Error reduction in quantum annealing using boundary cancellation: Only the end matters

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Error Reduction in Quantum Annealing using Boundary Cancellation: Only the End Matters

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The adiabatic theorem of quantum mechanics states that the error between an instantaneous eigenstate of a time-dependent Hamiltonian and the state given by quantum evolution of duration τ is upper bounded by C/τ for some positive constant C. It has been known for decades that this error can be reduced to C_k/τ^{k+1} if the Hamiltonian has vanishing derivatives up to order k at the beginning and end of the evolution. Here we extend this result to open systems described by a time-dependent Liouvillian superoperator. We find that the same results holds provided the Liouvillian has vanishing derivatives up to order k only at the end of the evolution. This asymmetry is ascribable to the arrow of time inherent in open system evolution. We further investigate whether it is possible to satisfy the required assumptions by controlling only the system, as required for realistic implementations. Surprisingly, we find the answer to be affirmative. We establish this rigorously in the setting of the Davies-Lindblad adiabatic master equation, and numerically in the setting of two different time-dependent Redfield-type master equations we derive. The results are shown to be stable with respect to imperfections in the preparation. Finally, we prove that the results hold also in a fully Hamiltonian model.

I. INTRODUCTION

Quantum annealing and adiabatic quantum computation are promising candidates in the search for quantum-enhanced information processing [1, 2]. Both can be viewed as adiabatic state preparation protocols [3], where the target state is typically the solution to a computational problem such as optimization, or a state from a distribution that one wishes to sample from. In the simplest scenario one simply interpolates linearly from a Hamiltonian with an easily prepared ground state to a target Hamiltonian whose ground state encodes the solution to a given computational problem [4, 5]. In this closed-system, ideal, zero-temperature case the time needed to reach an accuracy ϵ scales inversely proportional to ϵ and to some power of the inverse minimum gap [6]. A similar result holds also for preparing thermal equilibrium (Gibbs) states in a realistic, open-system setting, in that the time needed to reach an accuracy ϵ from the Gibbs state is still inversely proportional to ϵ [7]. The dependence on the problem size is, however, more complicated in the open system setting (where the dynamics is generated by a Liouvillian rather than a Hamiltonian), primarily because in this case not only the Hamiltonian gap but also the Liouvillian gap plays a role [7, 8]. Moreover, in the open-system setting one does not expect a speedup with respect to classical preparation algorithms if the temperature is sufficiently high. Arguments to substantiate this statement on general grounds were given in [8], and it can be rigorously proven in certain specific cases [9].

Given this state of affairs and the intense efforts to realize adiabatic quantum state preparation experimentally with an eye towards quantum speedups [10], it is critical to find general protocols for preparing quantum states using the adiabatic approach that offer provable advantages over naive protocols such as linear interpolation. It is well known that protocols that slow down near the quantum critical point are beneficial [11] and sometimes even necessary for achieving a quan-

tum speedup [12]. In the closed system setting there exists another general method that allows for a reduction of the adiabatic error (the distance between the desired state and the state that has been actually prepared) from $\propto 1/\tau$ where τ is the total evolution time (annealing, or preparation time) to $\propto 1/\tau^{k+1}$ where the exponent $q \geq 1$ can be made arbitrarily large [13]. In fact, it is even possible to achieve an adiabatic error exponentially small in τ which in turns means an annealing time logarithmic in $1/\epsilon$ [14–19]. This method simply requires the time-dependent Hamiltonian to have vanishing derivatives up to order k at the initial and final time. In other words, the schedule should be sufficiently flat at the beginning and at the end of the anneal.

Here we generalize the boundary cancellation method to the open system case, where the dynamics are generated by a time-dependent Liouvillian $\mathcal{L}_\tau(t)$. We find that, in contrast to the familiar closed-system result, an asymmetry with respect to the Hamiltonian case appears, in that the same result holds provided the *Liouvillian* has vanishing derivatives only at the *end* of the evolution. The origin of this asymmetry traces back to the time-asymmetry of non-unitary evolution, which admits an arrow of time. We then consider whether it is possible to satisfy the required condition on the Liouvillian by controlling *only the system* (and not the bath degrees of freedom), as would be required, e.g., for applications using experimental quantum annealers. To this end we first consider the time-dependent Davies-Lindblad type adiabatic master equation [20, 21] and, encouragingly, find the answer to be positive, in that it suffices to enforce that the system Hamiltonian alone has vanishing derivatives in order for the adiabatic error to be upper bounded by C_k/τ^{k+1}. This result requires complete positivity, a condition that is automatically satisfied in this case. To check the robustness of this result to different levels of approximations we also derive time-dependent adiabatic as well as non-adiabatic Redfield-type master equations. These master equations have not appeared previously, to the

