EFFICIENT QUANTUM GIBBS SAMPLERS WITH KUBO–MARTIN–SCHWINGER DETAILED BALANCE CONDITION

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Abstract. Lindblad dynamics and other open-system dynamics provide a promising path towards efficient Gibbs sampling on quantum computers. In these proposals, the Lindbladian is obtained via an algorithmic construction akin to designing an artificial thermostat in classical Monte Carlo or molecular dynamics methods, rather than treated as an approximation to weakly coupled system-bath unitary dynamics. Recently, Chen, Kastoryano, and Gilyén (arXiv:2311.09207) introduced the first efficiently implementable Lindbladian satisfying the Kubo–Martin–Schwinger (KMS) detailed balance condition, which ensures that the Gibbs state is a fixed point of the dynamics and is applicable to non-commuting Hamiltonians. This Gibbs sampler uses a continuously parameterized set of jump operators, and the energy resolution required for implementing each jump operator depends only logarithmically on the precision and the mixing time. In this work, we build upon the structural characterization of KMS detailed balanced Lindbladians by Fagnola and Umanità, and develop a family of efficient quantum Gibbs samplers that only use a discrete set of jump operators (the number can be as few as one). Our methodology simplifies the implementation and the analysis of Lindbladian-based quantum Gibbs samplers, and encompasses the construction of Chen, Kastoryano, and Gilyén as a special instance.

1. Introduction

For a given quantum Hamiltonian $H \in \mathbb{C}^{N\times N}$, preparing the associated Gibbs state $\sigma_\beta = e^{-\beta H}/\mathcal{Z}_\beta$ (also called quantum Gibbs sampling) has a wide range of applications in condensed matter physics, quantum chemistry, and optimization. Here $N = 2^n$ is the dimension of the underlying Hilbert space, β is the inverse temperature, and $\mathcal{Z}_\beta = \mathrm{tr}(e^{-\beta H})$ is the partition function. We assume efficient quantum access to the Hamiltonian simulation $\exp(-itH)$. The cost of a quantum algorithm is often dominated by the total Hamiltonian simulation time of H.

The Davies generator [Dav74, Dav76, Dav79], which is in the form of a Lindbladian (or Lindblad generator) [Lin76, GKS76], satisfies the desirable property that the Gibbs state is a fixed point of the generated dynamics, and hence can be viewed as a natural candidate for quantum Gibbs samplers. The Davies generator is typically derived as a simplified representation of weakly interacting system-bath models, following the Born-Markov-Secular[1] approximation route [BP02, Lid19]. Thus its applicability range seems to be constrained by the limitations of these approximations. However, there has been a recent revival of interest in designing quantum Gibbs samplers based on the Lindblad dynamics [ML20, RWW23, CB21, CKBG23, CKG23, WT23]. These Lindbladians are constructed purely algorithmically, and may not mimic specific system-bath unitary dynamics in nature.

The key object in these Lindblad dynamics-based approaches is the following frequency-dependent jump operator

$$\widehat{A}^a_f(\omega) := \int_{-\infty}^{\infty} f(t) e^{-i\omega t} e^{iHt} A^a e^{-iHt}\,\mathrm{d}t, \quad \omega \in \mathbb{R}\,, \tag{1.1}$$

which is a f-weighted Fourier transform of the Heisenberg evolution $A^a(t) := e^{iHt}A^a e^{-iHt}$ of A^a. Here $f : \mathbb{R} \to \mathbb{C}$ is a filtering function that is central to this work and will be discussed in detail, and $\{A^a\}_{a\in\mathcal{A}}$ is a set of (frequency-independent) coupling operators provided by the user, which represent the coupling between the system and the fictitious environment, akin to designing an artificial thermostat

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[1]The secular approximation is also referred to as the rotating wave approximation (RWA).

in classical Monte Carlo or molecular dynamics methods [FS02]. The choice of $\{A^a\}_{a\in\mathcal{A}}$ can be flexible and relatively simple (such as Pauli operators). The Lindblad generator for the algorithmic purpose is then formulated as

$$\mathcal{L}^\dagger[\rho] = -i[G,\rho] + \sum_{a\in\mathcal{A}} \int_{-\infty}^{\infty} \gamma(\omega) \left(\widehat{A}^a_f(\omega)\rho \left(\widehat{A}^a_f(\omega)\right)^\dagger - \frac{1}{2}\left\{ \left(\widehat{A}^a_f(\omega)\right)^\dagger \widehat{A}^a_f(\omega), \rho \right\} \right) \mathrm{d}\omega\,. \tag{1.2}$$

Here $-i[G,\cdot]$ is called the coherent part of the dynamics, and the simplest choices are $G = H$ (system Hamiltonian) or $G = 0$ (no coherent term). The remaining term on the right-hand side of Eq. (1.2) is referred to as the dissipative part. In particular, the Davies generator corresponds to taking $f(t) \equiv 1$, with a carefully chosen function $\gamma : \mathbb{R} \to \mathbb{R}$, and a coherent part $-i[H,\cdot]$ (see Section 2.1).

The Gibbs state is a fixed point of the Lindblad dynamics if $\mathcal{L}^\dagger[\sigma_\beta] = 0$. A sufficient condition to ensure this is that the generator $\mathcal{L}$ satisfies certain quantum detailed balance conditions (DBC). Here $\mathcal{L}$ and $\mathcal{L}^\dagger$ are adjoint to each other with respect to the Hilbert–Schmidt inner product. For a given precision $\epsilon > 0$, we define the mixing time of the dynamics generated by $\mathcal{L}^\dagger$ as

$$t_{\mathrm{mix}} := \inf\left\{ t \geq 0\,;\ \left\| e^{t\mathcal{L}^\dagger}(\rho) - \sigma_\beta \right\|_1 \leq \epsilon,\ \forall\, \text{quantum state } \rho \right\}, \tag{1.3}$$

where $\|\cdot\|_1$ denotes the trace norm. It is worth mentioning that the quantum DBC is also instrumental for proving the finite mixing time (if it is the case), and its scaling with respect to β and the system size [TKR+10, KT13, BCG+23, RFA24]. However, due to the non-commutativity of operators in quantum mechanics, there is no unique definition of quantum DBC [TKR+10, CM17, CM20].

1.1. **Related works.** The most widely studied form of quantum DBC is in the sense of Gelfand–Naimark–Segal (GNS). The seminal result by Alicki [Ali76] states that any Lindblad generator satisfying the GNS DBC must choose $f(t) \equiv 1$ in Eq. (1.2), leading to the same dissipative part as in the Davies generator. Since this filtering function does not decay in t, the exact implementation of $\widehat{A}^a_f(\omega)$ requires simulating the Heisenberg evolution $A^a(t)$ for an infinitely long period. This implies that in the frequency space, the energy levels of H have to be distinguished to infinite precision, which cannot be achieved in general, except for some special systems such as Hamiltonians with commuting terms. It is possible to select certain decaying filter functions f in (1.2) such that $\mathcal{L}$ approximates a Davies generator, while these approximate generators cannot satisfy the GNS DBC and their fixed points are not known *a priori*. Consequently, estimating the deviation of the fixed point of the approximate dynamics from σ_β involves tracking the accumulated error along the dynamic trajectory. In order to approximate the Gibbs state to precision ϵ, the dynamics should distinguish the energy levels of H to precision $\mathrm{poly}(\beta^{-1}t_{\mathrm{mix}}^{-1}\epsilon)$, where t_{mix} is given in Eq. (1.3) [CKBG23, Theorems I.1, I.3]. It means that the integral in Eq. (1.1) could be truncated to $T = \mathrm{poly}(\beta t_{\mathrm{mix}}\epsilon^{-1})$. However, this cost may still be prohibitively high for practical applications.

Recently, [CKG23] introduced the first algorithm that requires a finite energy resolution in constructing $\widehat{A}^a_f(\omega)$, where $\mathcal{L}^\dagger$ in Eq. (1.2) exactly satisfies a less stringent version of DBC called the Kubo–Martin–Schwinger (KMS) DBC. It involves a nontrivial choice of the coherent term G that is neither H or 0. Under the KMS DBC, the Gibbs state σ_β remains a fixed point of the Lindblad dynamics, and one no longer needs to keep track of the accumulated deviation from the trajectory generated by a Davies-like generator. In this setup, to prepare σ_β to precision ϵ, the integral in Eq. (1.1) can be truncated to $T = \mathcal{O}(\beta \log(t_{\mathrm{mix}}/\epsilon))$ [CKG23, Theorem I.2].

The integral with respect to ω in Eq. (1.2) involves a continuously parameterized set of jump operators if $\gamma(\omega)$ is a continuous function. Although one can discretize such an integral using a quadrature scheme, the algorithm must be meticulously designed to efficiently simulate the resulting Lindblad dynamics [CW17, CKBG23, CKG23]. To the best of our knowledge, high-order Lindblad simulators designed for a finite number of jump operators, which allow for simpler implementations [LW23, DLL24], are not suitable for this task.

1.2. **Contribution.** In parallel to Alicki's characterization of Lindblad generators satisfying the GNS DBC, Fagnola, and Umanità [FU07, FU10] have prescribed the necessary and sufficient conditions for a quantum Markov semigroup to satisfy the KMS DBC. This leads to a set of conditions on the jump operators and the Hamiltonian for its corresponding Lindblad generator (also see [AC21]). Building upon these works, we introduce a family of quantum Gibbs samplers satisfying the KMS DBC. This includes the construction of [CKG23] as a special instance. In particular, $\gamma(\omega)$ can be chosen to be a discrete sum of δ functions, leading to a *finite* number of jump operators. In fact, it is sufficient to choose $\gamma(\omega)=\delta(\omega)$, which means a single jump operator if $|\mathcal{A}|=1$. Our jump operators can be constructed using the standard linear combination of unitaries (LCU) routine [BCC+14, GSLW19]. As a result, our Lindblad dynamics can be efficiently simulated using *any* high-order simulation algorithms, including those in [LW23, DLL24]. In addition, we show that this new family of Gibbs samplers enables the selection of $f(t)$, whose Fourier transform is smooth and compactly supported. This approach simplifies the error analysis for controlling the discretization error, through the application of the Poisson summation formula. Table 1 compares the performance of a number of quantum Gibbs samplers based on the Lindblad dynamics.

Algorithms	**Properties**				**Remark**
	Detailed balance	Truncation time	Jump #	Total cost	
[CB21]	$\approx$ GNS	N/A	∞	$\mathrm{poly}(\beta\epsilon^{-1}t_{\mathrm{mix}})$	Weak coupling Refreshable bath
[RWW23, Theorem 1]	$\approx$ GNS	$\widetilde{\mathcal{O}}(\beta\epsilon^{-2})$	∞	$\widetilde{\mathcal{O}}(\beta^3 t_{\mathrm{mix}}\epsilon^{-7})$	Rounding promise
[CKBG23, Theorem I.1]	$\approx$ GNS	$\widetilde{\mathcal{O}}(\beta t_{\mathrm{mix}}^2\epsilon^{-2})$	∞	$\widetilde{\mathcal{O}}(\beta t_{\mathrm{mix}}^3\epsilon^{-2})$	Rectangular filter
[CKBG23, Theorem I.3]	$\approx$ GNS	$\widetilde{\mathcal{O}}(\beta t_{\mathrm{mix}}\epsilon^{-1})$	∞	$\widetilde{\mathcal{O}}(\beta t_{\mathrm{mix}}^2\epsilon^{-1})$	Gaussian filter
[CKG23, Theorem I.2]	KMS	$\widetilde{\mathcal{O}}(\beta\log(t_{\mathrm{mix}}/\epsilon))$	∞	$\widetilde{\mathcal{O}}(\beta t_{\mathrm{mix}}\mathrm{polylog}(1/\epsilon))$	Gaussian / Metropolis filter
This work [Theorem 19]	KMS	$\widetilde{\mathcal{O}}(\beta\log^{1+o(1)}(t_{\mathrm{mix}}/\epsilon))$	≥ 1	$\widetilde{\mathcal{O}}(\beta^2 S\cdot t_{\mathrm{mix}}\mathrm{polylog}(1/\epsilon))$	A family of filters

TABLE 1. A comparison of quantum Gibbs samplers using techniques related to Lindblad dynamics. Here the truncation time T is used to truncate the integral in Eq. (1.1) to $[-T,T]$ in simulation. The number of jump operators for the Libladian is denoted by ∞ if $\gamma(\omega)$ is a continuous function in Eq. (1.2). The total cost refers to the total Hamiltonian simulation time using the best available Lindblad simulation algorithm. The $o(1)$ factor in the truncation time of this work stems from our choice of the filtering function and $o(1)$ can be chosen to be arbitrarily small without much added cost. In this work, the factor $\beta^2 S$ scaling in the total cost is due to that our jump operator allows the Bohr frequency difference to be of size S (see Remark 23). When $S=\mathcal{O}(1/\beta)$, this recovers the linear dependence on β in the total cost. When $S=\mathcal{O}(1)$, the dependence on β is quadratic. The mixing time t_{mix} is method dependent, and their values are generally difficult to compare with each other in theory. The weak coupling assumption may be unphysical for large quantum systems. The rounding promise-based method prepares an ensemble of density operators, and the total cost for preparing each density operator in the ensemble may be improved to $\widetilde{\mathcal{O}}(t_{\mathrm{mix}}\beta\epsilon^{-2})$ (see [RWW23, Remark of Theorem 1]).

1.3. **Discussion and open questions.** There exist a series of algorithms [PW09, CS17, VAGGdW17, GSLW19, ACL23] that require only quantum access to H without additional information (such as coupling operators). The cost of these algorithms is deterministic and scales as $\mathcal{O}(\sqrt{N/\mathcal{Z}_\beta}\,\mathrm{poly}(\beta,\log\epsilon^{-1}))$. These algorithms can perform efficiently in the high-temperature regime, where β is small and $\sqrt{N/\mathcal{Z}_\beta}\sim 1$ (assuming the smallest eigenvalue of H is zero). However, they become significantly less efficient in the low-temperature regime, where β is large, and $\sqrt{N/\mathcal{Z}_\beta}\sim\sqrt{N}$. Furthermore, the factor $\sqrt{N/\mathcal{Z}_\beta}$ is explicitly present in the algorithm, and the average-case complexity is not very different from the worst-case scenario. On the other hand, the computational cost of open-system quantum dynamics is primarily determined by the mixing time, which can vary significantly across different systems. Besides the Lindblad dynamics, alternative open-system dynamics formalisms are also viable [TOV+11, YAG12, SM23, Cub23] for Gibbs state preparation. We may anticipate that for certain classes of physical Hamiltonians, even at low temperatures, Gibbs sampling could be executed efficiently. This possibility does not contradict the statement that preparing the ground state of H (when $\beta = \infty$) remains QMA-hard in the worst-case scenario [KSV02, AGIK09].

Although rigorous bounding of the mixing time has been achieved for certain quantum Gibbs samplers operating on commuting Hamiltonians [KB16, BCG+23], establishing the mixing time for non-commuting Hamiltonians at moderate or even low temperatures presents a substantial theoretical challenge. There are two interesting works along this line. The first is that Rouzé et al [RFA24] established the spectral gap of KMS detailed balanced Lindbladians for certain k-local Hamiltonians at high temperatures using Lieb-Robinson estimates. The analysis in [RFA24] may be applicable in our setting and we plan to investigate this in detail in a future work. On the other hand, Bakshi et al [BLMT24] demonstrated that at the high temperature, the Gibbs State of certain k-local Hamiltonian becomes a linear combination of tensor products of stabilizer states, can be prepared in polynomial time using randomized classical algorithms. This suggests that exploring the relationship between the complexity of Gibbs states and mixing times could be a fruitful avenue for future research.

It is also noteworthy that introducing a coherent term to any detailed balanced Lindbladian disrupts the detailed balance condition, but the Gibbs state remains a fixed point. The influence of the coherent term on the mixing time may be significant and its characterization remains an open question. Finally, the mixing time t_{mix} may be very different across different quantum Gibbs samplers. Both theoretical and numerical evidence are needed in order to quantify the mixing time and to compare the efficiency of quantum Gibbs samplers for physical systems of interest.

1.4. **Notation.** We denote by $\mathcal{H}$ a finite-dimensional Hilbert space with dimension $N = 2^n$, and by $\mathcal{B}(\mathcal{H})$ the space of bounded operators. For simplicity, we usually write $A \geq 0$ (resp., $A > 0$) for a positive semidefinite (resp., definite) operator. The identity element in $\mathcal{B}(\mathcal{H})$ is denoted by $\mathbf{1}$. Moreover, we denote by $\mathcal{D}(\mathcal{H})$ the set of quantum states (i.e., $\rho \geq 0$ with $\mathrm{tr}(\rho) = 1$), and $\mathcal{D}_+(\mathcal{H})$ the subset of full-rank states. Let $X^\dagger$ be the adjoint operator of X. We denote by $\langle \cdot, \cdot \rangle$ the Hilbert-Schmidt inner product on $\mathcal{B}(\mathcal{H})$: $\langle X, Y \rangle := \mathrm{tr}(X^\dagger Y)$. Then, with a slight abuse of notation, the adjoint of a superoperator $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ with respect to $\langle \cdot, \cdot \rangle$ is also denoted by $\Phi^\dagger$. Unless specified otherwise, $\|X\|$ denotes the operator norm for $X \in \mathcal{B}(\mathcal{H})$, while $\|x\|_s := (\sum_j |x_j|^s)^{1/s}$ denotes the s-norm of the vector $x \in \mathbb{C}^N$ ($s \geq 1$). The diamond norm of a superoperator $\mathcal{E}$ on $\mathcal{B}(\mathcal{H})$ is defined by $\|\mathcal{E}\|_\diamond = \|\mathcal{E} \otimes \mathrm{id}\|_1$, where id is the identity map on $\mathcal{B}(\mathcal{H})$.

We adopt the following asymptotic notations beside the usual big $\mathcal{O}$ one. We write $f = \Omega(g)$ if $g = \mathcal{O}(f)$; $f = \Theta(g)$ if $f = \mathcal{O}(g)$ and $g = \mathcal{O}(f)$. The notations $\widetilde{\mathcal{O}}$, $\widetilde{\Omega}$, $\widetilde{\Theta}$ are used to suppress subdominant polylogarithmic factors. Specifically, $f = \widetilde{\mathcal{O}}(g)$ if $f = \mathcal{O}(g \,\mathrm{polylog}(g))$; $f = \widetilde{\Omega}(g)$ if $f = \Omega(g \,\mathrm{polylog}(g))$; $f = \widetilde{\Theta}(g)$ if $f = \Theta(g \,\mathrm{polylog}(g))$. Note that these tilde notations do not remove or suppress dominant polylogarithmic factors. For instance, if $f = \mathcal{O}(\log g \log\log g)$, then we write $f = \widetilde{\mathcal{O}}(\log g)$ instead of $f = \widetilde{\mathcal{O}}(1)$.

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Note: In completing this work, we became aware of the concurrent research by Chen, Doriguello, and Gilyén that similarly aims to develop quantum Gibbs samplers with a finite number of jump operators.

2. Structures of detailed balanced Lindbladians

In this section, we present the canonical forms of the Lindbladians with detailed balance conditions and discuss their feasibility for implementation on a quantum computer.

We first recall that a quantum channel $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is a completely positive trace preserving (CPTP) map, while a quantum Markov semigroup (QMS) $(\mathcal{P}_t)_{t\geq 0} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, also called Lindblad dynamics, is defined as a C_0-semigroup of completely positive, unital maps. The generator

$$\mathcal{L}(X) := \lim_{t\to 0} t^{-1}(\mathcal{P}_t(X) - X)$$

is usually referred to as the Lindbladian, which has the following GKSL form [Lin76, GKS76].

Lemma 1. *For any generator $\mathcal{L}$ of a QMS $\mathcal{P}_t$, there exist operators $L_j, K \in \mathcal{B}(\mathcal{H})$ such that*

$$\mathcal{L}(X) = \Psi(X) + K^\dagger X + XK\,, \tag{2.1}$$

where $\Psi(\cdot)$ is completely positive with the Kraus representation:

$$\Psi(X) = \sum_{j\in\mathcal{J}} L_j^\dagger X L_j\,, \tag{2.2}$$

with $\mathcal{J}$ being the index set with cardinality $|\mathcal{J}| \leq N^2$.

The operators L_j in (2.2) are called jump operators, which are non-unique for a given Lindbladian. From $\mathcal{L}(\mathbf{1}) = 0$, by (2.1), the operator K can be written as

$$K = V - iG \quad \text{with} \quad V = -\frac{1}{2}\sum_{j\in\mathcal{J}} L_j^\dagger L_j\,, \tag{2.3}$$

where $V := \frac{K^\dagger + K}{2}$ and $G := \frac{K^\dagger - K}{2i}$ are self-adjoint operators, and then there holds

$$\mathcal{L}(X) = i[G,X] + \sum_{j\in\mathcal{J}} \left(L_j^\dagger X L_j - \frac{1}{2}\left\{L_j^\dagger L_j, X\right\}\right),$$

where $i[G,X]$ and $\mathcal{L}(X) - i[G,X]$ are the coherent and dissipative parts of the dynamic, respectively.

For the purpose of quantum state preparation, we are interested in those QMS converging to a given full-rank state $\sigma > 0$, i.e.,

$$\lim_{t\to\infty} \mathcal{P}_t^\dagger(\rho) = \sigma\,, \quad \forall \rho \in \mathcal{D}(\mathcal{H})\,, \tag{2.4}$$

equivalently, the irreducible QMS $\mathcal{P}_t^\dagger$ [Wol12, Proposition 7.5]. For the reader's convenience, we recall the definition of irreducibility and some further equivalent conditions. We say that a quantum channel Φ is irreducible if all the orthogonal projections P satisfying $\Phi(P\mathcal{B}(\mathcal{H})P) \subset P\mathcal{B}(\mathcal{H})P$ are trivial, i.e., zero or identity. The following results are adapted from [Wol12, ZB23].

