde{W}$ with eigenphase 0 is the purification

$$|\tilde{\sigma}\rangle = (\tilde{\sigma} \otimes I)|\Omega\rangle$$

(114)

where $\tilde{\sigma}$ denotes the thermal state for $\tilde{H}$ at the inverse temperature $\beta$. One can see that

$$\langle \sigma | \tilde{\sigma} \rangle = \frac{1}{\sqrt{Z_\tilde{Z}}} \sum_k \sqrt{e^{-\beta(\tilde{\epsilon}_k + \tilde{\epsilon}_k)}} \text{Tr}(P_k)$$

(115)

$$\geq \sqrt{\frac{Z_\tilde{Z}}{Z}}$$

(116)

$$\geq e^{-\beta/2^{r-1}} \geq 1 - \beta/2^{r-1},$$

(117)

where we have used that $\tilde{\epsilon}_k = [\epsilon_k 2^r]/2^r < \epsilon_k$ for the first inequality. To ensure that the overlap between the ideal and approximate purifications is at least $1 - \kappa$, we need to have $r > \log_2(\beta/\kappa)$.

It is also important to point out that in general the correct Davies generator $L$ and the approximate Davies generator $\tilde{L}$ will have different spectral gaps. The difference between these gaps will decrease with increasing $r$.

---

\(^8\) We omit the energy register $B$ whose value is always reversibly reset to the initial state $|0^r\rangle$. 
4. Existence of Szegedy Walk Unitaries for Arbitrary Detailed Balanced Lindbladians

The goal of this section is to establish the existence of Szegedy walk unitaries for general detailed balanced Lindbladians by reducing their canonical form to the special case of Davies generators with reflections as coupling operators.

Our main result is the theorem below, which formally proves the existence of the Szegedy walk unitary.

**Theorem 4 (Quantization of detailed balanced Lindbladians).** Assume that the Lindbladian $\mathcal{L}$ is detailed balanced with respect to the state $\sigma$. Then, there exists a corresponding walk unitary $W(\mathcal{L})$ such that its unique eigenvector with eigenphase $0$ is the purification $|\sigma\rangle = (\sigma^{1/2} \otimes I)|\Omega\rangle$ and its phase gap is quadratically larger than the spectral gap of the Lindbladian $\mathcal{L}$. It can be obtained by standard methods for spectral gap amplification applied to the block encoding of the vectorized quantum discriminate matrix $Q$ for $\mathcal{L}$.

**Proof.** We may assume that the Lindbladian $\mathcal{L}$ is in canonical form as in Definition 3 since it is detailed balanced with respect to $\sigma$.

It will be convenient to use $\theta$ instead of $\omega$ to denote the Bohr frequencies of the Hamiltonian $h = -\ln \sigma$. For each Bohr frequency $\theta$, we now define the operator $\Lambda_\theta(A)$ by

$$\Lambda_\theta(A) = \sum_{(k,\ell)\in J_\theta} P_k A P_\ell,$$

(118)

where $A$ is an arbitrary matrix. We now argue that for each $\alpha$ there always exists a Hermitian matrix $X^\alpha$ such that the jump operators $X^\alpha(\theta)$ for all $\theta$ arise from $X^\alpha$ by the projection

$$\Lambda_\theta(X^\alpha) = X^\alpha(\theta).$$

(119)

This is seen as follows. Observe that the condition in (33) in the canonical form for detailed balanced Lindbladians means that the jump operators $X^\alpha(\theta)$ are all eigenvectors of the so-called modular operator $\Delta_\sigma$ defined by $\Delta_\sigma(A) = \sigma A\sigma^{-1}$. The modular operator is a Hermitian operator with respect to the Hilbert-Schmidt trace inner product. This implies that these eigenvectors $X^\alpha(\theta)$ are necessarily all orthogonal to each other as the eigenvalues $e^{-\theta}$ are all different. It turns out that the operators $\Lambda_\theta$ are precisely the orthogonal projectors onto the eigenspaces of $\Delta_\sigma$ with eigenvalues $e^{-\theta}$. The desired matrix $X^\alpha$ is given by $X^\alpha = \sum_\theta X^\alpha(\theta)$.