best of our knowledge, and should be of independent interest. In the Redfield case the lack of a complete positivity guarantee prevents us from satisfying the assumptions required for our previous result to hold. However, our numerical simulations confirm that, in a parameter regime for which positivity is satisfied, enforcing vanishing derivatives of the system Hamiltonian alone results in a greatly diminished adiabatic error.

The important question that remains to be answered concerns the scaling of the adiabatic error with other parameters such as the number of qubits N or the temperature. The scaling with N is not yet fully understood in the closed system case, and the situation for open systems with or without boundary cancellation is even more complicated. We show that within the range of parameters tested in our numerical simulations, boundary cancellation provides an advantage for all annealing times, with an advantage that is more pronounced in the large τ region.

In Section II we formulate boundary cancellation in terms of condition on the derivatives of the Liouvillian at the end of the evolution. To do so we first give the general setting for the theory in terms of trace and hermitian preserving superoperators and describe a useful adiabatic expansion in powers of the evolution time τ. We also provide a stability and time-scale analysis. In Section III we apply the general theory in the setting of various master equations derived from first-principles, and show both analytically and numerically that—remarkably—boundary cancellation works by controlling only the system Hamiltonian. We conclude in Section IV, and provide additional technical details in the Appendix.

II. BOUNDARY CANCELLATION IN OPEN SYSTEMS

A. Setup

For simplicity we consider a system with a finite-dimensional dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^n$ and let $L(\mathcal{H})$ be the algebra of linear operators over it. We fix the norm on $L(\mathcal{H})$ to be the trace norm: $\|X\|_1 := \mathrm{Tr}\sqrt{X^\dagger X}$ for $X \in L(\mathcal{H})$. Let a time-dependent Liouvillean superoperator $\mathcal{L}_\tau(t)$ acting on $L(\mathcal{H})$ be given. The evolution of the system (characterized by the quantum state $\rho_\tau(t)$ at time t) is described by a time-dependent linear differential equation

$$\frac{\partial \rho_\tau(t)}{\partial t} = \mathcal{L}_\tau(t)\rho_\tau(t). \tag{1}$$

In some cases $\mathcal{L}_\tau(t)$ depends on t only through the rescaled time variable $s = t/\tau$ and we define $\mathcal{L}(s) := \mathcal{L}_\tau(t)$. The time-scale τ is the total evolution ("anneal") time. Note that $\mathcal{L}(s)$ depends on τ if $\mathcal{L}_\tau$ is not simply a function of t/τ. Switching to the variable s and defining $\rho(s) := \rho_\tau(t)$ allows us to rewrite Eq. (1) in the form

$$\dot{\rho}(s) = \tau \mathcal{L}(s)\rho(s), \tag{2}$$

where henceforth the dot denotes differentiation with respect to s. Evolution up to time τ thus becomes evolution up to

$s = 1$. For convenience we also define $\zeta = 1/\tau$. Below we use both the time t and rescaled time s, whichever is more convenient. We use $\mathcal{L}(s)$ to denote a linear, trace preserving and hermitian preserving (TPHP) superoperator for all $s \geq 0$. Occasionally we will assume more, namely that $\mathcal{L}(s)$ generates a contraction semigroup with respect to the induced norm $\|\mathcal{T}\|_{1,1} := \sup_{x \neq 0} \|\mathcal{T}(x)\|_1 / \|x\|_1$, meaning that $\left\|e^{t\mathcal{L}(s)}\right\|_{1,1} \leq 1$ for all $s, t \geq 0$. This includes generators that are in Lindblad form for all $s \geq 0$.

The propagator or evolution operator is the solution of the following differential equation:

$$\partial_s \mathcal{E}(s, s') = \tau \mathcal{L}(s)\mathcal{E}(s, s'), \quad \mathcal{E}(s, s) = \mathbb{1}. \tag{3}$$

The adiabatic approximation or expansion refers to the solution of Eq. (2) when $\tau \to \infty$. When a gap condition is satisfied the adiabatic expansion is an expansion in powers of τ^{-1}. By gap condition we mean that the eigenvalue being followed is separated from the rest of the spectrum by a finite gap uniformly for all s in the evolution window $[0, 1]$. In finite dimensions this is the only possibility if one excludes level crossings.