Lemma 2. *A QMS $\mathcal{P}_t^\dagger = e^{t\mathcal{L}^\dagger}$ is irreducible if and only if one of the following conditions holds:*

- *$\mathcal{P}_t^\dagger$ (as a quantum channel) is irreducible for some $t_0 > 0$.*
- *There exists a unique full-rank invariant state σ, i.e., $\mathcal{L}^\dagger(\sigma) = 0$.*
- *The multiplicative algebra generated by the jump operators $\{L_j\}$ and $K = -\frac{1}{2}\sum_j L_j^\dagger L_j - iG$ gives the whole algebra $\mathcal{B}(\mathcal{H})$.*
- *The operators $\{L_j\}$ and K have no trivial common invariant subspace.*

Lemma 3 ([Wol12, Theorem 7.2])**.** *If the QMS $\mathcal{P}_t^\dagger$ admits a full-rank invariant state, then*

$$\{G, L_j, L_j^\dagger\}' = \ker(\mathcal{L})\,,$$

where the commutant $\{G, L_j, L_j^\dagger\}'$ *is defined by all the operators commuting with* L_j, $L_j^\dagger$ *and* G*. It follows that in this case, the irreducibility is also equivalent to*

$$\{G, L_j, L_j^\dagger\}' = \{z\mathbf{1}\,;\ z \in \mathbb{C}\}\,. \tag{2.5}$$

We next discuss the quantum detailed balance condition (DBC), which provides a sufficient criterion to guarantee the Lindbladian's steady state. For a given $\sigma \in \mathcal{D}_+(\mathcal{H})$, we define the modular operator:

$$\Delta_\sigma(X) = \sigma X \sigma^{-1} :\ \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})\,,$$

and the weighting operator:

$$\Gamma_\sigma X = \sigma^{\frac{1}{2}} X \sigma^{\frac{1}{2}} :\ \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})\,.$$

We also let $L_\sigma(X) = \sigma X$ and $R_\sigma(X) = X\sigma$ be the left and right multiplication operators, respectively. Then, for any $f : (0,\infty) \to (0,\infty)$ satisfying $f(1) = 1$ and $\sigma \in \mathcal{D}_+(\mathcal{H})$, we define the following operator:

$$J_\sigma^f := R_\sigma f(\Delta_\sigma) : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})\,, \tag{2.6}$$

and the associated inner product:

$$\langle X, Y\rangle_{\sigma,f} := \langle X, J_\sigma^f(Y)\rangle\,. \tag{2.7}$$

In particular, for $f = x^{1-s}$ with $s \in \mathbb{R}$, the above inner product gives

$$\langle X, Y\rangle_{\sigma,s} := \operatorname{tr}(\sigma^s X^\dagger \sigma^{1-s} Y)\,, \quad \forall X, Y \in \mathcal{B}(\mathcal{H})\,, \tag{2.8}$$

where $\langle\cdot,\cdot\rangle_{\sigma,1}$ and $\langle\cdot,\cdot\rangle_{\sigma,1/2}$ are the Gelfand-Naimark-Segal (GNS) and Kubo-Martin-Schwinger (KMS) inner products, respectively.

Definition 4. *A QMS* $\mathcal{P}_t = e^{t\mathcal{L}}$ *satisfies the* J_σ^f*-DBC for some* $\sigma \in \mathcal{D}_+(\mathcal{H})$ *if the Lindbladian* $\mathcal{L}$ *is self-adjoint with respect to the inner product* $\langle\cdot,\cdot\rangle_{\sigma,f}$*, equivalently,*

$$J_\sigma^f \mathcal{L} = \mathcal{L}^\dagger J_\sigma^f\,.$$

In the cases of $f = 1$ *and* $x^{1/2}$*, it is called* σ-GNS DBC *and* σ-KMS DBC*, respectively.*

By the above definition, we find that if $\mathcal{P}_t$ satisfies the J_σ^f-DBC, there holds

$$0 = \langle X, \mathcal{L}(\mathbf{1})\rangle_{\sigma,f} = \langle \mathcal{L}(X), J_\sigma^f(\mathbf{1})\rangle = \langle X, \mathcal{L}^\dagger(\sigma)\rangle\,, \quad \forall X \in \mathcal{B}(\mathcal{H})\,,$$

which gives $\mathcal{L}^\dagger(\sigma) = 0$, namely, σ is an invariant state of $\mathcal{P}_t^\dagger$. The following lemma relates different concepts of detailed balance conditions; see [CM17, Lemma 2.5 and Theorem 2.9].

Lemma 5. *Let* $\sigma \in \mathcal{D}_+(\mathcal{H})$ *be a full-rank quantum state and* $\mathcal{P}_t = e^{t\mathcal{L}}$ *be a QMS. Then,*

- *If* $\mathcal{P}_t$ *satisfies the* σ-GNS DBC*, then it satisfies the* J_σ^f*-DBC for any* f *and the generator* $\mathcal{L}$ *commutes with the modular operator* Δ_σ*.*
- *If* $\mathcal{P}_t$ *satisfies the* J_σ^f*-DBC for* $f = x^{1-s}$*,* $s \in [0,1]\backslash\{\frac{1}{2}\}$*, then it also satisfies* σ-GNS DBC*.*

The above lemma means that the quantum DBC for the inner products $\langle\cdot,\cdot\rangle_{\sigma,s}$ with $s \in [0,1]\backslash\{\frac{1}{2}\}$ are all equivalent, and they are stronger notions than σ-KMS DBC (i.e., $s = \frac{1}{2}$). In fact, one can show that the class of QMS with σ-KMS DBC is strictly larger than the class of QMS satisfying σ-GNS DBC [CM17, Appendix B]. These properties underscore the special roles played by the KMS and GNS detailed balance when analyzing Lindblad dynamics.

2.1. **Davies generator and GNS-detailed balance.** Let H be a quantum Hamiltonian on the Hilbert space $\mathcal{H}$ with the eigendecomposition:

$$H = \sum_i \lambda_i P_i \,, \tag{2.9}$$

where P_i is the orthogonal projector to the eigenspace associated with the energy λ_i. Given an inverse temperature $\beta > 0$, the corresponding Gibbs state σ_β is defined by

$$\sigma_\beta := e^{-\beta H}/\mathcal{Z}_\beta \,, \tag{2.10}$$

with $\mathcal{Z}_\beta = \operatorname{tr}(e^{-\beta H})$ being the normalization constant, called partition function. It is easy to see that any full-rank quantum state can be written as a Gibbs state $\sigma = e^{-h}$ with $h = -\log(\sigma)$.

Recall that the main aim of this work is to develop an efficient quantum Gibbs sampler via QMS. An important class of Lindbladians for this purpose are Davies generators, which describe the weak coupling limit of a system coupled to a large thermal bath [Dav76, Dav79]. It has natural applications in thermal state preparations but with inherent difficulties from the energy-time uncertainty principle [ML20, RWW23, CKBG23]; see Remark 7. We next review the canonical form of Davies semigroups and show that they essentially characterize the Lindbladians with GNS-DBC [KFGV77].

For the Hamiltonian (2.9), we define the set of Bohr frequencies by

$$B_H = \{\nu = \lambda_i - \lambda_j \,;\ \lambda_i, \lambda_j \in \operatorname{Spec}(H)\} \,, \tag{2.11}$$

which is a sequence of real numbers symmetric with respect to 0. Here, $\operatorname{Spec}(H)$ denotes the spectral set of H. Then, for any bounded operator $A \in \mathcal{B}(\mathcal{H})$, one can write

$$A = \sum_{\lambda_i, \lambda_j \in \operatorname{Spec}(H)} P_i A P_j = \sum_{\nu \in B_H} A_\nu \,, \tag{2.12}$$

where

$$A_\nu := \sum_{\lambda_i - \lambda_j = \nu} P_i A P_j \,, \quad \text{with} \quad (A_\nu)^\dagger = (A^\dagger)_{-\nu} \,, \tag{2.13}$$

is an eigenstate of the modular operator Δ_{σ_β} (see Eq. (2.21) below). Such a decomposition (2.12) naturally relates to the Heisenberg evolution of A:

$$A(t) := e^{iHt} A e^{-iHt} = \sum_{\nu \in B_H} A_\nu e^{i\nu t} \,, \quad \text{equivalently,} \quad [H, A_\nu] = \nu A_\nu \,. \tag{2.14}$$

Following [CKBG23], we introduce the weighted operator Fourier Transform, which is crucial for our following algorithmic design and its analysis. Given an operator $A \in \mathcal{B}(\mathcal{H})$ and a filter function $f : \mathbb{R} \to \mathbb{C}$ with certain regularity (e.g., L^1 integrable or tempered distribution), we define

$$\widehat{A}_f(\omega) := \int_{-\infty}^{\infty} A(t) e^{-i\omega t} f(t) \mathrm{d}t = 2\pi \sum_{\nu \in B_H} A_\nu \widehat{f}(\omega - \nu) \,, \tag{2.15}$$

where

$$\widehat{f}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} \mathrm{d}t$$

is the Fourier Transform of $f(t)$. In the case of $f(t) = 1$, we have $\widehat{f}(\omega) = \delta(\omega)$ and

$$\widehat{A}_{f=1}(\omega) = 2\pi \sum_{\nu \in B} A_\nu \delta(\omega - \nu) \,. \tag{2.16}$$

The Davies Lindbladian is generally of the form:

$$\mathcal{L}_\beta(X) := i[H, X] + \sum_{a \in \mathcal{A}} \sum_{\nu \in B_H} \mathcal{L}_{a,\nu}(X) \,, \quad X \in \mathcal{B}(\mathcal{H}) \,, \tag{2.17}$$

where the dissipative generators are given by

$$\mathcal{L}_{a,\nu}(X) = \gamma_a(\nu)\left((A_\nu^a)^\dagger X A_\nu^a - \frac{1}{2}\left\{(A_\nu^a)^\dagger A_\nu^a, X\right\}\right) . \tag{2.18}$$

Here, the index $a \in \mathcal{A}$ sums over all the coupling operators $A^a \in \mathcal{B}(\mathcal{H})$ to the environment that satisfy $\{A^a\}_{a\in\mathcal{A}} = \{(A^a)^\dagger\}_{a\in\mathcal{A}}$, and $\gamma_a(\cdot)$ are the Fourier transforms of the bath correlation functions, which are nonnegative and bounded. The jump operators $\{A_\nu^a\}$ associated with a coupling $A^a \in \mathcal{B}(\mathcal{H})$ are defined by Eqs. (2.12) and (2.13):

$$A^a = \sum_{\lambda_i,\lambda_j\in\mathrm{Spec}(H)} P_i A^a P_j = \sum_{\nu\in B_H} A_\nu^a, \tag{2.19}$$

which gives the transitions from the eigenvectors of H with energy E to those with $E+\nu$. In addition, the following relations hold, for any $a \in \mathcal{A}$ and ν,

$$\gamma_a(-\nu) = e^{\beta\nu}\gamma_a(\nu) , \tag{2.20}$$

and

$$\Delta_{\sigma_\beta}(A_\nu^a) = e^{-\beta\nu}A_\nu^a , \tag{2.21}$$

that is, A_ν^a is an eigenvector of Δ_{σ_β} with the eigenvalue $e^{-\beta\nu}$. Note that the condition (2.21) holds by the definition of A_ν^a, while the condition (2.20) is often referred to as KMS condition[2] [KFGV77], which, as we shall see below, ensures the GNS-reversibility of the Lindbladian.

The following canonical form for the QMS that satisfies the σ-GNS DBC is due to Alicki [Ali76].

Lemma 6. *For a Lindbladian $\mathcal{L}$ satisfying σ_β-GNS DBC, there holds*

$$\mathcal{L}(X) = \sum_{j\in\mathcal{J}}\left(e^{-\omega_j/2}L_j^\dagger[X, L_j] + e^{\omega_j/2}[L_j, X]L_j^\dagger\right) , \tag{2.22}$$

with $\omega_j \in \mathbb{R}$ and $|\mathcal{J}| \le N^2 - 1$, where $L_j \in \mathcal{B}(\mathcal{H})$ satisfies

$$\Delta_{\sigma_\beta}(L_j) = e^{-\omega_j}L_j , \quad \mathrm{tr}(L_j^\dagger L_k) = c_j\delta_{j,k} , \quad \mathrm{tr}(L_j) = 0 , \tag{2.23}$$

with normalization constants $c_j > 0$, and for each j, there exists $j' \in \mathcal{J}$ such that

$$L_j^\dagger = L_{j'} , \quad \omega_j = -\omega_{j'} . \tag{2.24}$$

It is easy to see that the Davies semigroup (2.17) is exactly the class of QMS with GNS-DBC, up to the coherent term $i[H,\cdot]$. Indeed, we define $g_a(\nu) := e^{\beta\nu/2}\gamma_a(\nu)$ and find $g_a(\nu) = g_a(-\nu)$ by the KMS condition (2.20). Then, letting $L_{a,\nu} := g_a(\nu)^{1/2}A_\nu^a$, it follows from (2.17) and (2.18) that

$$\begin{aligned}\mathcal{L}_\beta(X) &= i[H, X] + \sum_{a\in\mathcal{A}}\sum_{\nu\in B_H} e^{-\beta\nu/2}\left(L_{a,\nu}^\dagger X L_{a,\nu} - \frac{1}{2}\left\{L_{a,\nu}^\dagger L_{a,\nu}, X\right\}\right) \\ &= i[H, X] + \frac{1}{2}\sum_{a\in\mathcal{A}}\sum_{\nu\in B_H} e^{-\beta\nu/2}L_{a,\nu}^\dagger[X, L_{a,\nu}] + e^{\beta\nu/2}[L_{a,\nu}, X]L_{a,\nu}^\dagger ,\end{aligned}$$

with the dissipative part exactly satisfying the conditions in Lemma 6 by re-indexing $j = (a, \nu)$.

Remark 7. *The Davies generator $\mathcal{L}_\beta$ in (2.17) can be viewed as a quantum analog of a classical Markov chain, and therefore becomes a natural candidate for the Gibbs state preparation [RWW23, CKBG23]. However, implementing the Davies generator accurately requires being able to resolve and distinguish between all Bohr frequencies ν, while the gap between two Bohr frequencies ν, ν' could be exponentially small as the system size increases in a generic setting. In view of (2.15) and (2.16), by the energy-time uncertainty principle, this means an impractically long Hamiltonian simulation time and is a key obstacle in leveraging the Davies semigroup directly as a quantum Gibbs sampler.*

[2]The KMS condition should not be confused with the KMS detailed balance condition. These two terms are mathematically unrelated.

It is also worth mentioning that the sum over Bohr frequencies (2.17) is derived from a secular approximation [BP02], which may be regarded as theoretical evidence that the GNS detailed balance is an idealized construction and thus is difficult to be exactly implemented in practice.

2.2. **KMS-detailed balanced generators.** Recalling that the KMS DBC is a weaker property compared to the GNS one, but can still guarantee the Gibbs state as a fixed point of the dynamic, one may expect that the KMS-detailed balanced QMS can provide a more efficient class of Gibbs state preparation algorithms. In this section, we introduce the canonical form of the QMS satisfying σ_β-KMS DBC with a proof sketch, mainly following [FU07, AC21], which are fundamental for the subsequent discussion on quantum algorithms.

Let $\mathfrak{H} := \mathcal{B}(\mathcal{B}(\mathcal{H}))$ be the space of superoperators. We define the subspace $\mathfrak{H}_S$ consisting of $\Phi \in \mathfrak{H}$ of the form: for some $X, Y \in \mathcal{B}(\mathcal{H})$,

$$\Phi(A) = XA + AY\,, \tag{2.25}$$

and denote by $\mathfrak{H}_S^\perp$ its orthogonal complement. The following useful lemma characterizes the freedom of X, Y in (2.25)[3].

Lemma 8. *Let Φ be a superoperator with the representation (2.25). If some $X', Y' \in \mathcal{B}(\mathcal{H})$ gives the same Φ, then $X' = X + \eta \mathbf{1}$ and $Y' = Y - \eta\mathbf{1}$ for some $\eta \in \mathbb{C}$.*

Proof. Let F_α with $\alpha = (i,j)$ and $1 \le i,j \le N$ be a basis of $\mathcal{B}(\mathcal{H})$ satisfying $\langle F_\alpha, F_\beta\rangle/N = \delta_{\alpha\beta}$, $F_{(1,1)} = \mathbf{1}$, and $F_{(i,j)}^\dagger = F_{(j,i)}$, and let $E_{i,j}$ be another basis defined by $E_{i,j} = \sqrt{N}\,|u_i\rangle\langle u_j|$, where $\{u_j\}$ is an orthonormal basis of $\mathcal{H}$. Suppose that $\Phi(A) = XA + AY$ for some X, Y. We compute the coefficients for the expansion of $\Phi(A) = \sum_{\alpha,\beta}(C_\Phi)_{\alpha,\beta}F_\alpha^\dagger A F_\beta$:

$$\begin{aligned}
(C_\Phi)_{\alpha,\beta} &= \frac{1}{N^3}\sum_{i,j=1}^N \operatorname{tr}\left[(F_\alpha^\dagger E_{i,j}F_\beta)^\dagger \Phi(E_{i,j})\right] \\
&= \frac{1}{N^2}\left(\operatorname{tr}[F_\beta^\dagger]\operatorname{tr}[F_\alpha X] + \operatorname{tr}[F_\alpha]\operatorname{tr}[F_\beta^\dagger Y]\right) = \frac{1}{N}\left(\delta_{\beta,(1,1)}\operatorname{tr}[F_\alpha X] + \delta_{\alpha,(1,1)}\operatorname{tr}[F_\beta^\dagger Y]\right)\,,
\end{aligned}$$

which is zero if $\alpha, \beta \neq (1,1)$. It follows that

$$\Phi(A) = (C_\Phi)_{(1,1),(1,1)}A + \sum_{\alpha\neq(1,1)}(C_\Phi)_{\alpha,(1,1)}F_\alpha^\dagger A + \sum_{\beta\neq(1,1)}(C_\Phi)_{(1,1),\beta}AF_\beta\,.$$

Therefore, any X', Y' such that $\Phi(A) = X'A + AY'$ satisfy

$$X' = \sum_{\alpha\neq(1,1)}(C_\Phi)_{\alpha,(1,1)}F_\alpha^\dagger + a\mathbf{1}\,,\quad Y' = \sum_{\beta\neq(1,1)}(C_\Phi)_{(1,1),\beta}F_\beta + b\mathbf{1}\,,$$

for some $a, b \in \mathbb{C}$ with $a + b = (C_\Phi)_{(1,1),(1,1)}$. The proof is complete. □

We next discuss the structure of QMS satisfying σ_β-KMS DBC for some Gibbs state σ_β (2.10).

Lemma 9. *A Lindbladian $\mathcal{L}$ satisfies σ_β-KMS DBC if and only if $\mathcal{L}$ has the form:*

$$\mathcal{L}(X) = \Psi(X) + \Phi(X)\,, \tag{2.26}$$

with the CP operator $\Psi(\cdot)$ admitting the Kraus representation (2.2) and the operator

$$\Phi(X) := K^\dagger X + XK\,,\quad \textit{for some } K \in \mathcal{B}(\mathcal{H})\,, \tag{2.27}$$

and both Ψ and Φ are self-adjoint with respect to the KMS inner product. In this case, there exist the jump operators $\{L_j\}_{j\in\mathcal{J}}$ and the operator K in Eq. (2.27) satisfying

$$\Delta_{\sigma_\beta}^{-1/2}L_j = L_j^\dagger\,, \tag{2.28}$$

[3] This result is from [AC21, Lemma 3.10 and Remark 3.11], which include some typos in the arguments. We provide a short proof here for the reader's convenience.

and

$$\Delta_{\sigma_\beta}^{-1/2} K = K^\dagger . \tag{2.29}$$

Proof. It suffices to prove the *only if* part. Recalling the structure of a Lindbladian in Lemma 1, without loss of generality, we assume $\mathrm{tr}(L_j) = 0$ by replacing L_j with $L_j - \mathrm{tr}(L_j)\mathbf{1}$ and K with $K + \sum_j \mathrm{tr}(L_j^\dagger) L_j - \frac{1}{2}|\mathrm{tr}(L_j)|^2$. Then, by [AC21, Lemma 3.12], there holds $\Psi(\cdot) \in \mathfrak{H}_S^\perp$. According to [AC21, Lemma 3.13], the subspaces $\mathfrak{H}_S$ and $\mathfrak{H}_S^\perp$ are invariant under the adjoint with respect to the KMS inner product. By $\Phi \in \mathfrak{H}_S$ and $\Psi \in \mathfrak{H}_S^\perp$, it holds that adjoints $\Phi^\dagger_{\mathrm{KMS}} \in \mathfrak{H}_S$ and $\Psi^\dagger_{\mathrm{KMS}} \in \mathfrak{H}_S$, where $\Phi^\dagger_{\mathrm{KMS}}$ and $\Psi^\dagger_{\mathrm{KMS}}$ are adjoints of Φ and Ψ for the KMS inner product. Thus, the self-adjointness $\Psi^\dagger_{\mathrm{KMS}} + \Phi^\dagger_{\mathrm{KMS}} = \Psi + \Phi$ implies $\Psi^\dagger_{\mathrm{KMS}} = \Psi$ and $\Phi^\dagger_{\mathrm{KMS}} = \Phi$.