We need to assume that the Hermitian matrices $X^\alpha$ satisfy the norm constraint $\|X^\alpha\| \leq 1$. This norm constraint implies that there exist reflections $S^\alpha$ that are block encodings of the matrices $X^\alpha$ of the form

$$X^\alpha = (|0\rangle \otimes I) S^\alpha (|0\rangle \otimes I).$$

(120)

It is always possible to embed a Hermitian matrix of norm less or equal to 1 inside a reflection that acts on the original register plus a single ancilla register, that is, we may choose $s = 1$.

Using these block encodings, we generalize the circuits for $T_0$ and $T_1$ as follows. To simplify the discussion, we consider the case where $\alpha$ is arbitrary but fixed. We drop the index $\alpha$ in the following (Fig. 4).

It suffices to explain the circuit for $T_0$ as $T_1$ works analogously. We have added the new register block, anc1, and anc2 (compare to the circuits in Fig. 1.) The two
system registers \text{sys}1 and \text{sys}2 have the ancilla registers \text{anc}1 and \text{anc}2 attached, respectively. Both ancilla registers are prepared in $|0\rangle_s$. The state (either 0, 1, 2) of the block register indicates which block of $S$ is selected. Let $P_0 = |0\rangle\langle 0|$ and $P_1 = I - P_0$. The state 0 indicates the diagonal block $P_0SP_0$ encoding $X$, the state 1 the off-diagonal blocks $P_0SP_1$ or $P_1SP_0$, and the state 2 the diagonal block $P_1SP_1$. Let \( C \) denote the cyclic shift operator $|x\rangle \mapsto |x+1 \pmod{3}\rangle$. The controlled cyclic shift operator is defined by $P_0 \otimes I + P_1 \otimes C$. The controlled filter rotation $W$ is applied only if the state of block is $|0\rangle$, which means that the state of \text{anc}2 was $|0\rangle_s$ before and after the application of $S$. The gate $\Phi$ and $\Phi^\dagger$ denotes phase estimation with respect to the Hamiltonian $h$ acting on \text{sys}2 and are used to record the Bohr frequency in the register \text{freq}.

As before we use $\theta$ (instead of $\omega$) to denote the Bohr frequencies of the Hamiltonian $h$. Define the “macro” jump operator $S(\theta)$ by

$$S(\theta) = \sum_{(k, \ell) \in J_\theta} (I \otimes P_k)S(I \otimes P_\ell),$$

where the projectors $P_k$ and $P_\ell$ act on \text{sys}2. For $c \in \{0, 1, 2\}$, define the “micro” jump operators $S(c, \theta)$ acting on the tensor product of \text{anc}1 and \text{sys}1 by

$$S(0, \theta) = (Q_0 \otimes I)S(\theta)(Q_0 \otimes I)$$

$$S(1, \theta) = (Q_0 \otimes I)S(\theta)(Q_1 \otimes I) + (Q_1 \otimes I)S(\theta)(Q_0 \otimes I)$$

$$S(2, \theta) = (Q_1 \otimes I)S(\theta)(Q_1 \otimes I).$$

Here the projectors $Q_0$ and $Q_1$ act on \text{anc}2. Observe that that for all $\theta$ we have

$$(|0\rangle \otimes I)S(0, \theta)(|0\rangle \otimes I) = X(\theta).$$

The corresponding filter functions $G(c, \theta)$ are defined by

$$G(0, \theta) = G(\theta)$$

$$G(1, \theta) = 0$$

$$G(2, \theta) = 0.$$
Now assume that block and freq are properly initialized. We assume that the ancilla registers anc1 and anc2 are arbitrary. We obtain as the explicit expressions for the subisometries \( T_0 \) and \( T_1 \)

\[
T_0 = \sum_{c, \theta} S(c, \theta) \otimes I \otimes |c, \theta\rangle \otimes \left( \sqrt{1 - G(c, \theta)} |0\rangle + \sqrt{G(c, \theta)} |1\rangle \right)
\]

\[
T_1 = \sum_{c, \theta} I \otimes \tilde{S}(c, \theta) \otimes |c, \theta\rangle \otimes \left( \sqrt{1 - G(c, \theta)} |0\rangle + \sqrt{G(c, \theta)} |1\rangle \right).
\]

Note that the first (from the left) tensor component refers to anc2 and sys2 and the second tensor component to anc1 and sys1, and the third tensor component to block and bohr.