Let $P(s)$ be the eigenprojector of $\mathcal{L}(s)$ with eigenvalue 0. A 0 eigenvalue always exist whenever $\mathcal{L}(s)$ is trace-preserving. Moreover if $\mathcal{L}(s)$ generates a contraction semi-group, the eigenvalue 0 does not have a nilpotent term (these and various other useful facts about Eq. (2) are collected in [7]). Let us also denote by $Q(s) = \mathbb{1} - P(s)$ the complementary projection. For simplicity we assume the system to be finite-dimensional although all the results still hold in the infinite-dimensional case, possibly after introducing some extra assumptions.[1]

B. Adiabatic expansion

We first provide an adiabatic expansion for the case of a non-degenerate steady state – the corresponding generators are generally called *ergodic*. This is essentially Theorem 6 of Avron *et al.* [22] with some additional simplifying assumptions.

Proposition 1. *Assume that $\mathcal{L}(s)$ in Eq. (2) is C^{k+2} ($k+2$ times differentiable), TPHP for each fixed $s \geq 0$, satisfies the gap condition and has a unique steady state. We denote by $\sigma(s)$ the unique steady state of $\mathcal{L}(s)$, i.e., $\mathcal{L}(s)\sigma(s) = 0$, $\mathrm{Tr}[\sigma(s)] = 1$. Let $\rho(s)$ denote the solution of Eq. (2) with the*

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[1] Essentially, in the infinite-dimensional case, one needs extra assumptions to ensure that $L(\mathcal{H}) = \mathrm{Ker}(\mathcal{L}) \oplus \mathrm{Ran}(\mathcal{L})$ or $L(\mathcal{H}) = \mathrm{Ker}(\mathcal{L}) \oplus \overline{\mathrm{Ran}(\mathcal{L})}$, where now $L(\mathcal{H})$ indicates a Banach algebra. This condition does not follow from the fact that $\mathcal{L}$ generates a contraction and must be assumed separately; see [22].

initial condition $\rho(0) = \sigma(0)$. Then

$$\rho(s) = \sigma(s) + \sum_{n=1}^{k} \zeta^n b_n(s) + \zeta^{k+1} r_k(\zeta, s) \quad (4a)$$

$$b_1(s) = S(s)\dot{P}(s)\sigma(s) = S(s)\dot{\sigma}(s) \quad (4b)$$

$$b_{n+1}(s) = S(s)\dot{b}_n(s), \quad n = 1, 2, \dots \quad (4c)$$

where $S(s)$ is the reduced resolvent, i.e.,

$$S(s) = \lim_{z \to 0} Q(s) \left(\mathcal{L}(s) - z \right)^{-1} Q(s), \quad (5)$$

and the remainder is

$$r_k(\zeta, s) = b_{k+1}(s) - \mathcal{E}(s, 0)b_{k+1}(0) - \int_0^s \mathcal{E}(s, s')\dot{b}_{k+1}(s')ds'. \quad (6)$$

The proof is provided in Appendix A.

Note that the Liouvillian has dimension of 1/time. We could rescale $\mathcal{L}(s) = \frac{1}{\tau_0}\tilde{\mathcal{L}}(s)$ where $\tilde{\mathcal{L}}(s)$ is now dimensionless and τ_0 is the natural time-scale of the process. The exact value of τ_0 is to some extent arbitrary (it can be fixed by fixing the norm of $\tilde{\mathcal{L}}(s)$ at some s). More concretely, in quantum information processing experiments, $\mathcal{L}(s)$ is typically a perturbation of some Hamiltonian evolution, and so it is reasonable to take $\tau_0 = 1/J$ where J is the energy scale of the Hamiltonian (we use units in which $\hbar = 1$). After this rescaling all the formulas remain unchanged and $\tau \mapsto \tau/\tau_0$. We see then that in Eq. (4a) the expansion parameter is effectively the appropriately dimensionless quantity $\zeta = \tau_0/\tau$, while all the other quantities are also dimensionless. This expansion parameter is small when $\tau \gg \tau_0$ where τ is the timescale on which we change the Liouvillian.

The following is a strengthening of a similar result contained in [22], and introduces the assumption of vanishing boundary derivatives.