Next, since Ψ is a KMS-detailed balanced CP map, (2.28) is implied by the structure result [AC21, Theorem 4.1]. To show (2.29), by the invariance of $\Phi = K^\dagger X + XK$ for adding a pure imaginary $ic\mathbf{1}$ ($c \in \mathbb{R}$) to K, without loss of generality, we can assume $\mathrm{tr}(K) \in \mathbb{R}$, which further implies $\mathrm{tr}(\Delta_{\sigma_\beta}^{-1/2} K) \in \mathbb{R}$. It follows from σ_β-KMS DBC of Φ that $\Gamma_{\sigma_\beta}\Phi = \Phi^\dagger \Gamma_{\sigma_\beta}$, equivalently,

$$K^\dagger X + XK = (\Delta_{\sigma_\beta}^{-1/2} K) X + X (\Delta_{\sigma_\beta}^{1/2} K^\dagger) .$$

Then, by Lemma 8, we derive $K^\dagger = \Delta_{\sigma_\beta}^{-1/2} K + \eta \mathbf{1}$ for some $\eta \in \mathbb{C}$, where η must be zero, thanks to $\mathrm{tr}(K^\dagger) = \mathrm{tr}(K) = \mathrm{tr}(\Delta_{\sigma_\beta}^{-1/2} K) \in \mathbb{R}$. The proof is complete. $\square$

We proceed to derive an explicit formula for the operator K. Recalling the decomposition (2.3) and $V = -\frac{1}{2}\sum_{j\in\mathcal{J}} L_j^\dagger L_j$, it suffices to find an expression for the involved operator G. To do so, we reformulate the constraint (2.29) above as a Lyapunov equation:

$$G\sigma_\beta^{1/2} + \sigma_\beta^{1/2} G = i(\sigma_\beta^{1/2} V - V\sigma_\beta^{1/2}) .$$

It can be uniquely solved as

$$G = i \int_0^\infty e^{-t\sigma_\beta^{1/2}} (\sigma_\beta^{1/2} V - V \sigma_\beta^{1/2}) e^{-t\sigma_\beta^{1/2}} \, \mathrm{d}t . \tag{2.30}$$

To simplify the formula, we note that for any $\lambda, \mu > 0$,

$$\int_0^\infty e^{-t\lambda^{1/2}} e^{-t\mu^{1/2}} \, \mathrm{d}t = \frac{1}{\lambda^{1/2} + \mu^{1/2}} ,$$

and $\tanh(\log(x^{1/4})) = \frac{x^{1/2}-1}{x^{1/2}+1}$. Then, by functional calculus and (2.30), there holds

$$G = i \frac{L_{\sigma_\beta}^{1/2} - R_{\sigma_\beta}^{1/2}}{L_{\sigma_\beta}^{1/2} + R_{\sigma_\beta}^{1/2}} (V) = i \frac{\Delta_{\sigma_\beta}^{1/2} - I}{\Delta_{\sigma_\beta}^{1/2} + I}(V) = i \tanh \circ \log(\Delta_{\sigma_\beta}^{1/4})(V) . \tag{2.31}$$

We summarize the above discussion in the following proposition.

Theorem 10. *A Lindbladian $\mathcal{L}$ satisfies σ_β-KMS DBC if and only if there exist linear operators $L_j, G \in \mathcal{B}(\mathcal{H})$ such that*

$$\mathcal{L}(X) = i[G, X] + \sum_{j\in\mathcal{J}} \left(L_j^\dagger X L_j - \frac{1}{2}\left\{ L_j^\dagger L_j, X \right\} \right) , \tag{2.32}$$

with L_j satisfying (2.28), and G being self-adjoint and given by

$$G := -i \tanh \circ \log(\Delta_{\sigma_\beta}^{1/4}) \left(\frac{1}{2} \sum_{j\in\mathcal{J}} L_j^\dagger L_j \right) . \tag{2.33}$$

We have shown in Lemma 5 that the Lindbladians with σ_β-GNS DBC is a subclass of those with σ_β-KMS DBC, but this property cannot be easily seen from the corresponding structural results (cf. Lemma 6 and Theorem 10), noting that an eigenvector L of the operator Δ_{σ_β} is generally not a solution to (2.28). To fill this gap, we next show that the canonical form (2.22) of a QMS with GNS DBC can be indeed reformulated as the one (2.32) for KMS DBC.

Corollary 11. *Let $\mathcal{L}$ be a Lindbladian with σ_β-GNS DBC of the form:*

$$\mathcal{L}(X) = \sum_{j\in\mathcal{J}} \mathcal{L}_j(X) \quad \text{with} \quad \mathcal{L}_j(X) = 2e^{-\omega_j/2}\left(L_j^\dagger X L_j - \frac{1}{2}\left\{L_j^\dagger L_j, X\right\}\right), \tag{2.34}$$

where the jumps $\{L_j\}_{j\in\mathcal{J}}$ satisfy the conditions in Lemma 6. Then, we can reformulate it in the form of a KMS detailed balanced Lindbladian (2.32):

$$\mathcal{L}(X) = \sum_{j\in\mathcal{J},\, L_j^\dagger = L_j} \mathcal{L}_j(X) + \frac{1}{2}\sum_{j\in\mathcal{J},\, L_j^\dagger \neq L_j} \widetilde{\mathcal{L}}_j(X)\,,$$

with

$$\widetilde{\mathcal{L}}_j(X) = \widetilde{L}_{j,1}^\dagger X \widetilde{L}_{j,1} + \widetilde{L}_{j,2}^\dagger X \widetilde{L}_{j,2} - \frac{1}{2}\left\{\widetilde{L}_{j,1}^\dagger \widetilde{L}_{j,1}, X\right\} - \frac{1}{2}\left\{\widetilde{L}_{j,2}^\dagger \widetilde{L}_{j,2}, X\right\},$$

where

$$\widetilde{L}_{j,1} := e^{-\omega_j/4} L_j + e^{\omega_j/4} L_j^\dagger\,, \quad \widetilde{L}_{j,2} := i(-e^{-\omega_j/4} L_j + e^{\omega_j/4} L_j^\dagger)$$

satisfy the constraint (2.28).

Proof. If L_j is self-adjoint, there hold $\omega_j = 0$ and $\Delta_{\sigma_\beta}^{-1/2} L_j = L_j = L_j^\dagger$. By the formula (2.31) of G, the associated Hamiltonian is given by

$$G_j := -\frac{i}{2}\frac{\Delta_{\sigma_\beta}^{1/2} - I}{\Delta_{\sigma_\beta}^{1/2} + I}(L_j^2) = 0\,.$$

Thus, in this case, $\mathcal{L}_j$ in (2.34) satisfies the canonical form (2.32) in Theorem 10.

We next consider the case where L_j is not self-adjoint. Let j' be the adjoint index for j specified in (2.24). It follows that

$$\mathcal{L}_j(X) + \mathcal{L}_{j'}(X) = 2e^{-\omega_j/2}\left(L_j^\dagger X L_j - \frac{1}{2}\left\{L_j^\dagger L_j, X\right\}\right) + 2e^{\omega_j/2}\left(L_j X L_j^\dagger - \frac{1}{2}\left\{L_j L_j^\dagger, X\right\}\right).$$

We consider the equation $\Delta_{\sigma_\beta}^{-1/2}\widetilde{L} = \widetilde{L}^\dagger$ with ansatz $\widetilde{L} = aL_j + bL_j^\dagger$, $a, b \in \mathbb{C}$:

$$\Delta_{\sigma_\beta}^{-1/2}(aL_j + bL_j^\dagger) = ae^{\omega_j/2}L_j + be^{-\omega_j/2}L_j^\dagger = \bar{a}L_j^\dagger + \bar{b}L_j\,.$$

It is easy to check that the coefficients (a, b) being real linear combinations of vectors $(e^{-\omega_j/2}, 1)$ and $(-e^{-\omega_j/2}i, i)$ satisfy $a = \bar{b}e^{-\omega_j/2}$, and the corresponding $\widetilde{\mathcal{L}}$ solves $\Delta_{\sigma_\beta}^{-1/2}\widetilde{L} = \widetilde{L}^\dagger$. We define

$$\widetilde{L}_1 = e^{-\omega_j/4}L_j + e^{\omega_j/4}L_j^\dagger\,, \quad \widetilde{L}_2 = i(-e^{-\omega_j/4}L_j + e^{\omega_j/4}L_j^\dagger)\,. \tag{2.35}$$

A direct computation gives, for $X \in \mathcal{B}(\mathcal{H})$,

$$\widetilde{L}_1^\dagger X \widetilde{L}_1 + \widetilde{L}_2^\dagger X \widetilde{L}_2 = 2e^{-\omega_j/2}L_j^\dagger X L_j + 2e^{\omega_j/2}L_j X L_j^\dagger\,,$$

and

$$\begin{aligned} G &= -\frac{i}{2}\frac{\Delta_{\sigma_\beta}^{1/2} - I}{\Delta_{\sigma_\beta}^{1/2} + I}\left(\widetilde{L}_1^\dagger \widetilde{L}_1 + \widetilde{L}_2^\dagger \widetilde{L}_2\right) \\ &= -i\frac{\Delta_{\sigma_\beta}^{1/2} - I}{\Delta_{\sigma_\beta}^{1/2} + I}\left(e^{-\omega_j/2}L_j^\dagger L_j + e^{\omega_j/2}L_j L_j^\dagger\right) = 0\,, \end{aligned}$$

by noting that $L_j^\dagger L_j$ and $L_j L_j^\dagger$ are eigenvectors of Δ_{σ_β} associated with eigenvalue one. Therefore, for non-self-adjoint L_j, the Lindbladian $\mathcal{L}_j + \mathcal{L}_{j'}$ also matches with the form (2.32). The proof is complete by the linearity of Lindbladians. □

3. A family of efficient quantum Gibbs samplers

In this section, we present a general framework for designing efficient quantum Gibbs samplers via Lindblad dynamics satisfying σ_β-KMS DBC.

3.1. **Quantum Gibbs samplers via KMS-detailed balanced Lindbladian.** Thanks to Theorem 10, the class of KMS detailed balanced Lindbladians can be parameterized by

- a set of jump operators for the Lindbladian $\{L_j\}_{j\in\mathcal{J}}$ satisfying (2.28): $\Delta_{\sigma_\beta}^{-1/2} L_j = L_j^\dagger$;
- a coherent term G defined as in (2.33) via $\{L_j\}_{j\in\mathcal{J}}$.

Note that the condition (2.28) is equivalent to $\Delta_{\sigma_\beta}^{-1/4} L_j = \Delta_{\sigma_\beta}^{1/4} L_j^\dagger$, namely, $\Delta_{\sigma_\beta}^{-1/4} L_j$ is self-adjoint. Thus, the admissible set of jump operators is

$$\{L \in \mathcal{B}(\mathcal{H})\,;\; L = \Delta_{\sigma_\beta}^{1/4} \widetilde{A} \;\text{ with }\; \widetilde{A} = \widetilde{A}^\dagger\}\,.$$

From the eigendecomposition of H in (2.9), we have

$$L = \Delta_{\sigma_\beta}^{1/4} \widetilde{A} = \sum_{i,j} e^{-\beta(\lambda_i - \lambda_j)/4} P_i \widetilde{A} P_j = \sum_{\nu \in B_H} e^{-\beta\nu/4} \widetilde{A}_\nu\,, \tag{3.1}$$

where $\widetilde{A}_\nu$ is defined by (2.13) for some self-adjoint $\widetilde{A}$.

Suppose that we are given a set of self-adjoint coupling operators $\{A^a\}_{a\in\mathcal{A}}$. For each a, we choose a weighting function $q^a(\nu) : \mathbb{R} \to \mathbb{C}$, which satisfies:

$$q^a(-\nu) = \overline{q^a(\nu)}, \quad \widehat{f^a}(\nu) := q^a(\nu) e^{-\beta\nu/4} \in L^1(\mathbb{R})\,. \tag{3.2}$$

Here $\widehat{f^a}(\nu)$ can be viewed as a filtering function in the frequency domain, and its Fourier transform gives the filtering function in the time domain:

$$f^a(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} q^a(\nu) e^{-\beta\nu/4} e^{-it\nu}\, \mathrm{d}\nu\,. \tag{3.3}$$

The choice of q^a is a key component in our algorithm and will be discussed in detail in Section 3.2. Moreover, for each pair (A^a, q^a), we define an operator $\widetilde{A}^a := \sum_{\nu\in B_H} \widetilde{A}^a_\nu$ with $\widetilde{A}^a_\nu = q^a(\nu) A^a_\nu$, which can be easily verified to be self-adjoint:

$$(\widetilde{A}^a)^\dagger = \sum_{\nu\in B_H} (\widetilde{A}^a)^\dagger_\nu = \sum_{\nu\in B_H} \overline{q^a(\nu)} (A^a_\nu)^\dagger = \sum_{\nu\in B_H} q^a(-\nu) A^a_{-\nu} = \widetilde{A}^a\,.$$

Then the jump operator for the Lindbladian, defined by

$$L_a = \sum_{\nu\in B_H} q^a(\nu) e^{-\beta\nu/4} A^a_\nu = \sum_{\nu\in B_H} \int_{-\infty}^{\infty} f^a(t) A^a_\nu e^{i\nu t}\, \mathrm{d}t = \int_{-\infty}^{\infty} f^a(t) A^a(t) \mathrm{d}t\,, \tag{3.4}$$

satisfies the requirement in (2.28). We see that each L_a is a linear combination of the Heisenberg evolution $A^a(t) = e^{iHt} A^a e^{-iHt}$.

Remark 12. *Noting that L_a in Eq. (3.4) is the same as $\widehat{A}^a_{f^a}(\omega = 0)$ in Eq. (1.2), if we let $f^a = f$ for all a, then the dissipative part of Lindbladian constructed via $\{L_a\}_{a\in\mathcal{A}}$ fits into the ansatz (1.2) with $\gamma(\omega) = \delta(\omega)$. This reduces a continuously parameterized set of jump operators to a discrete set.*

We proceed to construct the coherent part via the formula (2.33):

$$
\begin{aligned}
G &:= -i \tanh \circ \log(\Delta_{\sigma_\beta}^{1/4}) \left(\frac{1}{2} \sum_{a \in \mathcal{A}} L_a^\dagger L_a \right) \\
&= \sum_{a \in \mathcal{A}} \sum_{\nu, \nu' \in B_H} \widehat{g^a}(\nu, \nu') \, (A_{\nu'}^a)^\dagger \, A_\nu^a \,,
\end{aligned}
$$

with the coefficient function $\widehat{g^a}$ in the frequency domain given by

$$
\widehat{g^a}(\nu, \nu') = \frac{1}{2i} \tanh(\beta(\nu' - \nu)/4) e^{-\beta(\nu+\nu')/4} q^a(\nu) \overline{q^a(\nu')} \,. \tag{3.5}
$$

We define g^a in the time domain via a two-sided Fourier transform as follows:

$$
g^a(t, t') = \frac{1}{(2\pi)^2} \iint_{\mathbb{R}^2} \widehat{g^a}(\nu, \nu') e^{-i(\nu t - \nu' t')} \, \mathrm{d}\nu \, \mathrm{d}\nu' \,. \tag{3.6}
$$

Since $|\tanh(\cdot)| \le 1$ and $q^a(\nu) e^{-\beta\nu/4} \in L^1(\mathbb{R})$, $g^a(t, t')$ is well defined. Then, it is direct to compute, by $(A^a)^\dagger = A^a$ and (2.14),

$$
\begin{aligned}
G &= \sum_{a \in \mathcal{A}} \sum_{\nu, \nu' \in B_H} \widehat{g^a}(\nu, \nu') \, (A_{\nu'}^a)^\dagger \, A_\nu^a \\
&= \sum_{a \in \mathcal{A}} \sum_{\nu, \nu' \in B_H} \iint_{\mathbb{R}^2} e^{i\nu t} g^a(t, t') e^{-i\nu' t'} A_{-\nu'}^a A_\nu^a \, \mathrm{d}t \, \mathrm{d}t' \\
&= \sum_{a \in \mathcal{A}} \iint_{\mathbb{R}^2} g^a(t, t') A^a(t) A^a(t') \, \mathrm{d}t \, \mathrm{d}t' \,.
\end{aligned} \tag{3.7}
$$

Therefore, letting G and $\{L_a\}_{a \in \mathcal{A}}$ be constructed in (3.7) and (3.4), respectively, the Lindbladian

$$
\mathcal{L}(X) = i[G, X] + \sum_{a \in \mathcal{A}} \left(L_a^\dagger X L_a - \frac{1}{2} \left\{ L_a^\dagger L_a, X \right\} \right) , \tag{3.8}
$$

satisfies σ_β-KMS DBC by Theorem 10. Then the corresponding Lindblad master equation reads

$$
\partial_t \rho = \mathcal{L}^\dagger(\rho) = -i[G, \rho] + \sum_{a \in \mathcal{A}} \left(L_a \rho L_a^\dagger - \frac{1}{2} \left\{ L_a^\dagger L_a, \rho \right\} \right) . \tag{3.9}
$$

Remark 13. *To ensure that the constructed Lindblad dynamics* (3.8) *eventually relaxes to the desired Gibbs state, by Lemma 3, we should carefully choose the coupling operators A^a and weighting functions q^a such that the resulting $\{L^a\}$ and G satisfy Eq.* (2.5)*. This is always possible, due to the finite dimensionality of the system. Moreover, it is known* [TKR⁺10] *that for a primitive KMS detailed balanced QMS, the mixing time* (1.3) *can be characterized by the spectral gap of the Lindbladian. The recent work* [RFA24] *estimated the spectral gap of the efficient quantum Gibbs sampler in* [CKG23] *in the high-temperature regime, by mapping the Lindbladian $\mathcal{L}_\beta$ with KMS DBC to a Hamiltonian $\widetilde{\mathcal{L}}_\beta := \sigma_\beta^{-1/4} \mathcal{L}_\beta(\sigma_\beta^{1/4} X \sigma_\beta^{1/4}) \sigma_\beta^{-1/4}$ and then analyzing its spectral properties with perturbation theory. The extension of such a mixing time analysis framework to our case with the optimal selection of $\{(A^a, q^a)\}_{a \in \mathcal{A}}$ will be discussed in a forthcoming work.*

We have discussed the choice of self-adjoint coupling operators $\{A^a\}_{a \in \mathcal{A}}$ above. In fact, one can also generally consider a set of couplings such that $\{A^a\}_{a \in \mathcal{A}} = \{(A^a)^\dagger\}_{a \in \mathcal{A}}$, and construct the corresponding jump operators $\{L_a\}_{a \in \mathcal{A}}$ and the Lindbladian $\mathcal{L}$ as in Eqs. (3.4) and (3.8), respectively. It is easy to see that the Lindblad dynamics defined in this way still satisfies the KMS detailed balance. Indeed, let L_a and $L_{a,\mathrm{adj}}$ be the jumps associated with some A^a and $(A^a)^\dagger$ by (3.4) (without loss of generality, $A^a \neq (A^a)^\dagger$). We then define self-adjoint operators

$$
A_+^a = \frac{A^a + (A^a)^\dagger}{\sqrt{2}} \,, \quad A_-^a = \frac{A^a - (A^a)^\dagger}{\sqrt{2} i} \,,
$$

such that $\sqrt{2}A^a = A^a_+ + iA^a_-$ and denote by $L_{a,+}$ and $L_{a,-}$ the associated jumps (3.4). A direct computation by using the time-domain representation (3.4) gives

$$\begin{aligned} L_a\rho L_a^\dagger + L_{a,\mathrm{adj}}\rho L_{a,\mathrm{adj}}^\dagger &= \iint_{\mathbb{R}^2} f^a(t)\overline{f^a(t')}\left(A^a(t)\rho(A^a(t'))^\dagger + (A^a(t))^\dagger\rho A^a(t')\right) \\ &= \iint_{\mathbb{R}^2} f^a(t)\overline{f^a(t')}\left(A^a_+(t)\rho A^a_+(t') + A^a_-(t)\rho A^a_-(t')\right) \\ &= L_{a,+}\rho L_{a,+}^\dagger + L_{a,-}\rho L_{a,-}^\dagger\,, \end{aligned}$$

thanks to

$$\begin{aligned} &A^a(t)\rho(A^a(t'))^\dagger + (A^a(t))^\dagger\rho A^a(t') \\ =&\frac{1}{2}\left(A^a_+(t) + iA^a_-(t)\right)\rho\left(A^a_+(t') - iA^a_-(t')\right) + \frac{1}{2}\left(A^a_+(t) - iA^a_-(t)\right)\rho\left(A^a_+(t') + iA^a_-(t')\right) \\ =&A^a_+(t)\rho A^a_+(t') + A^a_-(t)\rho A^a_-(t')\,. \end{aligned}$$

Here f^a is defined via (3.3) with $q^a(\nu)$ satisfies (3.2). Similarly, one can check

$$\{L_a^\dagger L_a, \rho\} + \{L_{a,\mathrm{adj}}^\dagger L_{a,\mathrm{adj}}, \rho\} = \{L_{a,+}^\dagger L_{a,+}, \rho\} + \{L_{a,-}^\dagger L_{a,-}, \rho\}\,,$$

and hereby our claim holds.