The full isometry \( T \) is obtained by coherently adding the above two sub-isometries \( T_0 \) and \( T_1 \) and is given by

\[
T = \sum_{c, \theta} S(c, \theta) \otimes I \otimes |c, \theta\rangle \otimes \left( \sqrt{1 - G(c, \theta)} |0\rangle + \sqrt{G(c, \theta)} |1\rangle \right) \otimes |0\rangle + \sum_{c, \theta} I \otimes \tilde{S}(c, \theta) \otimes |c, \theta\rangle \otimes \left( \sqrt{1 - G(c, \theta)} |0\rangle + \sqrt{G(c, \theta)} |1\rangle \right) \otimes |1\rangle.
\]

We call a pair of the form \((c, \theta)\) an extended Bohr frequency, where \(c \in \{0, 1, 2\}\) and \(\theta\) is a Bohr frequency of \(h\). We reserve the symbol \(\omega\) to exclusively denote extended Bohr frequencies. For an arbitrary extended Bohr frequency \(\omega = (c, \theta)\), we define \(-\omega = (c, -\theta)\). Observe that this definition makes sense as the property (i)

\[
S(-\omega) = S^\dagger(\omega)
\]

holds. It is straightforward to check that the property (ii)

\[
\sum_\omega S^\dagger(\omega)S(\omega) = I
\]

holds as well, where \(I\) denotes the identity acting on the tensor product anc1 and sys1.

Using the definition of \(-\omega\) for extended Bohr frequencies, we now define the reflection operator \(R\) as

\[
R = I \otimes I \otimes I \otimes |0\rangle \langle 0| \otimes I
\]

\[
+ I \otimes I \otimes F \otimes |1\rangle \langle 1| \otimes X.
\]

Observe that \(R\) applies the flip \(\omega = (c, \theta) \leftrightarrow -\omega = (c, -\theta)\) and the bit flip \(0 \leftrightarrow 1\) whenever the control qubit filter is in the state \(|1\rangle\).

The entire analysis of the method for quantizing Davies generators now carries over because properties (i) and (ii) hold. We obtain a block encoding of the matrix

\[
I \otimes I + \sum_\omega \sqrt{G(\omega)G(-\omega)} S(\omega) \otimes \tilde{S}(\omega) - \frac{G(\omega)}{2} \left( S^\dagger(\omega)S(\omega) \otimes I + I \otimes \tilde{S}^\dagger(\omega)\tilde{S}(\omega) \right).
\]

This is not yet the desired quantum discriminate \(Q\) of the Lindbladian \(L\) because the ancilla registers have not been specialized. The first tensor component corresponds to
anc1 and sys1 and the second tensor component to anc2 and sys2. Observe now that we can drop all terms with \( c = 1, 2 \) because the corresponding filter functions \( G(c, \theta) \) are 0. Therefore, if we initialize both ancilla registers anc1 and anc2 in \( |0\rangle \), we obtain the desired block encoding

\[
Q = I \otimes I + \sum_{\theta} \sqrt{G(\theta)G(-\theta)} X(\theta) \otimes \bar{X}(\theta) - \frac{G(\theta)}{2} \left( \bar{X}^{\dagger}(\theta)X(\theta) \otimes I + I \otimes \bar{X}^{\dagger}(\theta)\bar{X}(\theta) \right),
\]

where we used using the identity in (125).

To summarize the above construction shows that any detailed balanced Lindbladian can be written as a Davies generator in a larger Hilbert space and all coupling operators of the Davies generator are reflections. It enables us to reduce the problem of quantizing detailed balanced Lindbladians to the special case of Davies generators.

Remark 4. It is important to realize that the above construction only proves the existence of Szegedy walk unitaries for arbitrary detailed balanced Lindbladians. It does not necessarily yield an efficient quantum algorithm for implementing these walk unitaries.

If we are given an arbitrary Lindbladian \( \mathcal{L} \) that is detailed balanced with respect to \( \sigma \), then the corresponding Hamiltonian \( h = -\ln \sigma \) arising in the canonical form is not necessarily a physically realistic Hamiltonian, or a Hamiltonian that can be efficiently encoded on a quantum computer.