Proposition 2. *Under the same assumptions as in Proposition 1, with the additional assumptions that $\mathcal{L}(s)$ is independent of τ, generates a contraction semigroup, i.e., $\left\| e^{r\mathcal{L}(s)} \right\|_1 \leq 1$ for each $r, s \geq 0$, and that $\mathcal{L}^{(j)}(1) = 0$ for $j = 1, 2, \dots, k$ (vanishing derivatives at the final time):*

$$\|\rho(1) - \sigma(1)\|_1 \leq \frac{C_k}{\tau^{k+1}}, \quad (7)$$

where C_k is a constant independent of τ.

Proof. We first note that if $\mathcal{L}^{(j)}(s_0) = 0$ for $j = 1, 2, \dots, k$ then, $\partial_s^{(j)}[(\mathcal{L}(s) - z)^{-1}]_{s=s_0} = 0$. This follows from

$$\frac{\partial}{\partial s}\frac{1}{\mathcal{L} - z} = -\frac{1}{\mathcal{L} - z}\dot{\mathcal{L}}\frac{1}{\mathcal{L} - z} \quad (8)$$

and iterating. Since the projector can be written as

$$P(s) = \frac{1}{2\pi i}\oint_\gamma \frac{dz}{z - \mathcal{L}(s)} \quad (9)$$

where γ is a path that encircles only the zero eigenvalue in anti-clockwise direction, it follows that also $P^{(j)}(s_0) = 0$ for

$j = 1, 2, \dots, k$. Moreover, it also follows immediately that $Q^{(j)}(s_0) = S^{(j)}(s_0) = 0$ and $\sigma^{(j)}(s_0) = P^{(j)}(s_0)\sigma(s_0)$ for $j = 1, 2, \dots, k$. We now use the assumptions and Proposition 1. From Eqs. (4b) and (4c) we see that $b_n(1)$ is a sum of products of terms which contain P and S and their derivatives up to order n at $s = 1$. All of these derivatives vanish up to order k, and so $b_n(1) = 0 \; \forall n \leq k$. Hence

$$\rho(1) = \sigma(1) + \zeta^{k+1} r_k(\zeta, 1). \quad (10)$$

At this point we need to bound the error $r_k(\zeta, 1)$. Since by assumption $\mathcal{L}(s)$ generates a contraction, it follows that $\mathcal{E}(s_1, s_0)$ is a contraction for $s_1 \geq s_0$ (simply use the Trotter formula to write the propagator as a limit of products), and we can bound the final remainder as:

$$\|r_k(\zeta, 1)\|_1 \leq \|b_{k+1}(s)\|_1 + \|\mathcal{E}(s, 0)b_{k+1}(0)\|_1$$
$$+ \int_0^s \left\| \mathcal{E}(s, s')\dot{b}_{k+1}(s') \right\|_1 ds' \quad (11a)$$
$$\leq \Big(\|b_{k+1}(1)\|_1 + \|b_{k+1}(0)\|_1$$
$$+ \sup_{s \in [0,1]} \left\| \dot{b}_{k+1}(s) \right\|_1 \Big) =: C_k. \quad (11b)$$

The quantity in Eq. (11b) does not depend on τ and is bounded because $S(s)$, $P(s)$ and their derivatives are bounded by the assumption that $\mathcal{L}(s)$ is smooth. $\qquad \square$

As noted above, there is an asymmetry between the boundary cancellation result for dissipative generators (that can admit a one-dimensional kernel) and the corresponding result for unitary evolutions. In the latter case, in order to have the analogue of Eq. (7) one needs the derivatives of the generators to be zero *both at the end and at the beginning* of the evolution (see [13]) up to order k. The technical reason is that $P(s)$ must be rank 1 (ergodicity) and that the kernel of $P(s)$ must be independent of s. The latter condition follows from trace preservation, i.e., conservation of probabilities, of the evolution map $\mathcal{E}$. However the rank 1 condition cannot be satisfied by unitary dynamics. In other words, the difference between Proposition 2 and the corresponding result for the unitary case is due to the fact that in the former we are dealing with irreversible dynamics, i.e., there is an arrow of time.