3.2. **Choice of the weighting function** $q(\nu)$**.** In order to efficiently implement the jump operators $\{L_a\}_{a\in\mathcal{A}}$ in (3.4) and the coherent term G in (3.7), we need to approximate the involved integrals on $\mathbb{R}$ and $\mathbb{R}^2$ by a numerical quadrature in a finite region. This requires $f^a(t), g^a(t,t')$ to be smooth functions that decay rapidly as $|t|, |t'| \to \infty$. To this end, we assume that q^a is a compactly supported Gevrey function. We first recall the definition of Gevrey functions below [AHR17].

Definition 14 (Gevrey function)**.** *Let $\Omega \subseteq \mathbb{R}^d$ be a domain. A complex-valued C^∞ function $h : \Omega \to \mathbb{C}$ is a* Gevrey function *of order $s \geq 0$, if there exist constants $C_1, C_2 > 0$ such that for every d-tuple of nonnegative integers $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$,*

$$\|\partial^\alpha h\|_{L^\infty(\Omega)} \leq C_1 C_2^{|\alpha|}|\alpha|^{|\alpha|s}\,, \tag{3.10}$$

where $|\alpha| = \sum_{i=1}^d |\alpha_i|$. For fixed constants C_1, C_2, s, the set of Gevrey functions is denoted by $\mathcal{G}^s_{C_1,C_2}(\Omega)$. Furthermore, $\mathcal{G}^s = \bigcup_{C_1,C_2>0}\mathcal{G}^s_{C_1,C_2}$.

Some useful properties of Gevrey functions are collected in Appendix C. In particular, the product of two Gevrey functions is a Gevrey function (Lemma 26); Certain compositions of Gevrey functions are Gevrey functions (Lemma 28). The Fourier transform of compactly supported Gevrey functions satisfies Paley-Wiener type estimates (Lemma 29).

Assumption 15 (Weighting function)**.** *For $\beta > 0$, suppose that $q(\nu)$ is a weighting function of the form $q(\nu) = u(\beta\nu)w(\nu)$ with the following conditions:*

- (Symmetry) *For any $\nu \in \mathbb{R}$, $u(\nu) = \overline{u(-\nu)}, w(\nu) = \overline{w(-\nu)}$.*
- (Compact support) *There exists $S > 0$ such that* $\mathrm{supp}(w) \subset [-S, S]$.
- (Gevrey) *There exists $A_q, A_u, A_w \geq 1$, $s_u, s_w \geq 1$ such that*

$$u(\nu)e^{-\nu/4} \in \mathcal{G}^{s_u}_{A_q,A_u}(\mathbb{R})\,, \quad w \in \mathcal{G}^{s_w}_{A_q,A_w}(\mathbb{R})\,.$$

In addition, we assume $\frac{\mathrm{d}}{\mathrm{d}\nu}(u(\nu)e^{-\nu/4}) \in L^1(\mathbb{R})$ and denote

$$C_{1,u} := \left\|\frac{\mathrm{d}}{\mathrm{d}\nu}(u(\nu)e^{-\nu/4})\right\|_{L^1(\mathbb{R})}.$$

For the weighting function in Assumption 15, there holds (Lemma 26)

$$q(\nu) = \overline{q(-\nu)}\,, \quad \mathrm{supp}(q) \subset [-S, S]\,, \tag{3.11}$$

and

$$q(\nu)e^{-\beta\nu/4} \in \mathcal{G}^{s,}_{A_q^2,\beta A_u+A_w}(\mathbb{R})\,, \quad s := \max\{s_u, s_w\}\,. \tag{3.12}$$

Intuitively, one may expect that the functions $u(\nu)$ and $w(\nu)$ control the magnitude and support of the energy transition induced by a jump operator L, respectively. We can prove that the associated filtering functions $f(t)$ and $g(t,t')$ in the time domain decay rapidly (Lemma 30). This further allows us to show that a simple quadrature scheme (trapezoidal rule) can efficiently approximate $\{L_a\}_{a\in\mathcal{A}}$ and G with high accuracy. Specifically, given $M = 2^{\mathfrak{m}-1}$ with $\mathfrak{m} \in \mathbb{N}_+$ and $\tau > 0$, the quadrature points are given by

$$t_m = -M\tau + m\tau\,, \quad 0 \le m < 2M\,. \tag{3.13}$$

The quadrature error can be controlled as follows, and its proof is given in Appendix D.

Proposition 16 (Quadrature error)**.** *Under Assumption 15, we assume $\beta > 0$, $\|A^a\| \le 1$ for any $a \in \mathcal{A}$. When $\tau < \frac{2\pi}{2\|H\|+S}$ and*

$$(M-1)\tau = \Omega\left((\beta A_u + A_w)\log(\beta A_u + A_w)\right)\,, \tag{3.14}$$

Then, it holds that

$$\left\| L_a - \sum_{m=0}^{2M-1} f^a(t_m)A^a(t_m)\tau \right\| \le C_f \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s}e}\right)\,, \tag{3.15}$$

with

$$C_f = \mathcal{O}\left(A_q^2 S(\beta A_u + A_w)^{1/s}\right)\,, \tag{3.16}$$

and

$$\left\| G - \sum_{a\in\mathcal{A}}\sum_{n,m=0}^{2M-1} g^a(t_n,t_m)A^a(t_n)A^a(t_m)\tau^2 \right\| \le C_g|\mathcal{A}|\exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s}e}\right)\,, \tag{3.17}$$

with

$$C_g = \mathcal{O}\left(A_q^4 S^2(\beta A_u + A_w)^{1/s}\right)\,. \tag{3.18}$$

Here $\Omega(\cdot)$, $\mathcal{O}(\cdot)$ absorbs some constant depending on s.

Thanks to Proposition 16, to approximately block encode $\{L_a\}$ and G, it suffices to construct block-encodings for the discretized quantities

$$\sum_{m=0}^{2M-1} f^a(t_m)e^{iHt_m}A^a e^{-iHt_m}\tau\,,$$

and

$$\sum_{a\in\mathcal{A}}\sum_{n,m=0}^{2M-1} g^a(t_n,t_m)e^{iHt_n}A^a e^{-iH(t_n-t_m)}A^a e^{-iHt_m}\tau^2\,.$$

In our algorithm, we construct these two block encodings using LCU (see Appendix B). This utilizes block encodings of A^a (3.23), controlled Hamiltonian simulation (3.24), and prepare oracles for f (Eqs. (3.26) and (3.27)) or g (Eqs. (3.29) and (3.30)). The detailed constructions are presented in the next subsection (see (3.32) and (3.33)).

Remark 17. *Bounding the approximation error for $\{L_a\}_{a\in\mathcal{A}}$ and G in the operator norm is a non-trivial task.* [CKBG23] *introduces a "rounding Hamiltonian" technique to bound the quadrature error in the frequency domain. By choosing weighting functions in Assumption 15, we can use the Poisson summation formula to simplify the quadrature error analysis. In particular, we can bound the quadrature error in the time domain without using the "rounding Hamiltonian" technique.*

According to [AHR17, Corollary 2.8], for any $s_w > 1$, there exists a "bump function" $w \in \mathcal{G}^{s_w}_{C_w,A_w}$ such that $\mathrm{supp}(w) \subset [-1,1]$ and $w(\nu) = 1$ when $|\nu| \le 1/2$. Here S is an adjustable parameter to control the support of q. Then $w(\nu/S)$ is supported on $[-S,S]$ and $w(\nu/S) \in \mathcal{G}^{s_w}_{C_w,A_w/S}$. Now we provide two specific examples of q satisfying Assumption 15.

- Metropolis-type:

$$q(\nu) = e^{-\sqrt{1+\beta^2\nu^2}/4} w(\nu/S) \quad \text{with} \quad u(\nu) = e^{-\sqrt{1+\nu^2}/4}, \tag{3.19}$$

where $u(\nu)e^{-\frac{\nu}{4}} = e^{-\frac{\sqrt{1+\nu^2}+\nu}{4}} \in \mathcal{G}^1_{1,7/2}$ is a Gevrey function of order $s_u = 1$ and its derivative is L^1-integrable; see Lemma 28. Therefore $s = \max\{s_u, s_w\} = s_w$. When $\beta \gg 1$, $q(\nu)$ in Eq. (3.19) gives a smoothed version of the Metropolis-type filter (similar to the Glauber-type filter):

$$\widehat{f}(\nu) = q(\nu)e^{-\beta\nu/4} \approx \min\left\{1, e^{-\beta\nu/2}\right\}, \quad \nu \in [-S/2, S/2]. \tag{3.20}$$

- Gaussian-type[4]:

$$q(\nu) = e^{-(\beta\nu)^2/8} w(\nu/S) \quad \text{with} \quad u(\nu) = e^{-\nu^2/8}, \tag{3.21}$$

Here $u(\nu)e^{-\frac{\nu}{4}} = e^{-\frac{(\nu+1)^2-1}{8}}$ is a Gevrey function of order $s_u = \frac{1}{2}$ by [HR19, Proposition B.1] and the L^1-integrability of its derivative is straightforward. So we still have $s = \max\{s_u, s_w\} = s_w$. Setting $S = \mathcal{O}(1/\beta)$, there holds

$$\widehat{f}(\nu) = q(\nu)e^{-\nu/4} \propto e^{-(\beta\nu+1)^2/8}, \tag{3.22}$$

which is approximately a Gaussian function concentrated at $-\beta^{-1}$ with width $\mathcal{O}(\beta^{-1})$.

A comparison of the shapes of the Metropolis-type and Gaussian-type filtering function $\widehat{f}(\nu)$ is shown in Fig. 1. The support size for the Gaussian choice decreases as $\mathcal{O}(\beta^{-1})$, which can cause inefficiency because the magnitude of a local move in Monte Carlo simulations stays around order 1, regardless of the value of β.

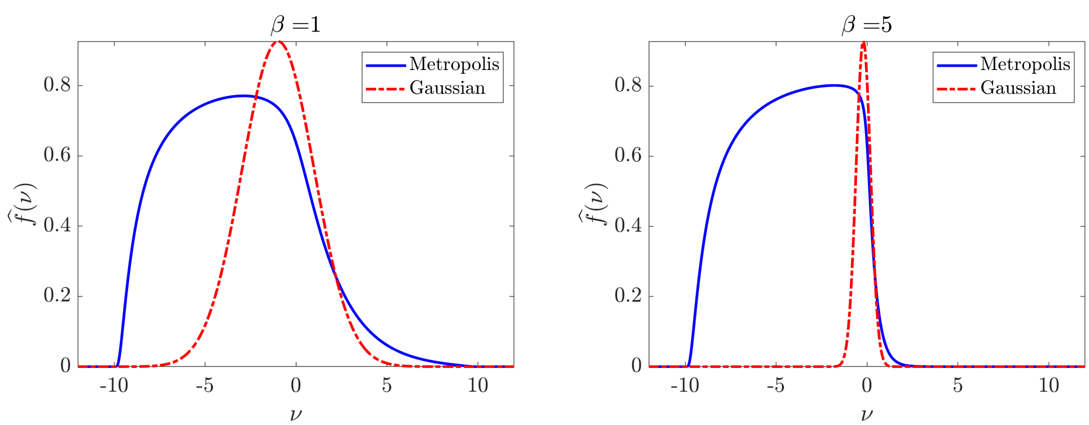


FIGURE 1. Comparison between Metropolis-type and Gaussian-type filtering functions $\widehat{f}(\nu)$ in the frequency domain with $\beta = 1$ (left) and $\beta = 5$ (right). For simplicity, the bump function is chosen to be $w(\nu/S) = \exp\left(-\frac{20}{1-(S\nu)^2}\right)$, and $S = 10$. The approximate support size of $\widehat{f}(\nu)$ remains $\mathcal{O}(1)$ for the Metropolis-type filter as $\beta \to \infty$, while it narrows to $\mathcal{O}(\beta^{-1})$ for the Gaussian-type filter.

[4]In this case, the Gaussian functions already decay rapidly. The multiplication with a bump function is for purely technical reasons to ensure $\hat{f}(\nu)$ is compactly supported.

3.3. **Efficient simulation of the Lindblad master equation** (3.9)**.** In this section, we discuss the efficient simulation of the Lindblad equation in (3.9). For simplicity, we assume that $q^a = q$, $f^a = f$, and $g^a = g$ and q satisfies Assumption 15. Our construction uses the block encoding input model and the linear combination of unitaries (see Appendices A and B). We also assume $\max_{a\in\mathcal{A}} \|A^a\| \le 1$ to ensure that efficient block encodings of A^a are available (see Eq. (3.23)).

Thanks to our algorithm's use of a discrete set of jump operators for the Lindbladian, we can directly apply efficient Lindblad simulation quantum algorithms, such as those in [CW17, LW23, CKG23, DLL24], to prepare the Gibbs state, once the efficient constructions of the block encodings of $\{L_a\}$ and G are available, which will be the focus of the rest of this section.

According to Proposition 16, in the following discussion, we set the integer $\mathfrak{m}$ large enough and consider the quadrature points $\{t_m\}_{m=0}^{2M-1}$ ($M = 2^{\mathfrak{m}-1}$) as in Eq. (3.13) such that Eq. (3.14) holds. Without loss of generality, we assume $|\mathcal{A}| = 2^{\mathfrak{a}}$ with $\mathfrak{a} \in \mathbb{N}_+$.

For the quantum simulation, we assume access to the following oracles:

- Block encoding $U_{\mathcal{A}}$ of the coupling operators $\{A^a\}_{a\in\mathcal{A}}$:

$$(\mathrm{I}_{\mathfrak{a}} \otimes \langle 0^{\mathfrak{b}}| \otimes \mathrm{I}_n) \cdot U_{\mathcal{A}} \cdot (\mathrm{I}_{\mathfrak{a}} \otimes |0^{\mathfrak{b}}\rangle \otimes \mathrm{I}_n) = \sum_a |a\rangle \langle a| \otimes A^a / Z_{\mathcal{A}}\,. \tag{3.23}$$

  We assume that the block encoding factor $Z_{\mathcal{A}}$ can be chosen to satisfy $\max_{a\in\mathcal{A}} \|A^a\| \le Z_{\mathcal{A}} \le 1$. Here $|0^{\mathfrak{b}}\rangle$ represents the ancilla qubits utilized in the block-encoding of A^a, $\mathrm{I}_{\mathfrak{a}}$ is the identity matrix acts on the index register.

- Controlled Hamiltonian simulations[5] for $\{t_m\}_{m=0}^{2M-1}$:

$$U_H = \sum_{m=0}^{2M-1} |t_m\rangle\langle t_m| \otimes \exp(-it_m H)\,. \tag{3.24}$$

- Prepare oracle for $a \in \mathcal{A}$, acting on the index register:

$$\mathbf{Prep}_{\mathcal{A}} = \mathrm{H}^{\otimes \mathfrak{a}} : |0^{\mathfrak{a}}\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{a\in\mathcal{A}} |a\rangle\ , \tag{3.25}$$

  which is used to implement LCU for the sum over a in $\mathcal{A}$ appearing in G. Here $\mathrm{H}^{\otimes\mathfrak{a}}$ are Hadamard gates acting the index register and are self-adjoint.

- Prepare oracles for the filtering functions f, acting on the time register:

$$\mathbf{Prep}_f : |0^{\mathfrak{m}}\rangle = \frac{1}{\sqrt{Z_f}} \sum_{m=0}^{2M-1} \sqrt{f(t_m)\tau}\, |t_m\rangle\ , \tag{3.26}$$

  and

$$\mathbf{Prep}_{\overline{f}} : |0^{\mathfrak{m}}\rangle = \frac{1}{\sqrt{Z_f}} \sum_{m=0}^{2M-1} \sqrt{\overline{f(t_m)}\tau}\, |t_m\rangle\ . \tag{3.27}$$

  Here the block encoding factor $Z_f := \sum_{m=0}^{2M-1} |f(t_m)|\tau$ is bounded by Lemma 32 with Eq. (D.3):

$$Z_f = \mathcal{O}\left((A_q C_{1,u} + A_q^2 S A_w)\log(\beta A_u + A_w)\right)\ . \tag{3.28}$$

- Prepare oracles for the g function, acting on the frequency register:

$$\mathbf{Prep}_g : |0^{\mathfrak{m}}\rangle\,|0^{\mathfrak{m}}\rangle = \frac{1}{\sqrt{Z_g}} \sum_{n,m=0}^{2M-1} \sqrt{g(t_n,t_m)\tau^2}\, |t_n\rangle\,|t_m\rangle\ , \tag{3.29}$$

  and

$$\mathbf{Prep}_{\overline{g}} : |0^{\mathfrak{m}}\rangle\,|0^{\mathfrak{m}}\rangle = \frac{1}{\sqrt{Z_g}} \sum_{n,m=0}^{2M-1} \sqrt{\overline{g(t_n,t_m)}\tau^2}\, |t_n\rangle\,|t_m\rangle\ , \tag{3.30}$$

[5] The circuit construction is similar to the controlled Hamiltonian simulations in the standard quantum phase estimation, and the total Hamiltonian simulation time required is $\mathcal{O}(M\tau)$.

with the block encoding factor $Z_g = \sum_{n,m=0}^{2M-1} |g(t_n, t_m)|\tau^2$ bounded as follows, by Lemma 32 with Eq. (D.4),

$$Z_g = \mathcal{O}\left((A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S) \log^2(\beta A_u + A_w) \right) . \tag{3.31}$$

Using these oracles, according to Proposition 16, we can apply LCU with (3.23), (3.24), (3.26), and (3.27) to construct a

$$\left(Z_f Z_{\mathcal{A}}, \mathfrak{m} + \mathfrak{b}, C_f \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s} e} \right) \right)$$

-block encoding U_L of $\sum_a |a\rangle\langle a| \otimes L_a$:

$$U_L = \underbrace{\left(\mathbf{Prep}_f^\dagger \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes \mathrm{I}_n \right)}_{\text{LCU prepare oracle}} \cdot \underbrace{\mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H^\dagger}_{e^{iHt_m}} \cdot \underbrace{(\mathrm{I}_{\mathfrak{m}} \otimes U_{\mathcal{A}})}_{|a\rangle\langle a| \otimes A^a} \cdot \underbrace{\mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H}_{e^{-iHt_m}} \cdot \underbrace{\left(\mathbf{Prep}_f \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes \mathrm{I}_n \right)}_{\text{LCU prepare oracle}} . \tag{3.32}$$

Here C_f is defined in Proposition 16. The circuit of U_L can be found in Fig. 2. In (3.32), the total Hamiltonian simulation time required by one query to U_L is $\mathcal{O}(M\tau)$.

Next, applying two layers of LCU (see Appendix B) with (3.23), (3.24), (3.25), (3.29), and (3.30), we construct the following

$$\left(Z_g Z_{\mathcal{A}}^2 \sqrt{|\mathcal{A}|}, 2\mathfrak{m} + \mathfrak{a} + \mathfrak{b}, C_g |\mathcal{A}| \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s} e} \right) \right)$$

-block encoding U_G of G:

(3.33)

$$\begin{aligned} U_G = & \underbrace{\left(\mathrm{I}_{\mathfrak{m}}^{\otimes 2} \otimes \mathbf{Prep}_{\mathcal{A}} \otimes \mathrm{I}_{\mathfrak{b}} \otimes \mathrm{I}_n \right)^\dagger \cdot \left(\mathbf{Prep}_g^\dagger \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes \mathrm{I}_n \right) \cdot}_{\text{Two layers of LCU prepare oracles}} \\ & \underbrace{\mathrm{I}_{\mathfrak{m}} \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H^\dagger}_{\exp(iHt_n)} \cdot \underbrace{(\mathrm{I}_{\mathfrak{m}}^{\otimes 2} \otimes U_{\mathcal{A}})}_{A^a} \cdot \underbrace{\mathrm{I}_{\mathfrak{m}} \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H}_{\exp(-iHt_n)} \cdot \underbrace{\mathrm{I}_{\mathfrak{m}} \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H^\dagger}_{\exp(iHt_m)} \cdot \underbrace{(\mathrm{I}_{\mathfrak{m}}^{\otimes 2} \otimes U_{\mathcal{A}})}_{A^a} \cdot \underbrace{\mathrm{I}_{\mathfrak{m}} \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes U_H}_{\exp(-iHt_m)} \\ & \underbrace{\cdot \left(\mathbf{Prep}_g \otimes \mathrm{I}_{\mathfrak{a}+\mathfrak{b}} \otimes \mathrm{I}_n \right) \cdot \left(\mathrm{I}_{\mathfrak{m}}^{\otimes 2} \otimes \mathbf{Prep}_{\mathcal{A}} \otimes \mathrm{I}_{\mathfrak{b}} \otimes \mathrm{I}_n \right)}_{\text{Two layers of LCU prepare oracles}} . \end{aligned}$$

Here C_g is defined in Proposition 16. We note that U_H for $\exp(-iHt_m)$ and $\exp(-iHt_n)$ are acting on different time registers. The circuit of U_G is given in Fig. 2. In (3.33), one query to U_G still requires $\mathcal{O}(M\tau)$ total Hamiltonian simulation time.

After acquiring the block encodings of $\{L_a\}_{a\in\mathcal{A}}$ and G, we can employ the algorithm proposed in [LW23] to simulate (3.9). The complexity of this algorithm is recalled below.