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Declarations

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Appendix A: Quantum–Quantum Metropolis Algorithm and Its Limitations

We mentioned in the introduction that the quantum-quantum Metropolis algorithm (QQMA) as presented in [23] only works when the spectrum of the Hamiltonian is non-degenerate. The goal of this appendix is to discuss the reasons for this limitation. One of the problems of QQMA in the degenerate case is the implementation of the projector \( \Lambda_1 \) defined below equation (6) in [23]. Before explaining this issue in detail, let us state some facts to put everything better into context.

It is stated that QQMA prepares a coherent encoding of the thermal state

\[
|\alpha_0\rangle = \sum_{i=0}^{N-1} \sqrt{\frac{e^{-\beta E_i}/Z_\beta}{|i\rangle}} \text{ with } |i\rangle \equiv |\varphi_i\rangle \otimes |\tilde{\varphi}_i\rangle.
\]

(A1)
where $|\varphi_i\rangle$ denote the eigenstates of the Hamiltonian with corresponding eigenvalues $E_i$. The tilde in $|\tilde{\varphi}_i\rangle$ denotes complex conjugation of the entries of the vectors $|\varphi_i\rangle$.

When the spectrum of the Hamiltonian is degenerate (and $\beta > 0$), it may seem at first that there could exist nonequivalent coherent encodings that depend on the particular chosen eigenbasis $|\varphi_i\rangle$. More precisely, let $U$ be any unitary that commutes with the Hamiltonian $H$ and set $|\psi_i\rangle = U|\varphi_i\rangle$ for $i = 0, \ldots, N - 1$. Define the corresponding "alternative" coherent encoding

$$|\beta_0\rangle = \sum_{i=0}^{N-1} \sqrt{\frac{e^{-\beta E_i}}{Z_\beta}} |\psi_i\rangle \otimes |\tilde{\psi}_i\rangle. \quad (A2)$$

Clearly, we have $(U \otimes \tilde{U})|\alpha_0\rangle = |\beta_0\rangle$. However, it already holds that $|\alpha_0\rangle = |\beta_0\rangle$ so that the coherent encoding does not depend on the chosen eigenbasis.

The central problem of QQMA in the degenerate case is the implementation of the projector $\Lambda_1$ defined below equation (6) in [23]. The operator $\Lambda_1$ is defined there as

$$\Lambda_1 = \sum_{i=0}^{N-1} |i\rangle \langle i| \otimes |0\rangle \langle 0| = \sum_{i=0}^{N-1} |\psi_i\rangle \langle \psi_i| \otimes |\tilde{\psi}_i\rangle \langle \tilde{\psi}_i| \otimes |0\rangle \langle 0|. \quad (A3)$$

It is obvious that only energy measurements (or measurements of energy differences) are performed in QQMA. It is essential to observe that it is impossible to realize this projector with energy measurements alone if the spectrum is degenerate. The issue is that the above projector does depend on the chosen eigenbasis $|\varphi_i\rangle$. More precisely, let

$$\Lambda'_1 = \sum_{i=0}^{N-1} |\psi_i\rangle \langle \psi_i| \otimes |\tilde{\psi}_i\rangle \langle \tilde{\psi}_i| \otimes |0\rangle \langle 0|. \quad (A4)$$

The problem is now that these two projectors are not equal, that is $\Lambda_1 \neq \Lambda'_1$. (A simple example that demonstrates inequality of the projectors $\Lambda_1$ and $\Lambda'_1$ is $|\phi_0\rangle = |0\rangle$, $|\phi_1\rangle = |1\rangle$ and $|\psi_0\rangle = |+\rangle$, $|\psi_1\rangle = |−\rangle$.) This is in contrast to the situation for the states $|\alpha_0\rangle$ and $|\beta_0\rangle$. Clearly, if one can only compare energies, then one cannot distinguish between different bases of a degenerate Hamiltonian. Thus, the authors implicitly assume that the Hamiltonian has non-degenerate spectrum in [23].