Two caveats should also be noted. First, while C_k does not depend on τ, it does contain an implicit dependence on the system size, and in general will grow with the latter, necessitating a corresponding growth of τ in order to keep the adiabatic error small. Second, since in physical models, the generator $\mathcal{L}$ also depends on the bath, it may seem impossible to fulfill the condition $\mathcal{L}^{(j)}(1) = 0$ for $j = 1, 2, \dots, k$ by controlling only the system. As we show later, this pessimistic view fortunately turns out to be wrong.

Proposition 2 guarantees that as long as $\tau \gg \tau_0$ the adiabatic error can be made arbitrarily small. More precisely (switching to the rescaled generator), taking

$$\tau \geq \tau_0 \left(\frac{\tilde{C}_k}{\epsilon} \right)^{\frac{1}{k+1}}, \quad (12)$$

where $\tilde{C}_k$ refers now to the dimensionless generator $\tilde{\mathcal{L}}(s)$, implies

$$\|\rho(1) - \sigma(1)\|_1 \leq \epsilon. \tag{13}$$

If the constants $\tilde{C}_k$ were independent of k, this would imply a $(k+1)$-root speedup with respect to the case $k = 0$. This hypothesis is likely overly optimistic: in the next subsection, using fairly crude bounds, we derive estimates for $\tilde{C}_k$ which predict a strong dependence on k. On the other hand, our numerical results in Sec. III are encouraging especially for large τ and show that asymptotically $\|\rho(1) - \sigma(1)\|_1 \sim \tau^{-(k+1)}$ (see Fig. 2).

C. Stability and time-scales

We next consider the practical feasibility of the boundary cancellation approach by asking what happens if we try to set a derivative to zero but only achieve a small norm? We focus on the case where one tries to set the first derivative of the generator to zero. We use Eq. (4a) with $k = 0$ and $k = 1$ and bound the difference $\rho(1) - \sigma(1)$. In Appendix B we show that then:

$$\|\rho(1) - \sigma(1)\|_1 \leq \min\left\{\frac{B_0}{\tau}, \frac{A_1}{\tau} + \frac{B_1}{\tau^2}\right\}, \tag{14}$$

where the constants are given by (all the superoperator norms are induced, 1-1 norms)

$$B_0 = \left(\|S\|^2 \left\|\dot{\mathcal{L}}\right\|\right)\Big|_0^1 + \sup_{s\in[0,1]}\left(6\|S\|^3\left\|\dot{\mathcal{L}}\right\|^2 + \|S\|^2\left\|\ddot{\mathcal{L}}\right\|\right) \tag{15a}$$

$$A_1 = \|S(1)\|^2\left\|\dot{\mathcal{L}}(1)\right\| < B_0 \tag{15b}$$

$$B_1 = \left(5\|S\|^4\left\|\dot{\mathcal{L}}\right\|^2 + \|S\|^3\left\|\ddot{\mathcal{L}}\right\|\right)\Big|_0^1 + \tag{15c}$$

$$\sup_{s\in[0,1]}\left(60\|S\|^5\left\|\dot{\mathcal{L}}\right\|^3 + 19\|S\|^4\left\|\dot{\mathcal{L}}\right\|\left\|\ddot{\mathcal{L}}\right\| + \|S\|^3\|\dddot{\mathcal{L}}\|\right)$$

and we used the notation $(X)\big|_0^1 = X(0) + X(1)$. Note that since $A_1 < B_0$ the minimum in Eq. (14) is achieved by the second (first) term in the region where τ is large (small). If boundary cancellation were enforced exactly we would have $A_1 = 0$ and B_k would be estimates of the constants C_k, for $k = 0, 1$, appearing in Proposition 2. It is apparent from Eq. (15) that B_k depends on k.

We now imagine changing the schedule in order to try to enforce boundary cancellation but we only achieve it imperfectly. We obtain a new generator $\mathcal{L}'(s)$ with derivatives of reduced norm for s close to the end (but not strictly zero) and hence obtain new constants $A_1' < A_1, B_0', B_1'$. In principle the modified schedule can unpredictably change B_0 and B_1. However, we have the following monotonicity result:

Proposition 3. *Assume that $\mathcal{L}(s), \mathcal{L}'(s) \in C^3([0,1])$ and we change the schedule only close to the end of the anneal, i.e.,*
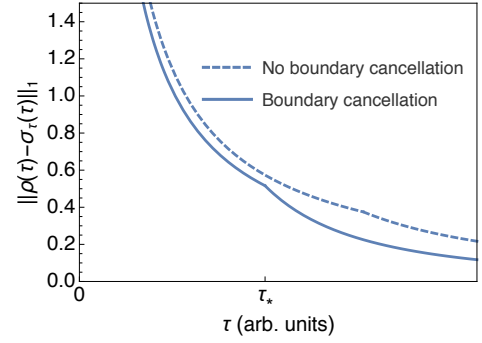