Theorem 18 ([LW23, Theorem 11]). *Suppose that we are given an $(A_g, \mathfrak{g}, \delta)$-block encoding U_G of G, and $(A_f, \mathfrak{f}, \delta)$-block encodings $\{U_a\}$ for the jumps $\{L_a\}$*[6]. *Let $\|\mathcal{L}\|_{\mathrm{be}} := A_g + \frac{1}{2}A_f^2|\mathcal{A}|$. For all t, ϵ with $\delta \le \epsilon/t\|\mathcal{L}\|_{\mathrm{be}}$, there exists a quantum algorithm for simulating (3.9) up to time t with an ϵ-diamond distance using*

$$\mathcal{O}\left(t\|\mathcal{L}\|_{\mathrm{be}} \log\left(t\|\mathcal{L}\|_{\mathrm{be}}/\epsilon \right) \right) \tag{3.34}$$

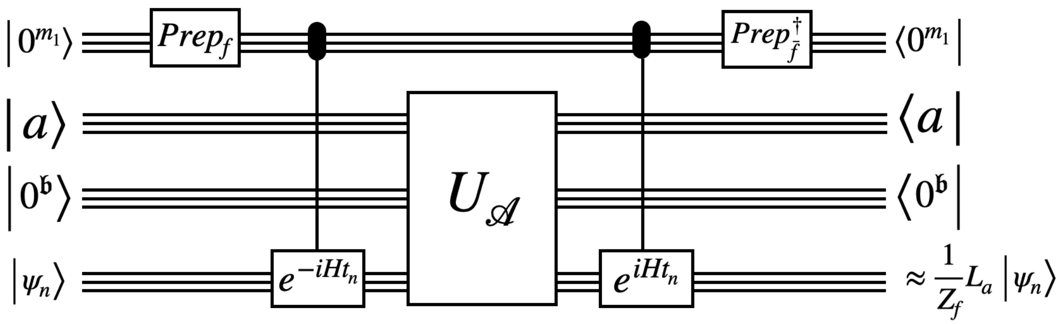
queries to U_G and $\{U_a\}_{a\in\mathcal{A}}$ and

$$\mathcal{O}\left(\log\left(t\|\mathcal{L}\|_{\mathrm{be}}/\epsilon \right) \left(\log|\mathcal{A}| + \log\left(t\|\mathcal{L}\|_{\mathrm{be}}/\epsilon \right) \right) \right)$$

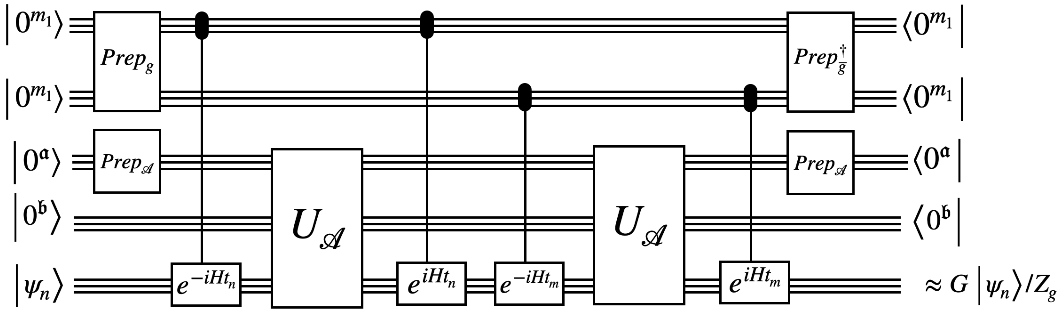
additional ancilla qubits.

Now, we are ready to give the simulation cost of our method as follows.

[6] In [LW23], the authors assume separate access to the block encodings U_a of L_a. This is slightly different from our setting assuming the block-encoding U_L of $|a\rangle\langle a| \otimes L_a$.



(A) Block encoding U_L of jump operators $\sum_{a\in\mathcal{A}} |a\rangle\langle a| \otimes L_a$.



(B) Block encoding U_G of the coherent term G.

FIGURE 2. Quantum circuits for block encodings of $\{L_a\}_{a\in\mathcal{A}}$ (top) and G (bottom). The simulation of e^{iHt_n} and e^{-iHt_m} involved in the block encoding U_G of G can be combined into a single step $e^{iH(t_n-t_m)}$ via Hamiltonian simulation controlled simultaneously by the top two registers.

Theorem 19. *Assume access to weighting functions $\{q^a\}$ satisfying Assumption 15 with any $s>1$, block encodings $U_{\mathcal{A}}$ in Eq. (3.23), controlled Hamiltonian simulation U_H in Eq. (3.24), and prepare oracles for filtering functions $\{f^a\}$ and $\{g^a\}$ in (3.26)–(3.30). The Lindbladian evolution (3.9) can be simulated up to time t_{mix} with an ϵ-diamond distance, and the total Hamiltonian simulation time is*

$$\widetilde{\mathcal{O}}\left(C_q t_{\mathrm{mix}} \beta^2 S |\mathcal{A}|^2 \log^{1+s}(1/\epsilon)\right) ,$$

where the constant C_q is defined as follows:

$$C_q := A_q^2 C_{1,u}^2/\beta S + A_q^4 A_w^2 S/\beta + A_q^3 C_{1,u} A_w/\beta + A_q^4 .$$

In addition, the algorithm requires

$$\widetilde{\mathcal{O}}\left(\log(A_q S) + \log^2(t_{\mathrm{mix}}|\mathcal{A}|/\epsilon) + \log^2(C_q\beta S) + \log A_u\right) .$$

number of additional ancilla qubits for the prepare oracles and simulation. The $\widetilde{\mathcal{O}}$ absorbs a constant only depending on s and subdominant polylogarithmic dependencies on parameters t_{mix}, $|\mathcal{A}|$, S, A_q, A_u, A_w, and β.

Remark 20. *In the above theorem, the total Hamiltonian simulation time scales quadratically in β, a complexity seemingly less favorable compared to the one in [CKG23], which is only linearly dependent in β (see Table 1). We will provide a detailed explanation of this distinction in Section 4. However, at first glance, we note that if q is chosen as a concentrated filtering function with support width $S=\mathcal{O}(1/\beta)$, one can readily recover a linear scaling of the total Hamiltonian simulation time in β. Although this choice offers a better theoretical simulation complexity, it confines energy transitions* *to a narrow range, potentially prolonging the mixing time. Balancing this trade-off by selecting S appropriately constitutes an intriguing avenue for future research.*

Proof. For simplicity, we let

$$\mathrm{C}_{q,\beta} := A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S \,. \tag{3.35}$$

By Theorem 18 with estimates in Eqs. (3.28) and (3.31), we have

$$\begin{aligned} \|\mathcal{L}\|_{\mathrm{be}} &= Z_g Z_{\mathcal{A}}^2 \sqrt{|\mathcal{A}|} + \frac{1}{2} Z_f^2 Z_{\mathcal{A}}^2 |\mathcal{A}| \\ &= \mathcal{O}\left(\mathrm{C}_{q,\beta} \log^2(\beta A_u + A_w)|\mathcal{A}|\right) , \end{aligned} \tag{3.36}$$

Recalling Proposition 16 and Lemma 32, we set a truncation time

$$T = \Theta\left((\beta A_u + A_w) \log^s \left(\frac{t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} (C_f + C_g |\mathcal{A}|)}{\epsilon} \right) \right) , \tag{3.37}$$

and the step size

$$\tau = \Theta\left(1/A_q^4 T^2 S^3\right) , \tag{3.38}$$

and then choose $M = 2^{\mathfrak{m}-1}$ such that $(M-1)\tau \leq T \leq M\tau$. This allows us to control the block-encoding error as follows:

$$(C_f + C_g|\mathcal{A}|) \exp\left(- \frac{s T^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s} e} \right) \leq \epsilon / t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} \,.$$

Note that one query to the block encoding of L_a requires one query to U_L, by Theorem 18 and Eq. (3.36), the simulation requires

$$\begin{aligned} &\mathcal{O}\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} \log\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}}/\epsilon\right) |\mathcal{A}|\right) = \widetilde{\mathcal{O}}\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} \log\left(1/\epsilon\right) |\mathcal{A}|\right) \\ =&\widetilde{\mathcal{O}}\left(t_{\mathrm{mix}} \mathrm{C}_{q,\beta} \log^2(\beta A_u + A_w) |\mathcal{A}|^2 \log\left(1/\epsilon\right)\right) \end{aligned}$$

queries to U_L. Similarly, we need

$$\widetilde{\mathcal{O}}\left(t_{\mathrm{mix}} \mathrm{C}_{q,\beta} \log^2(\beta A_u + A_w) |\mathcal{A}| \log\left(1/\epsilon\right)\right)$$

queries to U_G. Combining this with the cost $\mathcal{O}(M\tau) = \mathcal{O}(T)$ of one query to U_G and U_L, we can estimate the total Hamiltonian simulation time as follows:

$$\widetilde{\mathcal{O}}\left(t_{\mathrm{mix}} \mathrm{C}_{q,\beta} (\beta A_u + A_w) |\mathcal{A}|^2 \log^{1+s}\left(1/\epsilon\right)\right) = \widetilde{\mathcal{O}}\left(C_q t_{\mathrm{mix}} \beta^2 S |\mathcal{A}|^2 \log^{1+s}\left(1/\epsilon\right)\right) .$$

Next, we consider the number of extra ancilla qubits, again by Theorem 18. We first note

$$\log(t_{\mathrm{mix}} \left\|\mathcal{L}_{\mathrm{be}}\right\| / \epsilon) = \widetilde{\mathcal{O}}\left(\log(t_{\mathrm{mix}} |\mathcal{A}|/\epsilon) + \log \mathrm{C}_{q,\beta} + \log\log A_u\right)$$

and hence there holds

$$\begin{aligned} &\mathcal{O}\left(\log\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}}/\epsilon\right) \left(\log|\mathcal{A}| + \log\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}}/\epsilon\right)\right)\right) \\ =&\widetilde{\mathcal{O}}\left(\log^2(t_{\mathrm{mix}}|\mathcal{A}|/\epsilon) + (\log \mathrm{C}_{q,\beta} + \log\log A_u)^2\right) . \end{aligned}$$

For the preparation oracles, by Eqs. (3.37) and (3.38), we find

$$M = \Theta(A_q^4 T^3 S^3) = \Theta\left(A_q^4 S^3 (\beta A_u + A_w)^3 \log^{3s}\left(\frac{t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} (C_f + C_g |\mathcal{A}|)}{\epsilon} \right) \right)$$

This, along with Eqs. (3.16) and (3.18), implies that we need

$$\mathfrak{m} = \mathcal{O}\left(\log(A_q S) + \log(\beta A_u + A_w) + \log\left(t_{\mathrm{mix}} \|\mathcal{L}\|_{\mathrm{be}} |\mathcal{A}|/\epsilon\right)\right)$$

additional ancilla qubits for the preparation of $\mathbf{Prep}_f$, $\mathbf{Prep}_{\overline{f}}$, $\mathbf{Prep}_g$, and $\mathbf{Prep}_{\overline{g}}$. Finally, $\mathbf{Prep}_{\mathcal{A}}$ requires $\log(|\mathcal{A}|)$ ancilla qubits. Adding these quantities together concludes the proof. ∎

Remark 21. *In our simulation algorithm, thanks to the finite number of jump operators, we only need to construct the block encoding of $\sum_{a\in\mathcal{A}} |a\rangle\langle a| \otimes L_a$ for the efficient simulation. When $|\mathcal{A}| \gg 1$, by assuming oracle access to a different form of blocking encodings of A^a, we can simultaneously construct block encodings of all jump operators. Specifically, assuming oracle access to the block encoding of all coupling operators in the form $\sum_{a\in\mathcal{A}} |a\rangle\langle 0^{\mathfrak{a}}| \otimes A^a$, we can initially utilize* [CKBG23, Appendix B.1 Lemma III.1] *to construct a block encoding $U_{L,\mathrm{all}}$ for $\sum_{a\in\mathcal{A}} |a\rangle\langle 0^{\mathfrak{a}}| \otimes L_a$ and a block encoding U_G for G. Leveraging $U_{L,\mathrm{all}}$, we can implement the weak-measurement scheme proposed in* [CKG23, Section III.1] *to simulate* (3.9) *to first-order accuracy. Finally, by applying "compression" techniques as outlined in* [CW17] *to reduce the number of repetitions, the algorithm proposed in* [CKG23, Appendix F] *achieves optimal scaling in the number of uses of $U_{L,\mathrm{all}}$ and U_G.*

4. Recovery of the Gibbs sampler in [CKG23]

In this section, we discuss the connections between our proposed family of efficient quantum Gibbs samplers with KMS DBC and those constructed in [CKBG23, CKG23] and show that our framework can recover the one in [CKG23].

We have seen from (2.16) that Davies generator (2.17) without the coherent term (i.e., Lindbladian with σ_β-GNS DBC) corresponds to the algorithmic Lindbladian (1.2) with $\widehat{f}(\omega) = \delta(\omega)/2\pi$ and $G = 0$. As emphasized in Remark 7, such a choice of Dirac delta filtering function for the frequency makes it hard to approximate GNS detailed balanced Lindblad dynamic. Chen et al. [CKBG23, Theorem I.3] introduced a Gaussian smoothed version by taking f as

$$f(t) \propto \sqrt{\sigma_E}\exp(-t^2\sigma_E^2)\,, \tag{4.1}$$

with σ_E of order ϵ/β, which guarantees that the Gibbs state is an approximate fixed point. It follows that the parameter σ_E has to be small enough so that $\widehat{f}(\omega) \propto \exp(-\omega^2/4\sigma_E^2)/\sqrt{\sigma_E} \approx \delta(\omega)/2\pi$, to prepare the Gibbs state accurately. Then [CKG23] carefully constructed coherent term $i[G,\cdot]$ such that the resulting dynamics is σ_β-KMS detailed balanced and σ_E could be a moderate constant, which reduced the computational cost significantly; see Table 1.

We next prove that our construction in Section 3 can include the one in [CKG23] as a special case. Let us first recall the construction by Chen, Kastoryano, and Gilyén. Suppose that $\{A^a\}_{a\in\mathcal{A}}$ is a given set of operators satisfying $\{A^a\}_{a\in\mathcal{A}} = \{(A^a)^\dagger\}_{a\in\mathcal{A}}$. [CKG23, Corollary II.2, Proposition II.4] defined the Lindbladian of the form (1.2):

$$\begin{aligned}\mathcal{L}^\dagger[\rho] &= -i[G,\rho] + \sum_{a\in\mathcal{A}}\int_{-\infty}^{\infty}\gamma(\omega)\left(\widehat{A}^a_f(\omega)\rho\left(\widehat{A}^a_f(\omega)\right)^\dagger - \frac{1}{2}\left\{\left(\widehat{A}^a_f(\omega)\right)^\dagger\widehat{A}^a_f(\omega),\rho\right\}\right)\mathrm{d}\omega\\ &= -i[G,\rho] + \sum_{a\in\mathcal{A}}\sum_{\nu,\nu'\in B_H}\alpha_{\nu,\nu'}\left(A^a_\nu\rho\,(A^a_{\nu'})^\dagger - \frac{1}{2}\left\{(A^a_{\nu'})^\dagger A^a_\nu,\rho\right\}\right),\end{aligned} \tag{4.2}$$

with the Gaussian filtering function (4.1) for $\widehat{A}^a_f(\omega)$, the Gaussian-type transition weight function:

$$\gamma^{(g)}(\omega) = \exp\left(-\frac{(\beta\omega+1)^2}{2}\right), \tag{4.3}$$

or the Metropolis-type one:

$$\gamma^{(m)}(\omega) = \exp\left(-\beta\max\left(\omega+\frac{1}{2\beta},0\right)\right), \tag{4.4}$$

and the Hamiltonian

$$G := \sum_{a\in\mathcal{A}}\sum_{\nu,\nu'\in B_H}\frac{\tanh(-\beta(\nu-\nu')/4)}{2i}\alpha_{\nu,\nu'}\,(A^a_{\nu'})^\dagger A^a_\nu\,. \tag{4.5}$$

Here, the coefficients $\alpha_{\nu,\nu'} \in \mathbb{C}$ are given by

$$\alpha_{\nu,\nu'} := (2\pi)^2\int_{-\infty}^{\infty}\gamma(\omega)\widehat{f}(\omega-\nu)\overline{\widehat{f}(\omega-\nu')}\,\mathrm{d}\omega\,. \tag{4.6}$$

We then define the so-called Kossakowski matrix $\mathbf{C} := (\alpha_{\nu,\nu'})_{\nu,\nu'\in B_H}$ [GKS76], which is a real and positive semidefinite matrix by choosing $\hat{f}(\omega)$, $\gamma(\omega)$ to be non-negative functions. Then [CKG23] showed that if $\sigma_E = 1/\beta$, there holds

$$\alpha_{\nu,\nu'}e^{\beta(\nu+\nu')/4} = \alpha_{-\nu',-\nu}e^{-\beta(\nu+\nu')/4}\,, \tag{4.7}$$

which implies the KMS detailed balance of $\mathcal{L}$ constructed in (4.2) [CKG23, Theorem I.1].

To proceed, for notational simplicity, we assume $|\mathcal{A}| = 1$, which means that $\{A^a\}_{a\in\mathcal{A}}$ is a single self-adjoint operator $A = A^\dagger$. We introduce a new coefficient matrix:

$$\widetilde{\mathbf{C}} \in \mathbb{R}^{|B_H|\times|B_H|} \quad \text{with} \quad \widetilde{\mathbf{C}}_{\nu,\nu'} := \alpha_{\nu,\nu'}e^{\beta(\nu+\nu')/4}\,, \tag{4.8}$$

which is real and positive semidefinite and satisfy the centrosymmetry $\widetilde{\mathbf{C}}_{\nu,\nu'} = \widetilde{\mathbf{C}}_{-\nu',-\nu}$ by (4.7). We then consider the eigendecomposition of $\widetilde{\mathbf{C}}$:

$$\widetilde{\mathbf{C}} = QDQ^\dagger\,, \tag{4.9}$$

where Q is real orthogonal (hencd $Q^\dagger = Q^\top$) and D is real diagonal with elements also indexed by $(\nu,\nu') \in B_H \times B_H$. Moreover, by [CB76, Theorem 2], each eigenvector $Q_{\cdot,\nu'}$ is either symmetric (namely, $Q_{\nu,\nu'} = Q_{-\nu,\nu'}$) or skew-symmetric (namely, $Q_{\nu,\nu'} = -Q_{-\nu,\nu'}$). For $\nu' \in B_H$, we define

$$L_{\nu'} = \begin{cases} \sqrt{D_{\nu',\nu'}}\displaystyle\sum_{\nu\in B_H} Q_{\nu,\nu'}A_\nu\, e^{-\beta\nu/4}\,, & \text{if } Q_{\cdot,\nu'} \text{ is symmetric}\,,\\ i\sqrt{D_{\nu',\nu'}}\displaystyle\sum_{\nu\in B_H} Q_{\nu,\nu'}A_\nu e^{-\beta\nu/4}\,, & \text{if } Q_{\cdot,\nu'} \text{ is skew-symmetric}\,. \end{cases} \tag{4.10}$$

Then, Eq. (4.2) can be reformulated as

$$\mathcal{L}^\dagger = -i[G,\rho] + \sum_{\nu\in B_H} L_\nu\rho L_\nu^\dagger - \frac{1}{2}\left\{L_\nu^\dagger L_\nu,\rho\right\}\,,$$

and one can verify that G and $\{L_\nu\}_{\nu\in B_H}$ satisfy the requirements in Theorem 10.

For this, let us first consider G defined in (4.5). Noting from the construction (4.10) that

$$\log\left(\Delta_{\sigma_\beta}^{1/4}\right)\left(\sum_{\nu\in B_H} L_\nu^\dagger L_\nu\right) = \sum_{\nu,\nu'\in B_H} -\frac{\beta(\nu-\nu')}{4}\alpha_{\nu,\nu'}\left(A_{\nu'}^a\right)^\dagger A_\nu^a\,,$$

we compute, according to (4.5),

$$G = \sum_{\nu,\nu'\in B_H}\frac{\tanh(\beta(\nu'-\nu)/4)}{2i}\alpha_{\nu,\nu'}\left(A_{\nu'}^a\right)^\dagger A_\nu^a = -\frac{i}{2}\tanh\circ\log\left(\Delta_\beta^{1/4}\right)\left(\sum_{\nu\in B_H} L_\nu^\dagger L_\nu\right)\,, \tag{4.11}$$

which matches the general form (2.33). We next check the condition (2.28). We start with the case where $Q_{\cdot,\nu'}$ is symmetric. By (2.21) and (4.10), it holds that

$$\begin{aligned}\Delta_{\sigma_\beta}^{-1/2}(L_{\nu'}) =& \sqrt{D_{\nu',\nu'}}\sum_{\nu\in B_H} Q_{\nu,\nu'}A_\nu\, e^{-\beta\nu/4}e^{\beta\nu/2}\\ =& \sqrt{D_{\nu',\nu'}}\sum_{\nu\in B_H} Q_{\nu,\nu'}(A_\nu)^\dagger\, e^{-\beta\nu/4} = L_{\nu'}^\dagger\,,\end{aligned}$$

where we use $(A_\nu)^\dagger = A_{-\nu}$ and $Q_{\nu,\nu'} = Q_{-\nu,\nu'}$ in the second equality. For the case where $Q_{\cdot,\nu'}$ is skew-symmetric, a similar computation gives

$$\begin{aligned}\Delta_{\sigma_\beta}^{-1/2}(L_{\nu'}) =& i\sqrt{D_{\nu',\nu'}} \sum_{\nu\in B_H} Q_{\nu,\nu'} A_\nu \; e^{-\beta\nu/4} e^{\beta\nu/2} \\ =& i\sqrt{D_{\nu',\nu'}} \sum_{\nu\in B_H} Q_{-\nu,\nu'} A_{-\nu} \; e^{-\beta\nu/4} \\ =& -i\sqrt{D_{\nu',\nu'}} \sum_{\nu\in B_H} Q_{\nu,\nu'} (A_\nu)^\dagger \; e^{-\beta\nu/4} = L_{\nu'}^\dagger \,,\end{aligned}$$

where the third equality is by $(A_\nu)^\dagger = A_{-\nu}$ and $Q_{\nu,\nu'} = -Q_{-\nu,\nu'}$.