While projectors of the form $\Lambda_1$ are unphysical, it is possible to implement a projector (assuming perfect energy estimation) of the form

$$\sum_{E} P_E \otimes \tilde{P}_E, \quad (A5)$$

where $E$ ranges over the eigenvalues of the Hamiltonian and $P_E$ over the projectors onto the corresponding eigensubspaces.

Observe that in the classical setting there is a way out. Although some energies of the classical Hamiltonian are equal, there is always a unique preferred basis— namely, the computational basis. But such preferred eigenbasis does not exist in the quantum case for degenerate Hamiltonians unless some additional assumptions are made.
Appendix B: Gap Amplification

The appendix is an adaptation of [33, 17.2 How to quantize a Markov chain].

**Definition 6 (Quantization).** Let $Q \in \mathbb{C}^{M \times M}$ be a Hermitian matrix, $|\varphi_1\rangle, \ldots, |\varphi_M\rangle$ an orthonormal basis of $\mathbb{C}^M$ consisting of eigenvectors of $Q$ with eigenvalues $\lambda_1 = 1 \geq \lambda_2 = 1 - \Delta \geq \lambda_3 \geq \ldots \geq \lambda_M \geq -1$. We refer to $\Delta$ as the classical gap.

Assume that $T \in \mathbb{C}^{N \times M}$ is an isometry from $\mathbb{C}^M$ to $\mathbb{C}^N$ and $S \in \mathbb{C}^{N \times N}$ is a reflection acting on $\mathbb{C}^N$ such that

$$T^\dagger S T = Q. \tag{B6}$$

Then, we define the quantization of $Q$ to be

$$U = S(2\Pi I - I) \in \mathbb{C}^{N \times N}, \tag{B7}$$

where $\Pi = TT^\dagger$ is an orthogonal projector in $\mathbb{C}^{N \times N}$. Let $A$ denote the image of $T$ (or equivalently the image of $\Pi$). We refer to the value $\theta = \arccos(1 - \Delta)$ as the phase gap of the quantization $U$ of $Q$.

For $j \in \{1, \ldots, M\}$, define the states

$$|\chi_j\rangle = T|\varphi_j\rangle \in \mathbb{C}^N. \tag{B8}$$

Let $B$ be the subspace $A + S A$, where $S A = \{S|\chi\rangle : |\chi\rangle \in A\}$, and $B^\perp$ the orthogonal complement of $B$.

**Lemma 9.** The subspace spanned $|\chi_1\rangle, \ldots, |\chi_M\rangle$ coincides with the subspace $A$.

**Proof.** We have $\sum_{j \in [M]} |\chi_j\rangle \langle \chi_j| = \sum_{j \in [M]} T|\varphi_j\rangle \langle \varphi_j| T^\dagger = TT^\dagger = \Pi. \tag{B9}$

**Theorem 5 (Spectrum of quantization).** The subspace $B$ and its orthogonal complement $B^\perp$ are invariant under $U$. The spectrum of $U$ restricted to $B$ is as follows:

1. For $j = 1$, the one-dimensional subspace $\mathcal{V}_1$ spanned by $|\chi_1\rangle$ is invariant under $U$ and the eigenvector of $U$ in $\mathcal{V}_1$ is

$$|\psi_1\rangle = |\chi_1\rangle \in B \tag{B9}$$

with eigenvalue 1.

2. For $j \geq 2$, the two-dimensional subspace $\mathcal{V}_j$ spanned by $|\chi_j\rangle$ and $S|\chi_j\rangle$ is invariant under $U$ and the two orthogonal eigenvectors of $U$ in $\mathcal{V}_j$ are

$$|\psi_j^\pm\rangle = |\chi_j\rangle - \mu_j^\pm S|\chi_j\rangle \in B \tag{B10}$$

with corresponding eigenvalues $\mu_j^\pm$, where

$$\mu_j^\pm = \lambda_j \pm i\sqrt{1 - \lambda_j^2} = e^{\pm i \arccos(\lambda_j)}. \tag{B11}$$
Proof. Let \( j \) be arbitrary. We have

\[
U|\chi_j\rangle = S(2\Pi - I)|\chi_j\rangle \tag{B12}
\]

\[
= S(TT^\dagger - I)T|\varphi_j\rangle \tag{B13}
\]