Figure 1. Schematic plot of the adiabatic error before and after imperfect boundary cancellation at first order. The dashed line shows Eq. (14) for random values of A_1, B_0, B_1, while for the solid line these values are (slightly) diminished in accordance with the conditions of Proposition 3. There is an improvement for all values of τ, although a larger improvement is predicted for $\tau > \tau_* = B_1'/(B_0' - A_1')$.

$\mathcal{L}'(s) = \mathcal{L}(s)$ *for* $s \in [0, 1-\delta]$, *and that* $\|\mathcal{L}'^{(j)}(s)\| < \|\mathcal{L}^{(j)}(s)\|$ *for s in a neighborhood of $s = 1$ independent of δ, for $j = 1, 2, 3$. Then for sufficiently small δ, boundary cancellation provides an improvement for all values of the anneal time τ.*

Proof. By assumption $A_1' < A_1$. Consider B_0 given by Eq. (15a). We have $\|S'\|^2\|\dot{\mathcal{L}}'\|(0) = \|S\|^2\|\dot{\mathcal{L}}\|(0)$, while $\|S'\|^2\|\dot{\mathcal{L}}'\|(1) < \|S\|^2\|\dot{\mathcal{L}}\|(1)$. Now, consider the supremum term in Eq. (15a), which we write as $Y = \sup_{s\in[0,1]} X(s) = X(s_0)$; after changing the schedule we obtain $Y' = \sup_{s'\in[0,1]} X'(s') = X'(s_0')$. If $Y' \leq Y$ this schedule is good enough and we keep it. Conversely, assume that $X'(s_0') > X(s_0)$. By hypothesis $X'(s) = X(s)$ for $s \in [0, 1-\delta]$. We can now take δ small enough such that $[1-\delta, 1]$ is entirely in the region where $\|\mathcal{L}'^{(j)}(s)\| < \|\mathcal{L}^{(j)}(s)\|$ (for $j = 1, 2$). At this point we must have necessarily $X'(s_0') \leq X(s_0)$. Hence $B_0' < B_0$ by Eq. (15a). An entirely analogous argument holds for B_1, and so there exist a δ small enough such that $A_1' < A_1, B_0' < B_0$, and $B_1' < B_1$. This implies that the adiabatic error, as predicted by Eq. (14), is smaller after boundary cancellation is employed. $\square$

See Fig. 1 for a plot of the improvement predicted by boundary cancellation under these circumstances. Note that our discussion is framed in terms of upper bounds, and it is possible that a larger benefit exists in a larger region than $\tau > B_1'/(B_0' - A_1')$.

Estimating the scaling of the terms in Eq. (15) as a function of relevant parameters such as size and temperature, is of great importance for applications, e.g., the preparation of ground states or thermal Gibbs states in quantum annealing, where we are interested in the behavior of the adiabatic error $\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1$ with respect to the system size N (number of qubits). One is then led to estimate the norm of the (reduced) resolvent. In contrast to the closed-system case the

norm of S cannot be simply evaluated, i.e.:

$$\|S(s)\|_{1,1} \neq \frac{1}{\text{dist}(0, \sigma(\mathcal{L}(s)))} \tag{16}$$

where $\sigma(\mathcal{L}(s))$ is the spectrum of $\mathcal{L}(s)$. This fact makes the estimates complicated. For $k = 0$ in the low temperature regime, such estimates were given in [7, 8]. The result is that $\|S(s)\|_{1,1}$ depends not only on the Liouvillian gap but also on the Hamiltonian one.

III. APPLICATION OF BOUNDARY CANCELLATION WHILE CONTROLLING ONLY THE SYSTEM HAMILTONIAN

Our goal is to apply the boundary cancellation method under realistic conditions using master equations for time-dependent system-Hamiltonians. I.e., given a total Hamiltonian $H_{\text{tot}}(t) = H_S(t) + H_I + H_B$, the sum of system, interaction, and bath Hamiltonians respectively, we wish to consider master equations in the form of Eq. (1) with $\mathcal{L}_\tau(t)$ derived from first principles, while directly controlling the boundary terms of only the system Hamiltonian. We will consider three such master equations. Henceforth we write the interaction Hamiltonian explicitly in the general form $H_I = g \sum_\alpha A_\alpha \otimes B_\alpha$.