Finally, to see that our construction in Section 3.1 recovers the quantum Gibbs sampler in [CKG23], it suffices to define the weighting function:

$$q_{\nu'}(\nu) = \begin{cases} \sqrt{D_{\nu',\nu'}} Q_{\nu,\nu'} \,, & \text{if } Q_{\cdot,\nu'} \text{ is symmetric}\,, \\ i\sqrt{D_{\nu',\nu'}} Q_{\nu,\nu'} \,, & \text{if } Q_{\cdot,\nu'} \text{ is skew-symmetric}\,, \end{cases} \tag{4.12}$$

and find $q_{\nu'}(-\nu) = \overline{q_{\nu'}(\nu)}$ as required in (3.2) and that the jumps in (4.10) are the same as those in (3.4) with A and $q_{\nu'}(\nu)$ given above.

Remark 22. *Letting $\widehat{f}(\omega) \propto \exp(-\omega^2/4\sigma_E^2)$ be given as above, choosing $\gamma(\nu)$ to satisfy the KMS condition (2.20), in the limit $\sigma_E \to 0$, the matrix $\{\alpha_{\nu,\nu'}\}$ in (4.6) reduces to $\{\gamma(\nu)\delta_{\nu,\nu'}\}$ (up to some constant) and the associated Lindblad dynamic becomes GNS detailed balanced. One can similarly define the matrix $\widetilde{\mathbf{C}}$ as in (4.8) with decomposition (4.9). It holds that for each $\nu \in B_H$, there exists a symmetric eigenvector $Q_{\nu,\nu'} = \frac{1}{\sqrt{2}}(\delta_{\nu'} + \delta_{-\nu'})$ and a skew-symmetric one $Q_{\nu,\nu'} = \frac{1}{\sqrt{2}}(\delta_{\nu'} - \delta_{-\nu'})$, which corresponds to the eigenvalue $D_{\nu,\nu} = D_{-\nu,-\nu} \propto \gamma(\nu)e^{\beta\nu/2}$. In this case, $q_{\nu'}(\nu)$ in (4.12) is either $\sqrt{D_{\nu',\nu'}/2}(\delta_{\nu'}+\delta_{-\nu'})$ or $i\sqrt{D_{\nu',\nu'}/2}(\delta_{\nu'}-\delta_{-\nu'})$, and the jumps defined in (4.10) are consistent with those in (2.35).*

We now estimate the element distribution of the Kossakowski matrix $(\alpha_{\nu,\nu'})_{\nu,\nu'\in B_H}$, which in principle determines the KMS detailed balanced Lindbladian, in view of Eqs. (4.2) and (4.5). This would help us better understand the effects of the choice of q on the energy transition and how our proposed Gibbs sampler relates to those in [CKBG23, CKG23]. Recall the definition of $\alpha_{\nu,\nu'}$ in Eq. (4.6) and note that $\widehat{f}(\nu)$ was chosen as a Gaussian $\widehat{f}(\nu) \propto \sqrt{\beta}\exp(-(\beta\nu)^2/4)$. It follows that for any L^∞-bounded $\gamma(\omega)$,

$$|\alpha_{\nu,\nu'}| \le C \left\|\gamma\right\|_{L^\infty(\mathbb{R})} \beta \int_{-\infty}^{\infty} e^{-\frac{\beta^2((\omega-\nu)^2+(\omega-\nu')^2)}{4}} \mathrm{d}\omega \le C \left\|\gamma\right\|_{L^\infty(\mathbb{R})} e^{-\frac{\beta^2(\nu-\nu')}{8}} \,,$$

where C is a uniform constant. This means that for any fixed $\beta > 0$,

$$|\alpha_{\nu,\nu'}| = \Omega(1) \quad \text{only if} \quad |\nu - \nu'| = \mathcal{O}\left(\frac{1}{\beta}\right) \,, \tag{4.13}$$

that is, $\alpha_{\nu,\nu'}$ is concentrated around the diagonal part, which is the case for the Metropolis-type transition weight (4.4), due to $\gamma^{(m)} \equiv 1$ for $\omega \le 1/(2\beta)$. When $\beta \to \infty$, this narrow strip shrinks rapidly and the matrix $\alpha_{\nu,\nu'}$ approximately reduces to a diagonal one so that the sampler becomes GNS detailed balanced (Remark 22). For the case of Gaussian transition weight (4.3), we can see that the $\alpha_{\nu,\nu'}$ is actually concentrated around the origin:

$$\alpha_{\nu,\nu'} \propto e^{-\frac{(\beta\nu+\beta\nu'+2)^2}{16}} e^{-\frac{\beta^2(\nu-\nu')^2}{8}} = \Omega(1) \quad \text{if and only if} \quad |\nu|, |\nu'| = \mathcal{O}\left(\frac{1}{\beta}\right) .$$

by the explicit computation in [CKG23, Proposition II.3]. In contrast, for our Gibbs sampler constructed in Section 3.1, we have

$$\alpha_{\nu,\nu'} = e^{-\beta(\nu+\nu')/4} q^a(\nu) \overline{q^a(\nu')} \,,$$

which is always supported on $[-S, S]^2$ independent of β by Assumption 15. We refer the readers to Fig. 3 below for an illustration of the pattern of $\alpha_{\nu,\nu'}$ for various Gibbs samplers.

Remark 23. *Recall Remark 20 and note that in [CKG23], both choices of $\gamma^{(g)}$ and $\gamma^{(m)}$ in Eqs. (4.3) and (4.4) give the linear dependence of the total Hamiltonian simulation time on β. The discrepancy in complexity between our approach and theirs arises from the difference in the construction of jump operators and coherent terms. The discussion above shows that when $|\nu - \nu'| = \Omega(1/\beta)$, $\alpha_{\nu,\nu'} \ll 1$ (see Eq. (4.13)). Consequently, in (4.2), the energy transition ν in A_ν is always $\mathcal{O}(1/\beta)$ close to the energy transition ν' in $(A^a_{\nu'})^\dagger$. This property ensures that the norm of the coherent term G in [CKG23] and the normalization block encoding constant does not increase linearly in β. This differs from our case, where $\{\alpha_{\nu,\nu'}\}$ always includes a $\Omega(1)$-sized principal submatrix and the dynamics allows different energy transition terms $A_\nu \rho (A^a_{\nu'})^\dagger$ even when $|\nu - \nu'| \gg \Omega(1/\beta)$. Therefore, our coherent G has much more cross terms in the expansion, and the normalization constant for the block encoding increases linearly in β (3.31). This introduces an additional β factor in our complexity result (see Theorem 19).*

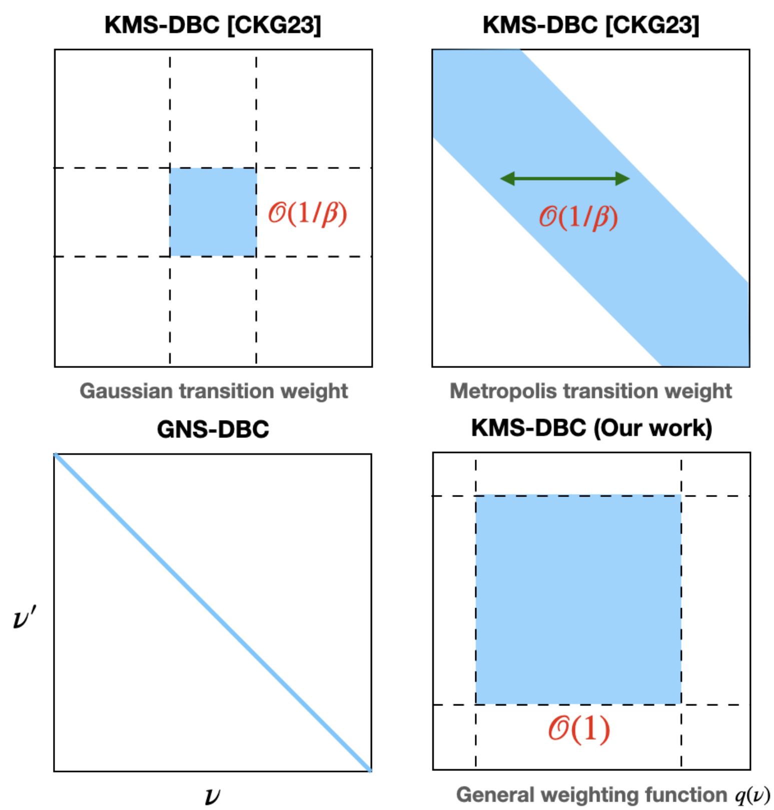


FIGURE 3. The matrix element distribution of the Kossakowski matrix $(\alpha_{\nu,\nu'})_{\nu,\nu' \in B_H}$ associated with a coupling A for various detailed balanced quantum Gibbs samplers. The blue shadow region indicates the dominant entries.

Conflict of interest statment. Authors have no conflict of interest to declare.

REFERENCES

[AC21] Érik Amorim and Eric A. Carlen. Complete positivity and self-adjointness. *Linear Algebra Appl.*, 611:389–439, 2021.

[ACL23] Dong An, Andrew M Childs, and Lin Lin. Quantum algorithm for linear non-unitary dynamics with near-optimal dependence on all parameters. *arXiv preprint arXiv:2312.03916*, 2023.

[AGIK09] Dorit Aharonov, Daniel Gottesman, Sandy Irani, and Julia Kempe. The power of quantum systems on a line. *Comm. Math. Phys.*, 287(1):41–65, 2009.

[AHR17] Ziad Adwan, Gustavo Hoepfner, and Andrew Raich. Global L^q-gevrey functions and their applications. *J. Geom. Anal.*, 27:1874–1913, 2017.

[Ali76] Robert Alicki. On the detailed balance condition for non-hamiltonian systems. *Rep. Math. Phys.*, 10(2):249–258, 1976.

[BCC+14] Dominic W Berry, Andrew M Childs, Richard Cleve, Robin Kothari, and Rolando D Somma. Exponential improvement in precision for simulating sparse hamiltonians. In *STOC 2014*, pages 283–292, 2014.

[BCG+23] Ivan Bardet, Ángela Capel, Li Gao, Angelo Lucia, David Pérez-García, and Cambyse Rouzé. Rapid thermalization of spin chain commuting Hamiltonians. *Phys. Rev. Lett.*, 130(6):060401, 2023.

[BLMT24] Ainesh Bakshi, Allen Liu, Ankur Moitra, and Ewin Tang. High-Temperature Gibbs States are Unentangled and Efficiently Preparable. *arXiv preprint arXiv:2403.16850*, 2024.

[Boy07] Khristo N. Boyadzhiev. Derivative polynomials for tanh, tan, sech and sec in explicit form. *Fibonacci Quart.*, page 291–303, 2007.

[BP02] Heinz-Peter Breuer and Francesco Petruccione. *The theory of open quantum systems*. OUP Oxford, 2002.

[CB76] Antonio Cantoni and Paul Butler. Properties of the eigenvectors of persymmetric matrices with applications to communication theory. *IEEE T COMMUN*, 24(8):804–809, 1976.

[CB21] Chi-Fang Chen and Fernando G.S.L. Brandão. Fast Thermalization from the Eigenstate Thermalization Hypothesis. *arXiv preprint arXiv:2112.07646*, 2021.

[CKBG23] Chi-Fang Chen, Michael J. Kastoryano, Fernando G.S.L. Brandão, and András Gilyén. Quantum thermal state preparation. *arXiv preprint arXiv:2303.18224*, 2023.

[CKG23] Chi-Fang Chen, Michael J. Kastoryano, and András Gilyén. An efficient and exact noncommutative quantum Gibbs sampler. *arXiv preprint arXiv:2311.09207*, 2023.

[CLVBY24] Daan Camps, Lin Lin, Roel Van Beeumen, and Chao Yang. Explicit quantum circuits for block encodings of certain sparse matrices. *SIAM J. Matrix Anal.Appl.*, 45(1):801–827, 2024.

[CM17] Eric A. Carlen and Jan Maas. Gradient flow and entropy inequalities for quantum markov semigroups with detailed balance. *J. Funct. Anal.*, 273(5):1810–1869, 2017.

[CM20] Eric A. Carlen and Jan Maas. Non-commutative calculus, optimal transport and functional inequalities in dissipative quantum systems. *J. Stat. Phys.*, 178(2):319–378, 2020.

[Com74] L. Comtet. *Advanced Combinatorics: The Art of Finite and Infinite Expansions*. Springer Netherlands, 1974.

[CS17] Anirban Narayan Chowdhury and Rolando D. Somma. Quantum algorithms for Gibbs sampling and hitting-time estimation. *Quantum Inf. Comput.*, 17(1-2):41–64, 2017.

[Cub23] Toby S. Cubitt. Dissipative ground state preparation and the dissipative quantum eigensolver. *arXiv preprint arXiv:2303.11962*, 2023.

[CW12] Andrew M. Childs and Nathan Wiebe. Hamiltonian simulation using linear combinations of unitary operations. *Quantum Inf. Comput.*, 12:901–924, 2012.

[CW17] Richard Cleve and Chunhao Wang. Efficient quantum algorithms for simulating Lindblad evolution. In *ICALP 2017*, 2017.

[Dav74] E. Brian Davies. Markovian master equations. *Commun. Math. Phys.*, 39:91–110, 1974.

[Dav76] E. Brian Davies. *Quantum theory of open systems*. Academic Press, 1976.

[Dav79] E. Brian Davies. Generators of dynamical semigroups. *J. Funct. Anal.*, 34(3):421–432, 1979.

[DLL24] Zhiyan Ding, Xiantao Li, and Lin Lin. Simulating open quantum systems using hamiltonian simulations. *arXiv preprint arXiv:2311.15533*, 2024.

[FS02] Daan Frenkel and Berend Smit. *Understanding Molecular Simulation: From Algorithms to Applications*. Academic Press, 2002.

[FU07] Franco Fagnola and Veronica Umanità. Generators of detailed balance quantum Markov semigroups. *Infin. Dimens. Anal. Quantum Probab. Relat. Top.*, 10(03):335–363, 2007.

[FU10] Franco Fagnola and Veronica Umanità. Generators of KMS symmetric Markov semigroups on symmetry and quantum detailed balance. *Commun. Math. Phys.*, 298(2):523–547, 2010.

[GKS76] Vittorio Gorini, Andrzej Kossakowski, and Ennackal Chandy George Sudarshan. Completely positive dynamical semigroups of n-level systems. *J. Math. Phys.*, 17:821–825, 1976.

[GSLW19] András Gilyén, Yuan Su, Guang Hao Low, and Nathan Wiebe. Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics. In *STOC 2019*, pages 193–204, 2019.

[HR19] Gustavo Hoepfner and Andrew Raich. Global L^q Gevrey Functions, Paley-Weiner Theorems, and the FBI Transform. *Indiana University Mathematics Journal*, 68(3):pp. 967–1002, 2019.

[KB16] Michael J. Kastoryano and Fernando G.S.L. Brandão. Quantum Gibbs samplers: The commuting case. *Commun. Math. Phys.*, 344:915–957, 2016.

[KFGV77] Andrzej Kossakowski, Alberto Frigerio, Vittorio Gorini, and Maurizio Verri. Quantum detailed balance and KMS condition. *Commun. Math. Phys.*, 57(2):97–110, 1977.

[KSV02] Alexei Yu Kitaev, Alexander Shen, and Mikhail N. Vyalyi. *Classical and quantum computation.* Number 47 in Graduate Studies in Mathematics. American Mathematical Soc., 2002.

[KT13] Michael J Kastoryano and Kristan Temme. Quantum logarithmic Sobolev inequalities and rapid mixing. *J. Math. Phys.*, 54(5):1–34, 2013.

[LC19] Guang Hao Low and Isaac L. Chuang. Hamiltonian simulation by qubitization. *Quantum*, 3:163, 2019.

[Lid19] Daniel A. Lidar. Lecture notes on the theory of open quantum systems. *arXiv preprint arXiv:1902.00967*, 2019.

[Lin76] Goran Lindblad. On the generators of quantum dynamical semigroups. *Commun. Math. Phys.*, 48:119–130, 1976.

[LW23] Xiantao Li and Chunhao Wang. Simulating Markovian Open Quantum Systems Using Higher-Order Series Expansion. In *ICALP 2023*, pages 87:1–87:20, 2023.

[ML20] Evgeny Mozgunov and Daniel Lidar. Completely positive master equation for arbitrary driving and small level spacing. *Quantum*, 4(1):1–62, 2020.

[NKL22] Quynh T. Nguyen, Bobak T. Kiani, and Seth Lloyd. Block-encoding dense and full-rank kernels using hierarchical matrices: applications in quantum numerical linear algebra. *Quantum*, 6:876, 12 2022.

[Pin08] Mark A. Pinsky. *Introduction to Fourier Analysis and Wavelets.* Graduate studies in mathematics. American Mathematical Society, 2008.

[PW09] David Poulin and Pawel Wocjan. Preparing ground states of quantum many-body systems on a quantum computer. *Phys. Rev. Lett.*, 102(13):130503, 2009.

[RFA24] Cambyse Rouzé, Daniel Stilck Franca, and Álvaro M. Alhambra. Efficient thermalization and universal quantum computing with quantum Gibbs samplers. *arXiv preprint arXiv:2403.12691*, 2024.

[RWW23] Patrick Rall, Chunhao Wang, and Pawel Wocjan. Thermal state preparation via rounding promises. *Quantum*, 7:1132, 2023.

[SCC23] Christoph Sünderhauf, Earl Campbell, and Joan Camps. Block-encoding structured matrices for data input in quantum computing. *arXiv preprint arXiv:2302.10949*, 2023.

[SM23] Oles Shtanko and Ramis Movassagh. Preparing thermal states on noiseless and noisy programmable quantum processors. *arXiv preprint arXiv:2112.14688*, 2023.

[TKR+10] Kristan Temme, Michael James Kastoryano, Mary Beth Ruskai, Michael Marc Wolf, and Frank Verstraete. The χ^2-divergence and mixing times of quantum Markov processes. *J. Math. Phys.*, 51(12), 2010.

[TOV+11] Kristan Temme, Tobias J. Osborne, Karl G. Vollbrecht, David Poulin, and Frank Verstraete. Quantum Metropolis sampling. *Nature*, 471(7336):87–90, 2011.

[VAGGdW17] Joran Van Apeldoorn, András Gilyén, Sander Gribling, and Ronald de Wolf. Quantum SDP-solvers: Better upper and lower bounds. In *FOCS 2017*, pages 403–414. IEEE, 2017.

[Wol12] Michael M. Wolf. Quantum channels & operations: guided tour. Lecture Notes. *URL http://www-m5. ma. tum. de/foswiki/pub M*, 2012.

[WT23] Pawel Wocjan and Kristan Temme. Szegedy walk unitaries for quantum maps. *Commun. Math. Phys.*, 402(3):3201–3231, 2023.

[YAG12] Man-Hong Yung and Alán Aspuru-Guzik. A quantum–quantum Metropolis algorithm. *PNAS*, 109(3):754–759, 2012.

[ZB23] Yikang Zhang and Thomas Barthel. Criteria for Davies irreducibility of Markovian quantum dynamics. *J. Phys. A: Math. Theor*, 2023.

Appendix A. Block encoding

Block encoding (see [LC19, GSLW19]) provides a general framework for encoding a non-unitary matrix using unitary matrices, which can be implemented on quantum devices.

Definition 24 (Block encoding). *Given a matrix $A \in \mathbb{C}^{2^n \times 2^n}$, if we can find $\alpha, \epsilon \in \mathbb{R}_+$, and a unitary matrix $U_A \in \mathbb{C}^{2^{n+m} \times 2^{n+m}}$ so that*

$$\|A - \alpha \left(\langle 0^m| \otimes I_n\right) U_A \left(|0^m\rangle \otimes I_n\right)\| \leq \epsilon, \tag{A.1}$$

then U_A is called an (α, m, ϵ)-block-encoding of A. The parameter α is referred to as the block encoding factor, or the subnormalization factor.

Intuitively, the block encoding matrix U_A encodes the rescaled matrix A/α in its upper left block:

$$U_A \approx \begin{pmatrix} A/\alpha & * \\ * & * \end{pmatrix}.$$

There have been substantial efforts on implementing the block encoding of certain structured matrices of practical interest [GSLW19, NKL22, CLVBY24, SCC23]. In this work, we assume that the query access to the block encoding of relevant matrices is available. We also assume that there is no error in the block encodings of the input matrices H, A^a, etc. If such errors are present, their impact should be treated using perturbation theories. Meanwhile, we need to carefully keep track of the error of the block encodings derived from the input matrices, such as the jump operators L_a.

Appendix B. Linear combination of unitaries

The linear combination of unitaries (LCU) [CW12] is an important quantum primitive, which allows matrices expressed as a superposition of unitary matrices to be coherently implemented using block encoding. Here we follow [GSLW19] and present a general version of the LCU that is applicable to possibly complex coefficients.