\[
= 2ST|\varphi_j\rangle - ST|\varphi_j\rangle \tag{B14}
\]

\[
= S|\chi_j\rangle \tag{B15}
\]

and

\[
US|\chi_j\rangle = S(2\Pi - I)ST|\varphi_j\rangle \tag{B16}
\]

\[
= S(2TT^\dagger - I)ST|\varphi_j\rangle \tag{B17}
\]

\[
= (2STT^\dagger ST - T)|\varphi_j\rangle \tag{B18}
\]

\[
= (2STQ - T)|\varphi_j\rangle \tag{B19}
\]

\[
= (2\lambda_j ST - T)|\varphi_j\rangle \tag{B20}
\]

\[
= (2\lambda_j S - I)|\chi_j\rangle. \tag{B21}
\]

We see that the subspace spanned by \(|\chi_j\rangle\) and \(S|\chi_j\rangle\) is invariant under \(U\) for each \(j\). Thus, we can find eigenvectors of \(U\) within this subspace.

First, we consider the case \(j = 1\). We have

\[
1 = \langle \varphi_1 | Q | \varphi_1 \rangle = \langle \varphi_1 | T^\dagger ST | \varphi_1 \rangle = \langle \chi_1 | S | \chi_1 \rangle, \tag{B22}
\]

implying that \(|\chi_1\rangle\) is an eigenvector of \(S\) with eigenvalue 1. Therefore, the subspace \(\mathcal{V}_1\) is one-dimensional. Moreover, we have

\[
U|\chi_1\rangle = S(2\Pi - I)|\chi_1\rangle = S|\chi_1\rangle = |\chi_1\rangle, \tag{B23}
\]

where we used \(\Pi|\chi_1\rangle = TT^\dagger T|\varphi_1\rangle = T|\varphi_1\rangle = |\chi_1\rangle\), implying that \(|\chi_1\rangle\) is an eigenvector of \(U\) with eigenvalue 1.

Second, we consider the case \(j \geq 2\), that is, \(\lambda_j\) is bounded away from 1 by at least the spectral gap \(\Delta\). Let

\[
|\psi_j^\pm\rangle = |\chi_j\rangle - \mu_j^\pm S|\chi_j\rangle \tag{B24}
\]

be an ansatz for the eigenvectors of \(U\) supported on \(\mathcal{V}_j\). We have

\[
U|\psi_j^\pm\rangle = S|\chi_j\rangle - \mu_j^\pm (2\lambda_j S - I)|\chi_j\rangle \tag{B25}
\]

\[
= \mu_j^\pm |\chi_j\rangle - (2\lambda_j \mu_j^\pm - 1) S|\chi_j\rangle. \tag{B26}
\]

Therefore, \(|\psi_j^\pm\rangle\) is an eigenvector of \(U\) with eigenvalue \(\mu_j^\pm\) provided that

\[
(\mu_j^\pm)^2 - 2\lambda_j \mu_j^\pm + 1 = 0, \tag{B27}
\]

that is,

\[
\mu_j^\pm = \lambda_j \pm i \sqrt{1 - \lambda_j^2} = e^{\pm i \arccos(\lambda_j)}. \tag{B28}
\]

This implies that the subspaces \(V_j\) with \(j \geq 2\) are two-dimensional.

The union of all the subspaces \(\mathcal{V}_j\) is \(\mathcal{B}\), implying that \(\mathcal{B}\) and its orthogonal complement \(\mathcal{B}^\perp\) are invariant under \(U\). \qed
Lemma 10 (Lower bound on quantum gap). Let $\Delta$ denote the classical gap of $Q$. The quantum gap of the corresponding unitary $U$ is $\theta = \arccos(1-\Delta)$ and is quadratically larger than the classical gap because

$$\theta \geq \sqrt{2\Delta}. \quad (B29)$$

Proof. Write the second largest eigenvalue as $\lambda_2 = 1 - \Delta = \cos(\theta)$ for a suitable $\theta$. We have

$$1 - \Delta = \cos(\theta) \geq 1 - \frac{\theta^2}{2}, \quad (B30)$$

which implies the bound $\theta \geq \sqrt{2\Delta}$. $\square$

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