A. Master equations

The first master equation is the Davies-Lindblad adiabatic master equation (DLAME) derived in [20]. Its generator is given by

$$\mathcal{L}_\tau(t) = -i[H_S(t) + H_{LS}(t), \bullet] + \mathcal{L}_\tau^D(t) \tag{17a}$$

$$\mathcal{L}_\tau^D(t) = \sum_{\alpha,\beta,\omega_n} \gamma_{\alpha,\beta}(\omega_n)\Big(A_\beta(\omega_n) \bullet A_\alpha^\dagger(\omega_n)$$
$$- \frac{1}{2}\big\{A_\alpha^\dagger(\omega_n)A_\beta(\omega_n), \bullet\big\}\Big). \tag{17b}$$

Here $H_{LS}(s)$ is the Lamb-shift term, $\gamma_{\alpha,\beta}(\omega)$ is the Fourier transform of the bath-correlation function

$$G_{\alpha,\beta}(t,s) := g^2\langle B_\alpha(t)B_\beta(s)\rangle = G_{\alpha,\beta}(t-s), \tag{18}$$

and $\omega_n(s)$ are the Bohr frequencies of $H_S(s)$ (to simplify notation we suppress their explicit time-dependence when convenient). The Lindblad jump operators $A_\alpha(\omega_n)$ that appear in the Davies generator $\mathcal{L}^D$ are given by

$$e^{itH(s)}A_\alpha e^{-itH(s)} = \sum_{\omega_n} e^{-it\omega_n}A_\alpha(\omega_n), \tag{19}$$

and

$$H_{LS} = \sum_{\alpha,\beta,\omega_n} S_{\alpha,\beta}(\omega_n)A_\alpha^\dagger(\omega_n)A_\beta(\omega_n), \tag{20}$$

with

$$S_{\alpha,\beta}(\omega) = \int_{-\infty}^{\infty} d\omega'\gamma_{\alpha\beta}(\omega')\mathcal{P}\left(\frac{1}{\omega - \omega'}\right), \tag{21}$$

where $\mathcal{P}$ is the Cauchy principal value. This master equation preserves complete positivity and assumes that the system evolves adiabatically.

The second master equation is the the Schrödinger picture Redfield master equation (SPRME), which we write as:

$$\frac{\partial\rho(t)}{\partial t} = -i[H_S(t), \rho(t)]$$
$$+ \sum_{\alpha,\beta} \int_0^t dr G_{\alpha,\beta}(r)[U_0(t,t-r)A_\beta U_0(t-r,t)\rho(t), A_\alpha]$$
$$+ \text{h.c.}, \tag{22}$$

where the unperturbed propagator is generated purely by the system Hamiltonian, i.e., is the solution of $\partial_t U_0(t,0) = -iH_S(t)U_0(t,0)$ with the boundary condition $U_0(0,0) = \mathbb{1}$. The SPRME is a generalization of the standard Redfield master equation, which is typically written in the interaction picture for time-independent system Hamiltonians [23].

The third master equation is obtained after performing an adiabatic-type approximation on Eq. (22), so we call it the adiabatic Redfield master equation (ARME):

$$\frac{\partial\rho(t)}{\partial t} = -i[H_S(t), \rho(t)] \tag{23}$$
$$+ \sum_{\alpha,\beta} \int_0^\infty dr G_{\alpha,\beta}(r)[A_\beta(-r,t)\rho(t), A_\alpha] + \text{h.c.}$$