LCU implements a block encoding of $\sum_{j=0}^{J-1} c_j U_j$, where U_j are unitary operators and c_j are complex numbers. For the coefficients, we assume access to a pair of *state preparation oracles* (also called prepare oracles for short) $(\mathbf{Prep}_{\overline{\gamma_l}}, \mathbf{Prep}_{\gamma_r})$ acting as (assume $J = 2^\ell$)

$$\mathbf{Prep}_{\overline{\gamma_l}} : |0^\ell\rangle \to \frac{1}{\|\gamma_l\|_2} \sum_{j=0}^{J-1} \overline{\gamma_{l,j}}\, |j\rangle\,,$$

$$\mathbf{Prep}_{\gamma_r} : |0^\ell\rangle \to \frac{1}{\|\gamma_r\|_2} \sum_{j=0}^{J-1} \gamma_{r,j}\, |j\rangle\,.$$

Here the coefficients should satisfy $\gamma_{l,j}\gamma_{r,j} = c_j, 0 \leq j \leq J-1$. To minimize the block encoding factor, the optimal choice is $|\gamma_{l,j}| = |\gamma_{r,j}| = \left|\sqrt{c_j}\right|$, and where $\sqrt{z}$ refers to the principal value of the square root of z. In this case, $\|\gamma_l\|_2 = \|\gamma_r\|_2 = \sqrt{\|c\|_1}$, where $\|c\|_1 = \sum_j |c_j|$ is the 1-norm of the vector c.

The unitaries U_j needs to be accessed via a *select oracle* **Select** as

$$\mathbf{Select} = \sum_{j=0}^{J-1} |j\rangle \langle j| \otimes U_j,$$

which can be constructed using controlled versions of the block encoding matrices U_j.

Lemma 25 (LCU). *Assume $J = 2^\ell$, $\|\gamma_l\|_2 = \|\gamma_r\|_2 = \sqrt{\|c\|_1}$, then the matrix*

$$W = \left(\mathbf{Prep}_{\overline{\gamma_l}}^\dagger \otimes I\right) \mathbf{Select} \left(\mathbf{Prep}_{\gamma_r} \otimes I\right)$$

is a $(\|c\|_1, \ell, 0)$-block-encoding of the linear combination of unitaries $\sum_{j=0}^{J-1} c_j U_j$.

Appendix C. Gevrey functions

In this section, we collect a few results for Gevrey functions that are useful for this work. While similar findings have been previously demonstrated in the literature, notably in [AHR17] and [HR19], we provide self-contained proofs here with explicit expressions for the constants involved.

Lemma 26 (Product of Gevrey functions). *Given $h \in \mathcal{G}^s_{C_1,C_2}(\mathbb{R}^d)$ and $h' \in \mathcal{G}^{s'}_{C_1',C_2'}(\mathbb{R}^d)$, then*

$$h \cdot h' \in \mathcal{G}^{\max\{s,s'\}}_{C_1C_1',C_2+C_2'}(\mathbb{R}^d)\,.$$

Proof. For a index vector $\alpha \in \mathbb{N}^d$, a direct application of Leibniz rule gives

$$\begin{aligned}
\left\|\partial^\alpha\left(h\cdot h'\right)\right\|_{L^\infty(\mathbb{R}^d)} &\leq \sum_{j=0}^{|\alpha|}\sum_{\beta\leq\alpha,|\beta|=j}\binom{\alpha}{\beta}\left\|\partial^\beta h\right\|_{L^\infty(\mathbb{R}^d)}\left\|\partial^{\alpha-\beta}h'\right\|_{L^\infty(\mathbb{R}^d)}\\
&\leq C_1C_1'\sum_{j=0}^{|\alpha|}\left((C_2)^j j^{js}(C_2')^{|\alpha|-j}(|\alpha|-j)^{(|\alpha|-j)s'}\left(\sum_{\beta\leq\alpha,|\beta|=j}\binom{\alpha}{\beta}\right)\right)\\
&\leq C_1C_1'\sum_{j=0}^{|\alpha|}\left(\binom{|\alpha|}{j}(C_2)^j j^{js}(C_2')^{|\alpha|-j}(|\alpha|-j)^{(|\alpha|-j)s'}\right)\\
&\leq C_1C_1'\left(C_2+C_2'\right)^{|\alpha|}|\alpha|^{|\alpha|\max\{s,s'\}}\,,
\end{aligned}$$

where the third inequality is by $\sum_{\beta\leq\alpha,|\beta|=j}\binom{\alpha}{\beta}=\binom{|\alpha|}{j}$. □

We next show that $\exp(-\frac{\sqrt{1+x^2}+x}{4})$ is a Gevrey function and its derivative is L^1-integrable. We first recall the Faà di Bruno's formula and the partial Bell polynomial for the chain rule of high-order derivatives [Com74, p.139].

Lemma 27 (Faà di Bruno's formula and partial Bell polynomial). *Let h, g be smooth function from $\mathbb{C}$ to $\mathbb{C}$, and $f(x) := h(g(x))$. Then the k-th order derivative of f is given by*

$$f^{(k)}(x) = \sum \frac{k!}{q_1!(1!)^{q_1}q_2!(2!)^{q_2}\cdots q_k!(k!)^{q_k}}h^{(\sum q_i)}(g(x))\prod_{i=1}^{k}\left(g^{(i)}(x)\right)^{q_i}$$

where the sum is over all k-tuples of nonnegative integers $(q_1, q_2, \cdots, q_k)$ satisfying $\sum iq_i = k$. The above formula can also be rewritten as

$$f^{(k)}(x) = \sum_{j=1}^{k}h^{(j)}(g(x))B_{k,j}\left(g^{(1)}(x), g^{(2)}(x), \ldots, g^{(k-j+1)}(s)\right)\,,$$

where $B_{k,j}$ is the partial Bell polynomial:

$$B_{k,j} = \sum_{\substack{1\leq i\leq k\,,\,q_i\in\mathbb{N}\\ \sum_{i=1}^k iq_i=k\\ \sum_{i=1}^k q_i=j}}\frac{k!}{q_1!q_2!\cdots q_{k-j+1}!}\prod_{i=1}^{k-j+1}\left(\frac{x_i}{i!}\right)^{q_i}\,.$$

Using Faà di Bruno's formula, we can calculate the high order derivatives of $\exp(-\frac{\sqrt{1+x^2}+x}{4})$ and verify that it belongs to a Gevrey class.

Lemma 28. *It holds that*

$$e^{-\frac{\sqrt{1+x^2}+x}{4}} \in \mathcal{G}^1_{1,\frac{7}{2}}\,,\quad \left(e^{-\frac{\sqrt{1+x^2}+x}{4}}\right)^{(1)} \in L^1(\mathbb{R})\,.$$

Proof. We first use the second formula of Lemma 27 and some properties of the partial Bell polynomials $B_{n,k}$ to calculate k-th order derivative for $\sqrt{1+x^2}$. For $k \geq 2$, we have (define $\binom{j}{k-j} = 0$ if $k > 2j$)

$$\begin{aligned}
&\left(\sqrt{1+x^2}\right)^{(k)} \\
=&\sum_{j=1}^{k} \frac{(-1)^{j+1}(2j-3)!!}{2^j(1+x^2)^{j-1/2}} B_{k,j}(2x,2,0,\dots,0) = \sum_{j=1}^{k} \frac{(-1)^{j+1}2^j(2j-3)!!}{2^j(1+x^2)^{j-1/2}} B_{k,j}(x,1,0,\dots,0) \\
=&\sum_{j=1}^{k} \frac{(-1)^{j+1}2^j(2j-3)!!}{2^j(1+x^2)^{j-1/2}} \frac{1}{2^{k-j}} \frac{k!}{j!} \binom{j}{k-j} x^{2j-k} = \frac{k!}{2^k} \sum_{j=1}^{k} \frac{(-1)^{j+1}2^j(2j-3)!!}{j!} \binom{j}{k-j} \frac{x^{2j-k}}{(1+x^2)^{j-1/2}} \,.
\end{aligned}$$

Using the fact that $\left|\frac{x^{2j-k}}{(1+x^2)^{j-1/2}}\right| \leq 1$, $(2j-3)!! \leq 2^j j!$, and $(1+2^2)^k = \sum_{j=0}^{k} \binom{k}{k-j} 2^{2j}$, we have

$$\left|\left(\sqrt{1+x^2}\right)^{(k)}\right| \leq \frac{k!}{2^k} \sum_{j=0}^{k} \frac{2^j(2j-3)!!}{j!} \binom{j}{k-j} \leq \frac{k!}{2^k} \sum_{j=0}^{k} 4^j \binom{k}{k-j} \leq (5/2)^k\, k! \,.$$

Next, by Faà di Bruno's formula for $\exp(-\frac{\sqrt{1+x^2}+x}{4})$, we obtain

$$\begin{aligned}
&\left(e^{-\frac{\sqrt{1+x^2}+x}{4}}\right)^{(k)} \\
=&\sum \frac{k!}{q_1!(1!)^{q_1} q_2!(2!)^{q_2} \cdots q_k!(k!)^{q_k}} \left(-\frac{1}{4}\right)^k e^{-\frac{\sqrt{1+x^2}+x}{4}} \prod_{j=1}^{k} \left(\left(\sqrt{1+x^2}\right)^{(j)} + x^{(j)}\right)^{q_j} \,.
\end{aligned} \tag{C.1}$$

Plugging the upper bound $\left|\left(\sqrt{1+x^2}\right)^{(j)}\right|$ gives

$$\begin{aligned}
\left|\left(e^{-\frac{\sqrt{1+x^2}+x}{4}}\right)^{(k)}\right| &< \sum \frac{k!}{q_1!(1!)^{q_1} q_2!(2!)^{q_2} \cdots q_k!(k!)^{q_k}} \left(\frac{1}{4}\right)^k \prod_{j=1}^{k} (7/2)^{jq_j} (j!)^{q_j} \\
=\sum \frac{k!}{q_1! q_2! \cdots q_k!} \left(\frac{1}{4}\right)^k \prod_{j=1}^{k} (7/2)^{jq_j} &= \sum \frac{(7/8)^k k!}{q_1! q_2! \cdots q_k!} \leq (7/8)^k k! \sum 1 \leq (7/2)^k k! \,,
\end{aligned}$$

where we use the fact that the number of k-tuples of nonnegative integers $(q_1, q_2, \cdots, q_k)$ satisfying $\sum j q_j = k$ is less than $\binom{2k}{k} \leq 2^{2k}$. This concludes $\exp(-\frac{\sqrt{1+x^2}+x}{4}) \in \mathcal{G}^1_{1,\frac{7}{2}}$. The L^1-integrablity of $(\exp(-\frac{\sqrt{1+x^2}+x}{4}))^{(1)}$ is a simple consequence of Eq. (C.1). □

Finally, we show that the Fourier transform of the Gevrey class with compact support decays rapidly, by a Paley-Wiener type estimate.

Lemma 29. *Given $h \in \mathcal{G}^s_{C_1,C_2}(\mathbb{R}^d)$ with compact support $\Omega = \mathrm{supp}(h)$ and $s \geq 1$, define*

$$H(y) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} h(x) e^{-ix\cdot y} \,\mathrm{d}x \,.$$

Then, for any $y \in \mathbb{R}^d$, there holds

$$|H(y)| \leq \frac{C_1|\Omega|}{(2\pi)^d} e^{\frac{esd}{2} - \frac{s}{C_2^{1/s} e} \|y\|_2^{1/s}} \,,$$

where $|\Omega| = \int_\Omega 1 \,\mathrm{d}x$ is the volume of Ω and $\|y\|_2$ is the 2-norm of the vector y.

Proof. By Definition 14, we have, for every d-tuple of nonnegative integers α with $|\alpha| = \sum_i |\alpha_i|$,

$$\|\partial^\alpha h\|_{L^\infty(\mathbb{R}^d)} \leq C_1 C_2^{|\alpha|} |\alpha|^{|\alpha| s} \,.$$

It follows that

$$|y^\alpha|\,|H(y)| = |y^\alpha H(y)| = \left|\frac{1}{(2\pi)^d} \int_\Omega \partial^\alpha h(x) e^{-ix\cdot y} \,\mathrm{d}x\right| \leq \frac{C_1|\Omega|}{(2\pi)^d} C_2^{|\alpha|} |\alpha|^{|\alpha| s} \,,$$

where $y^\alpha := \Pi_{i=1}^d y_i^{\alpha_i}$. Recall from [AHR17, Proposition 3.1] that

$$\inf_{m\in\mathbb{Z}_{\geq 0}} \left\{ \left(\frac{s}{ae}\right)^{ms} \frac{m^{ms}}{|t|^m} \right\} \leq e^{es/2} e^{-a|t|^{1/s}}\,, \quad \text{for any } a, s, t > 0\,.$$

Letting $a := s/(C_2^{1/s} e)$ and using the above inequality, we obtain

$$\begin{aligned} |H(y)| \leq \frac{C_1|\Omega|}{(2\pi)^d} \inf_{\alpha\in\mathbb{N}^d} \frac{C_2^{|\alpha|}|\alpha|^{|\alpha|s}}{|y^\alpha|} &\leq \frac{C_1|\Omega|}{(2\pi)^d} \prod_i \inf_{\alpha_i\in\mathbb{Z}_{\geq 0}} \left| \frac{C_2^{\alpha_i}|\alpha_i|^{\alpha_i s}}{|y_i|^{\alpha_i}} \right| \\ &\leq \frac{C_1|\Omega|}{(2\pi)^d} e^{esd/2} e^{-a\sum_{i=1}^d |y_i|^{1/s}} \\ &\leq \frac{C_1|\Omega|}{(2\pi)^d} e^{esd/2} e^{-a\|y\|_2^{1/s}}\,. \end{aligned}$$

□

Appendix D. Quadrature error analysis

In this section, for notational simplicity, sometimes we absorb the generic constant C_s depending on the parameter s of the filtering function $q(\nu)$ in Eq. (3.12) into $\mathcal{O}$. We first study the decaying and integrable property of the functions f and $g(t,t')$.

Lemma 30. *Let $f(t)$ and $g(t,t')$ be the functions defined in (3.3) and (3.6) with a weighting function $q(\nu)$ satisfying Assumption 15. Then, it holds that*

$$|f(t)| \leq \frac{A_q^2 S}{\pi} \exp\left(\frac{es}{2} - \frac{s}{(\beta A_u + A_w)^{1/s} e}|t|^{1/s}\right), \tag{D.1}$$

and

$$|g(t,t')| \leq \frac{A_q^4 S^2}{2\pi^2} \exp\left(es - \frac{s}{(2\beta A_u + 2A_w + \beta)^{1/s} e}\left(\sqrt{t^2 + (t')^2}\right)^{1/s}\right). \tag{D.2}$$

The integrals of f and g have the following asymptotics:

$$\int_{\mathbb{R}} |f(t)|\,\mathrm{d}t = \mathcal{O}\left((A_q C_{1,u} + A_q^2 S A_w)\log(\beta A_u + A_w)\right), \tag{D.3}$$

and

$$\iint_{\mathbb{R}^2} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t' = \mathcal{O}\left((A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S)\log^2(\beta A_u + A_w + \beta)\right). \tag{D.4}$$

Proof. We recall the definitions of $f(t)$ and $g(t,t')$:

$$f(t) = \frac{1}{2\pi}\int_{\mathbb{R}} u(\beta\nu) w(\nu) e^{-\beta\nu/4} e^{-it\nu}\,\mathrm{d}\nu\,, \tag{D.5}$$

and

$$g(t,t') = \frac{1}{(2\pi)^2}\iint_{\mathbb{R}^2} \frac{\tanh(\beta(\nu'-\nu)/4)e^{-\beta(\nu+\nu')/4}}{2i} u(\beta\nu)w(\nu)\overline{u(\beta\nu')w(\nu')}e^{-i(\nu t - \nu' t')}\,\mathrm{d}\nu\,\mathrm{d}\nu'\,. \tag{D.6}$$

Exponential decay of f. Thanks to Lemma 26 with Assumption 15, we have

$$\widehat{f}(\nu) = u(\beta\nu)w(\nu)e^{-\beta\nu/4} \in \mathcal{G}^s_{A_q^2, \beta A_u + A_w}(\mathbb{R}) \quad \text{with} \quad \mathrm{supp}(\widehat{f}) \in [-S, S]\,.$$

Then, Lemma 29 with $d = 1$ and $|\Omega| = 2S$ yields the estimate for f:

$$|f(t)| \leq \frac{A_q^2 S}{\pi} \exp\left(\frac{es}{2} - \frac{s|t|^{1/s}}{(\beta A_u + A_w)^{1/s} e}\right). \tag{D.7}$$

Exponential decay of g. By using [Boy07, Eq. (3.3)], we first have

$$\left\|\tanh^{(N)}(x)\right\|_{L^\infty(\mathbb{R})} \leq 2^N \sum_{k=0}^N k! \binom{N}{k} \leq 4^N N!\,,$$

which implies

$$\tanh((\nu'-\nu)/4) \in \mathcal{G}^1_{1,1}(\mathbb{R}^2)\,. \tag{D.8}$$

It follows from Lemma 26 with

$$(2i)\widehat{g}(\nu,\nu') = \tanh(\beta(\nu'-\nu)/4)e^{-\beta(\nu+\nu')/4}u(\beta\nu)w(\nu)\overline{u(\beta\nu')w(\nu')}$$

that

$$(2i)\widehat{g}(\nu,\nu') \in \mathcal{G}^s_{A_q^4,2\beta A_u+2A_w+\beta} \quad \text{with} \quad \operatorname{supp}(\widehat{g}) \in [-S,S]^2\,.$$

Again, applying Lemma 29 with $d=2$ and $|\Omega| = 4S^2$ gives

$$|g(t,t')| \le \frac{A_q^4 S^2}{2\pi^2}\exp\left(es - \frac{s}{(2\beta A_u + 2A_w+\beta)^{1/s}e}\left(\sqrt{t^2+(t')^2}\right)^{1/s}\right)\,, \tag{D.9}$$

which concludes the proof for the decay of g.

Estimate the integral of f. We note from Assumption 15 that the derivative of $u(\beta\nu)w(\nu)e^{-\beta\nu/4}$ is L^1-integrable. It follows that

$$itf(t) = \frac{1}{2\pi}\int_{\mathbb{R}}\frac{\mathrm{d}}{\mathrm{d}\nu}\left(u(\beta\nu)w(\nu)e^{-\beta\nu/4}\right)e^{-it\nu}\,\mathrm{d}\nu\,,$$

and then

$$\begin{aligned}2\pi\left\|tf(t)\right\|_{L^\infty(\mathbb{R})} &\le \left\|(u(\beta\nu)e^{-\beta\nu/4})^{(1)}\right\|_{L^1(\mathbb{R})}\left\|w\right\|_{L^\infty(\mathbb{R})} + \left\|u(\beta\nu)e^{-\beta\nu/4}\right\|_{L^\infty(\mathbb{R})}\left\|w^{(1)}\right\|_{L^1(\mathbb{R})}\\ &\le A_q C_{1,u} + 2SA_q^2A_w\,,\end{aligned}$$

by the invariance of $\left\|(u(\beta\nu)e^{-\beta\nu/4})^{(1)}\right\|_{L^1(\mathbb{R})}$ in β. Here, we use $w \in \mathcal{G}^s_{A_q,A_\omega}$ and $\operatorname{supp}(w) = [-S,S]$ to obtain $\left\|w^{(1)}\right\|_{L^1(\mathbb{R})} \le 2SA_qA_\omega$. In addition, because $\left\|u(\beta\nu)e^{-\beta\nu/4}\right\|_{L^\infty(\mathbb{R})} \le A_q$, there holds

$$\|f\|_{L^\infty(\mathbb{R})} \le \frac{1}{2\pi}\int_{[-S,S]}\left|u(\beta\nu)w(\nu)e^{-\beta\nu/4}\right|\,\mathrm{d}\nu \le \frac{1}{\pi}A_q^2S\,.$$

Thus, we readily have, for any $T>1$,

$$\begin{aligned}\int_{-T}^{T}|f(t)|\,\mathrm{d}t &\le \frac{2}{\pi}A_q^2S + 2\int_1^T|f(t)|\,\mathrm{d}t\\ &\le \frac{2}{\pi}A_q^2S + 2\frac{A_qC_{1,u}+2SA_q^2A_w}{2\pi}\log T = \mathcal{O}\left((A_qC_{1,u}+SA_q^2A_w)\log T\right)\,.\end{aligned} \tag{D.10}$$

Next, by Eq. (D.1), a direct computation via change of variable $t^{1/s} = u$ gives

$$\int_T^\infty |f(t)|\,\mathrm{d}t = \mathcal{O}\left(A_q^2S\int_{T^{1/s}}^\infty u^{s-1}\exp\left(-\frac{s}{(\beta A_u+A_w)^{1/s}e}u\right)\mathrm{d}u\right)\,,\quad T>0\,. \tag{D.11}$$

We define the constant T_f by

$$T_f(A_u,A_w) := \inf\left\{T>0\,;\ u^{s-1} \le \exp\left(\frac{s}{2(\beta A_u+A_w)^{1/s}e}u\right)\ \text{for any}\ u \ge T^{1/s}\right\}\,, \tag{D.12}$$

which satisfies the following asymptotics: as $\beta A_u + A_w \to \infty$,

$$T_f(A_u,A_w)/\log(T_f(A_u,A_w)) = \Theta\left(\beta A_u + A_w\right)\,.$$

Note that $x/\log x$ is decreasing on $(1,e]$ and increasing on $[e,+\infty)$ with global minimum e at $x=e$. For any $y \ge e$, the equation $x/\log x = y$ has a unique solution $y \le x \le y^2$, which readily gives $y\log y \le x = y\log x \le 2y\log y$ and thus, by (D.12),

$$T_f(A_u,A_w) = \Theta\left((\beta A_u+A_w)\log\left(\beta A_u+A_w\right)\right)\,. \tag{D.13}$$

We can then estimate the integral by Eqs. (D.10) and (D.11), as well as Eq. (D.13),

$$\begin{aligned}\int_{\mathbb{R}} |f(t)|\,\mathrm{d}t &= \int_{-T_f^k}^{T_f^k} |f(t)|\,\mathrm{d}t + \mathcal{O}\left(A_q^2 S \int_{T_f^{k/s}}^{\infty} \exp\left(-\frac{s}{2(\beta A_u + A_w)^{1/s} e} u\right) \mathrm{d}u\right) \\ &= \mathcal{O}\left((A_q C_{1,u} + A_q^2 S A_w)\log T_f + A_q^2 S \underbrace{(\beta A_u + A_w)^{1/s} \exp\left(-\frac{s}{2(\beta A_u + A_w)^{1/s} e} T_f^{k/s}\right)}_{o(1) \text{ as } \beta A_u + A_w \to \infty}\right) \\ &= \mathcal{O}\left((A_q C_{1,u} + A_q^2 S A_w)\log(\beta A_u + A_w)\right),\end{aligned} \tag{D.14}$$

for any positive $k > 1$. This gives Eq. (D.3).

Estimate the integral of g. Similarly, by Eq. (D.6) with Assumption 15 and $|\tanh((\nu'-\nu)/4)| \le 1$, we have $\|g(t,t')\|_{L^\infty(\mathbb{R}^2)} \le \frac{1}{2\pi^2} A_q^4 S^2$. A direct computation gives, for a fixed $\nu' \in \mathbb{R}$,

$$\frac{\mathrm{d}}{\mathrm{d}\nu} \tanh((\nu'-\nu)/4) = \frac{1}{4}(\tanh^2((\nu'-\nu)/4) - 1) \in L^1(\mathbb{R}) \bigcap L^\infty(\mathbb{R})$$

with its L^1 and L^∞ norms independent of $\nu' \in \mathbb{R}$. This implies

$$\partial_{\nu'}\left(\tanh((\nu'-\nu)/4)\right) \partial_\nu \left(e^{-\nu/4} u(\nu)\right) \in L^1(\mathbb{R}^2)\,.$$

In addition, we have the second-order partial derivative:

$$\partial_{\nu'\nu} \tanh((\nu'-\nu)/4) = \frac{1}{8}\tanh((\nu'-\nu)/4)(1 - \tanh^2((\nu'-\nu)/4)) \in L^1(\mathbb{R}^2)\,,$$

which is L^1-integrable in ν (for fixed ν'). Then, we can estimate

$$\begin{aligned}\|t' t g(t,t')\|_{L^\infty(\mathbb{R}^2)} &= \mathcal{O}\left(\iint_{\mathbb{R}^2} |\partial_{\nu'\nu} \widehat{g}(\nu,\nu')|\,\mathrm{d}\nu\,\mathrm{d}\nu'\right) \\ &= \mathcal{O}\left(A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S\right).\end{aligned}$$

by a straightforward computation:

$$\begin{aligned}&\partial_{\nu'\nu}\left(\tanh(\beta(\nu'-\nu)/4) e^{-\beta(\nu+\nu')/4} u(\beta\nu) w(\nu) \overline{u(\beta\nu') w(\nu')}\right) \\ &= \underbrace{\partial_{\nu'\nu}\left(\tanh(\beta(\nu'-\nu)/4)\right) \overline{w(\nu')}}_{\|\cdot\|_{L^1} = \mathcal{O}(A_q S \beta)} \underbrace{e^{-\beta\nu/4} u(\beta\nu) w(\nu) \overline{u(\beta\nu') e^{-\beta\nu'/4}}}_{\|\cdot\|_{L^\infty} \le A_q^3} \\ &+ \underbrace{\partial_{\nu'}\left(\tanh(\beta(\nu'-\nu)/4)\right) \partial_\nu \left(e^{-\beta\nu/4} u(\beta\nu)\right)}_{\|\cdot\|_{L^1} = \mathcal{O}(C_{1,u})} \underbrace{w(\nu) \overline{u(\beta\nu') e^{-\beta\nu'/4} w(\nu')}}_{\|\cdot\|_{L^\infty} \le A_q^3} \\ &+ \underbrace{\partial_\nu\left(\tanh(\beta(\nu'-\nu)/4)\right) \partial_{\nu'}\left(\overline{u(\beta\nu') e^{-\beta\nu'/4}}\right)}_{\|\cdot\|_{L^1} = \mathcal{O}(C_{1,u})} \underbrace{e^{-\beta\nu/4} u(\beta\nu) w(\nu) \overline{w(\nu')}}_{\|\cdot\|_{L^\infty} \le A_q^3} \\ &+ \underbrace{\left(\tanh(\beta(\nu'-\nu)/4)\right)}_{\|\cdot\|_{L^\infty} = \mathcal{O}(1)} \underbrace{\partial_\nu\left(e^{-\beta\nu/4} u(\beta\nu)\right) \partial_{\nu'}\left(\overline{u(\beta\nu') e^{-\beta\nu'/4}}\right)}_{\|\cdot\|_{L^1} \le C_{1,u}^2} \underbrace{w(\nu)\overline{w(\nu')}}_{\|\cdot\|_{L^\infty} \le A_q^2} \\ &+ \underbrace{\partial_\nu\left(\tanh(\beta(\nu'-\nu)/4) e^{-\beta\nu/4} u(\beta\nu) \overline{u(\beta\nu') e^{-\beta\nu'/4}}\right) \partial_{\nu'}\left(\overline{w(\nu')}\right)}_{\|\cdot\|_{L^1} = \mathcal{O}(C_{1,u} A_q^2 A_\omega S + A_q^3 A_\omega S)} \underbrace{w(\nu)}_{\|\cdot\|_{L^\infty} \le A_q} \\ &+ \underbrace{\partial_{\nu'}\left(\tanh(\beta(\nu'-\nu)/4) \overline{u(\beta\nu') e^{-\beta\nu'/4}} u(\beta\nu) e^{-\beta\nu/4}\right) (\partial_\nu w(\nu))}_{\|\cdot\|_{L^1} = \mathcal{O}(C_{1,u} A_q^2 A_\omega S + A_q^3 A_\omega S)} \underbrace{\overline{w(\nu')}}_{\|\cdot\|_{L^\infty} \le A_q} \\ &+ \underbrace{\tanh(\beta(\nu'-\nu)/4) \overline{u(\beta\nu') e^{-\beta\nu'/4}} u(\beta\nu) e^{-\beta\nu/4}}_{\|\cdot\|_{L^\infty} \le A_q^2} \underbrace{(\partial_\nu w(\nu)) \partial_{\nu'}\left(\overline{w(\nu')}\right)}_{\|\cdot\|_{L^1} \le A_q^2 A_\omega^2 S^2}.\end{aligned}$$

In the same manner as Eq. (D.10), we have

$$\int_{-T}^{T}\int_{-T}^{T} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t' = \mathcal{O}(A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S)\log^2(T)\,,\quad T>1\,. \tag{D.15}$$

We now consider the truncation time as in (D.12):

$$T_g(A_u,A_w) := \inf\left\{T>0\,;\ u^{2s-1} \le \exp\left(\frac{s}{2(2\beta A_u + 2A_w + \beta)^{1/s} e} u\right) \text{ for any } u \ge T^{1/s}\right\}, \tag{D.16}$$

which satisfy, as $2\beta A_u + 2A_w + \beta \to \infty$,

$$T_g(A_u,A_w) = \Theta\left((2\beta A_u + 2A_w + \beta)\log\left(2\beta A_u + 2A_w + \beta\right)\right)\,.$$

It follows from Eqs. (D.2) and (D.15) and some similar estimates as in Eq. (D.14) that

$$\begin{aligned}\iint_{\mathbb{R}^2} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t' &= \int_{-T_g}^{T_g}\int_{-T_g}^{T_g} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t' + \mathcal{O}\left(A_q^4 S^2 \int_{T_g}^{\infty} \exp\left(-\frac{s}{(2\beta A_u + 2A_w + \beta)^{1/s} e} r^{1/s}\right) r\,\mathrm{d}r\right) \\ &= \int_{-T_g}^{T_g}\int_{-T_g}^{T_g} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t' + \mathcal{O}\left(A_q^4 S^2 \int_{T_g^{1/s}}^{\infty} \exp\left(-\frac{s}{(2\beta A_u + 2A_w + \beta)^{1/s} e} u\right) u^{2s-1}\,\mathrm{d}u\right) \\ &= \mathcal{O}\left((A_q^2 C_{1,u}^2 + A_q^4 S^2 A_w^2 + A_q^3 C_{1,u} S A_w + A_q^4 \beta S)\log^2(\beta A_u + A_w + \beta)\right)\,.\end{aligned}$$

The proof is complete. □

We next prove Proposition 16. We shall employ the Poisson summation formula recalled in the following lemma [Pin08, Theorem 4.4.2].

Lemma 31 (Poisson summation formula)**.** *Given any $h \in L^1(\mathbb{R}^d)$ with inverse Fourier transform:*

$$\widehat{h}(y) = \int_{\mathbb{R}^d} h(x) e^{ix\cdot y}\,\mathrm{d}x\,,$$

for any $y \in \mathbb{R}^d$ and $\tau > 0$, there holds

$$\sum_{\boldsymbol{n}\in\mathbb{Z}^d} \widehat{h}\left(y + \frac{2\pi \boldsymbol{n}}{\tau}\right) = \sum_{\boldsymbol{n}\in\mathbb{Z}^d} \tau^d h\left(\boldsymbol{n}\tau\right) e^{iy\cdot\boldsymbol{n}\tau}\,.$$

We are now ready to show Proposition 16.

Proof of Proposition 16. In the proof, we shall consider an infinite time grid defined by $\{m\tau\}_{m\in\mathbb{Z}}$. The grid $\{t_m\}_{m=0}^{2M-1}$ is given by the subset $\{m\tau\}_{m=-M}^{M-1}$ as in the statement of Proposition 16. We omit the upper index a in f^a and g^a.

Estimate for the jump L_a. Thanks to Lemma 30, there holds

$$\begin{aligned}&\left\|\sum_{m=-\infty}^{\infty} f(m\tau) A^a(m\tau)\tau - \sum_{m=0}^{2M-1} f(t_m) A^a(t_m)\tau\right\| \le \|A^a\| \sum_{|m|\ge M} |f(m\tau)|\tau \\ &\le \sum_{|m|\ge M} \frac{A_q^2 S}{\pi} \exp\left(\frac{es}{2} - \frac{s}{(\beta A_u + A_w)^{1/s} e}|m\tau|^{1/s}\right)\tau\,.\end{aligned} \tag{D.17}$$

By the monotonicity of the exponential function, we have

$$\begin{aligned}&\sum_{|m|\ge M} \exp\left(-\frac{s}{(\beta A_u + A_w)^{1/s} e}|m\tau|^{1/s}\right)\tau \\ \le& 2\int_{(M-1)\tau}^{\infty} \exp\left(-\frac{s}{(\beta A_u + A_w)^{1/s} e}|t|^{1/s}\right)\mathrm{d}t \\ \le& 2s\int_{((M-1)\tau)^{1/s}}^{\infty} u^{s-1}\exp\left(-\frac{s}{(\beta A_u + A_w)^{1/s} e} u\right)\mathrm{d}u\,.\end{aligned} \tag{D.18}$$

Let $T_f(A_u, A_w)$ be the constant defined as in Eq. (D.12). Then, when $(M-1)\tau \geq T_f(A_u, A_w)$, we can compute, by (D.18),

$$\begin{aligned}\sum_{|m|\geq M} \exp\left(-\frac{s}{(\beta A_u + A_w)^{1/s} e}\left|m\tau\right|^{1/s}\right)\tau &\leq 2s\int_{((M-1)\tau)^{1/s}}^{\infty} \exp\left(-\frac{s}{2(\beta A_u + A_w)^{1/s} e} u\right) \mathrm{d}u \\ &\leq 4s\frac{(\beta A_u + A_w)^{1/s} e}{s} \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s} e}\right).\end{aligned}$$

Combining this with Eq. (D.17), we find

$$\begin{aligned}&\left\|\sum_{m=-\infty}^{\infty} f(m\tau)A^a(m\tau)\tau - \sum_{m=0}^{2M-1} f(t_m)A^a(t_m)\tau\right\| \\ \leq &\sum_{|m|\geq M} \frac{A_q^2 S}{\pi} \exp\left(\frac{es}{2} - \frac{s}{(\beta A_u + A_w)^{1/s} e}\left|m\tau\right|^{1/s}\right)\tau \\ \leq &C_s A_q^2 S(\beta A_u + A_w)^{1/s} \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s} e}\right).\end{aligned} \tag{D.19}$$

Then, by the triangle inequality, we readily have

$$\begin{aligned}&\left\|L_a - \sum_{m=0}^{2M-1} f(t_m)A^a(t_m)\tau\right\| \\ \leq &\left\|\int_{-\infty}^{\infty} f(t)A^a(t)\,\mathrm{d}t - \sum_{m=-\infty}^{\infty} f(m\tau)A^a(m\tau)\tau\right\| + \left\|\sum_{m=-\infty}^{\infty} f(m\tau)A^a(m\tau)\tau - \sum_{m=0}^{2M-1} f(t_m)A^a(t_m)\tau\right\| \\ \leq &\left\|\int_{-\infty}^{\infty} f(t)A^a(t)\,\mathrm{d}t - \sum_{m=-\infty}^{\infty} f(m\tau)A^a(m\tau)\tau\right\| + C_f \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s} e}\right),\end{aligned} \tag{D.20}$$

with constant

$$C_f = \mathcal{O}\left(A_q^2 S(\beta A_u + A_w)^{1/s}\right).$$

Note from (3.4) that $\int_{-\infty}^{\infty} f(t)A^a(t)\,\mathrm{d}t = \sum_{i,j} \widehat{f}(\lambda_i - \lambda_j)P_i A^a P_j$, and from Assumption 15 that

$$|\lambda_i - \lambda_j| \leq 2\|H\| \text{ for any } \lambda_i, \lambda_j \in \mathrm{Spec}(H) \quad \text{and} \quad \mathrm{supp}(\widehat{f}) \subset [-S, S].$$

For $\tau < \frac{2\pi}{2\|H\|+S}$, by Poisson summation formula in Lemma 31, we have

$$\widehat{f}(\lambda_i - \lambda_j) = \sum_{m=-\infty}^{\infty} \widehat{f}\left(\lambda_i - \lambda_j + \frac{2\pi m}{\tau}\right) = \sum_{m=-\infty}^{\infty} f(m\tau)e^{i(\lambda_i - \lambda_j)m\tau}\tau.$$

Plugging the above formula into the first term of (D.20), there holds

$$\begin{aligned}&\int_{-\infty}^{\infty} f(t)A^a(t)\,\mathrm{d}t - \sum_{m=-\infty}^{\infty} f(m\tau)A^a(m\tau)\tau \\ = &\sum_{i,j}\left(\widehat{f}(\lambda_i - \lambda_j) - \sum_{m=-\infty}^{\infty} f(m\tau)e^{i(\lambda_i - \lambda_j)m\tau}\tau\right)P_i A^a P_j = 0,\end{aligned}$$

which then implies

$$\left\|L_a - \sum_{m=0}^{2M-1} f(t_m)A^a(t_m)\tau\right\| \leq C_f \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(\beta A_u + A_w)^{1/s} e}\right).$$

and concludes the proof of (3.15).

Estimate for the coherent term G. Again by Lemma 30 with similar estimates as in (D.19) for L_a, we obtain, when $(M-1)\tau > T_g(A_u, A_w)$,

$$\begin{aligned}
&\left\| \sum_{n,m=-\infty}^{\infty} g(n\tau, m\tau) A^a(n\tau) A^a(m\tau)\tau^2 - \sum_{n,m=0}^{2M-1} g(t_n, t_m) A^a(t_n) A^a(t_m)\tau^2 \right\| \\
\leq & \|A^a\|^2 \sum_{|n|,|m|\geq M} |g(n\tau, m\tau)|\,\tau^2 \leq C_g \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s} e}\right),
\end{aligned}$$

where the constant $T_g(A_u, A_w)$ is given in Eq. (D.16) and

$$C_g = \mathcal{O}\left(A_q^4 S^2 (2\beta A_u + 2A_w + \beta)^{1/s}\right).$$

It follows that

$$\begin{aligned}
&\left\| \iint_{\mathbb{R}^2} g(t,t') A^a(t) A^a(t')\, \mathrm{d}t\, \mathrm{d}t' - \sum_{n,m=0}^{2M-1} g(t_n, t_m) A^a(t_n) A^a(t_m)\tau^2 \right\| \\
\leq & \left\| \iint_{\mathbb{R}^2} g(t,t') A^a(t) A^a(t')\, \mathrm{d}t\, \mathrm{d}t' - \sum_{n,m=-\infty}^{\infty} g(n\tau, m\tau) A^a(n\tau) A^a(m\tau)\tau^2 \right\| \\
& + C_g \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s} e}\right).
\end{aligned} \tag{D.21}$$

Similarly, Poisson summation formula with $\mathrm{supp}(\widehat{g}) \subset [-S, S] \times [-S, S]$ gives

$$\widehat{g}(\nu, \nu') = \sum_{n,m=-\infty}^{\infty} \widehat{g}\left(\nu + \frac{2\pi n}{\tau}, \nu' + \frac{2\pi m}{\tau}\right) = \sum_{n,m=-\infty}^{\infty} g(n\tau, m\tau) e^{in\nu\tau} e^{-im\nu'\tau}\tau^2,$$

for $\tau < \frac{2\pi}{2\|H\|+S}$ and $(\nu, \nu') \in B_H \times B_H$, thanks to $|\nu|, |\nu'| \leq 2\|H\|$. It follows that the first term of (D.21) is zero. By definition (3.7) of G and above estimates, it holds that

$$\begin{aligned}
&\left\| G - \sum_{a\in\mathcal{A}} \sum_{n,m=0}^{2M-1} g(t_n, t_m) A^a(t_n) A^a(t_m)\tau^2 \right\| \\
\leq & \sum_{a\in\mathcal{A}} \left\| \iint_{\mathbb{R}^2} g(t,t') A^a(t) A^a(t')\, \mathrm{d}t\, \mathrm{d}t' - \sum_{n,m=0}^{2M-1} g(t_n, t_m) A^a(t_n) A^a(t_m)\tau^2 \right\| \\
\leq & C_g |\mathcal{A}| \exp\left(-\frac{s((M-1)\tau)^{1/s}}{2(2\beta A_u + 2A_w + \beta)^{1/s} e}\right).
\end{aligned}$$

The proof is complete. □

Finally, the simulation of the algorithm requires the preparation of oracles (3.26)-(3.30), where the normalization factors Z_f and Z_g affect the algorithm complexity. In the following theorem, we demonstrate that the discretization normalization constant can be bounded by the L^1 norm of f and g when the discretization step τ is sufficiently small.

Lemma 32. *Under Assumption 15, for any given $T > 0$, there exists small $\tau = \Theta\left(1/A_q^4 T^2 S^3\right)$ such that for any integer M with $M\tau \leq T$,*

$$\sum_{m=-M}^{M} |f(m\tau)|\,\tau \leq \|f\|_{L^1(\mathbb{R})} + 1, \tag{D.22}$$

and

$$\sum_{m=-M}^{M} \sum_{m'=-M}^{M} |g(m\tau, m'\tau)|\,\tau^2 \leq \|g\|_{L^1(\mathbb{R}^2)} + 1. \tag{D.23}$$

Proof. We note

$$|f'(t)| = \left|\frac{1}{2\pi}\int_{\mathbb{R}} u(\beta\nu)w(\nu)e^{-\beta\nu/4}\nu e^{-it\nu}\,\mathrm{d}\nu\right| \leq \frac{A_q}{2\pi}\int_{\mathbb{R}} |\nu w(\nu)|\,\mathrm{d}\nu = \mathcal{O}(A_q^2 S^2)\,.$$

Similarly, one can obtain

$$|\partial_t g(t,t')| = \mathcal{O}(A_q^4 S^3)\,, \quad |\partial_{t'} g(t,t')| = \mathcal{O}(A_q^4 S^3)\,.$$

Then, it follows from the mean-value theorem that

$$\left|\sum_{m=-M}^{M} |f(m\tau)|\,\tau - \int_{-M\tau}^{(M+1)\tau} |f(t)|\,\mathrm{d}t\right| = \mathcal{O}\left(A_q^2 S^2 M\tau^2\right)\,,$$

which implies

$$\sum_{m=-M}^{M} |f(m\tau)|\,\tau \leq \|f\|_{L^1(\mathbb{R})} + \mathcal{O}\left(A_q^2 S^2 M\tau^2\right)\,.$$

Then Eq. (D.22) follows. For the estimate of g, similarly, by the mean-value theorem, we find

$$\left|\sum_{m=-M}^{M}\sum_{m'=-M}^{M} |g(m\tau,m'\tau)|\,\tau^2 - \int_{-M\tau}^{(M+1)\tau}\int_{-M\tau}^{(M+1)\tau} |g(t,t')|\,\mathrm{d}t\,\mathrm{d}t'\right| = \mathcal{O}\left(A_q^4 S^3 M^2\tau^3\right)\,,$$

which means

$$\sum_{m=-M}^{M}\sum_{m'=-M}^{M} |g(m\tau,m'\tau)|\,\tau^2 \leq \|g\|_{L^1(\mathbb{R}^2)} + \mathcal{O}\left(A_q^4 S^3 M^2\tau^3\right)\,.$$

This concludes the proof of Eq. (D.23). □

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