where

$$A_\beta(-r,t) = e^{-irH_S(t)}A_\beta e^{irH_S(t)}. \tag{24}$$

We derive the SPRME and the ARME in Appendix C, where we also estimate the error of the approximations involved. As far as we know these forms of the Redfield equation have not appeared previously. To derive the SPRME one needs only the Born and Markov approximations. For the case of a "fast bath" (bath-correlation function exponentially decaying with time-constant τ_B) the Markov approximation introduces a relative error $O((\tau_B g)^2)$ and so requires a fast bath and/or small coupling. To derive the ARME one introduces an additional error $O((\tau_B/\tau)^2)$ which additionally requires a slow system Hamiltonian. It turns out that for an algebraically decaying bath correlation function, $|G_{\alpha,\beta}(t)| \sim t^{-\theta}$ ($\theta > 0$), the SPRME tolerates a slower bath. Indeed, in order to have a bounded error for the ARME one needs $\theta > 3$ while for the SPRME $\theta > 2$ suffices. Moreover, for the case $\theta = 2$, which includes the Ohmic bath case, the SPRME introduces a (tolerable) relative error growing as $\ln(\tau)$, while for the same bath the ARME introduces an error $\propto \tau$. More details are given in Appendix C. We note that the Davies generator is obtained from the ARME after the rotating wave (secular) approximation, i.e., the Redfield case requires one fewer approximations. However, while Redfield theory is TPHP, unlike the Davies-Lindblad case it is notoriously not completely positive (though various fixes have been proposed [24, 25]).

B. Application of boundary cancellation

We now investigate whether it is possible to satisfy the assumptions of Proposition 2 under realistic conditions.

1. The Davies-Lindblad adiabatic master equation

We begin by considering the DLAME, Eq. (17). We assume henceforth that the system Hamiltonian is a function of t/τ and not separately of t and τ. Note that for the time-dependent Davies generator this implies that the rescaled generator $\mathcal{L}(s)$ resulting from $\mathcal{L}_\tau(t)$ is τ-independent.

Proposition 4. *Assume a master equation with generator in time dependent Davies form $\mathcal{L}_\tau(t)$ given by Eq. (17). Moreover assume that the system Hamiltonian $H_S(t)$ is smooth and that the degeneracy of all the levels does not change for $t \in [0,\tau]$. If $\partial_t^{(j)}[H_S(t)]_{t=\tau} = 0$ for $j = 1,2,\ldots,k$ then $\partial_t^{(j)}[\mathcal{L}_\tau(t)]_{t=\tau} = 0$ for $j = 1,2,\ldots,k$. Furthermore, if the steady state of $\mathcal{L}_\tau(t)$ is unique for $t \in [0,\tau]$ then the assumptions of Proposition 2 all hold, so that*

$$\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1 \leq \frac{C_k}{\tau^{k+1}}. \quad (25)$$

Proof. The degeneracy assumption is needed since otherwise $\mathcal{L}_\tau(t)$ is not even continuous. Let $H_S(t) = \sum_n E_n(t)\Pi_n(t)$, where $E_n(t)$ and $\Pi_n(t)$ are the instantaneous energies and eigenprojectors, respectively. The assumptions imply that $E_n^{(j)}(\tau) = 0$ for $j = 1,2,\ldots,k$ and so the same holds for the Bohr frequencies $\omega_n^{(j)}(\tau)$. The Lindblad jump operators $A_\alpha(\omega_n)$ that appear in the Davies generator appear in Eq. (19), whereby:

$$A_\alpha(\omega_n) = \lim_{X \to \infty} \frac{1}{X} \int_0^X dt' e^{it'\omega_n(t)} e^{it'H(t)} A_\alpha e^{-it'H(t)}. \quad (26)$$

Now, using the Duhamel formula

$$\partial_t e^{B(t)} = \int_0^1 dr e^{rB(t)} (\partial_t B) e^{(1-r)B(t)} \quad (27)$$

repeatedly, together with $\omega_n^{(j)}(\tau) = 0$ for $j = 1,2,\ldots,k$, one obtains

$$\partial_t^{(j)}[A_\alpha(\omega)]_{t=\tau} = 0, \text{ for } j = 1,2,\ldots,k, \quad (28)$$

which ensures that both $\partial_t^{(j)}[\mathcal{L}_\tau^D]_{t=\tau}$ and $\partial_t^{(j)}[H_{LS}]_{t=\tau}$ [Eq. (17)] vanish, so that the Proposition 2 assumption that $\mathcal{L}^{(j)}(1) = 0$ for $j = 1,2,\ldots,k$ is also satisfied.

To prove the last assertion of the current Proposition note that the assumptions, together with finite dimensionality, imply that the zero eigenvalue is separated by a finite gap from the rest of the spectrum. Moreover, a theorem due to Kossakowski [26] (see also Theorem 3.3.1 of [27]) states that a Lindbladian generates a contraction semigroup, so we can apply Proposition 2. More specifically, the Lindbladian assumption implies that $\|\mathcal{E}(s,s')\|_1 \leq 1$ for $s \geq s'$, so that we can go
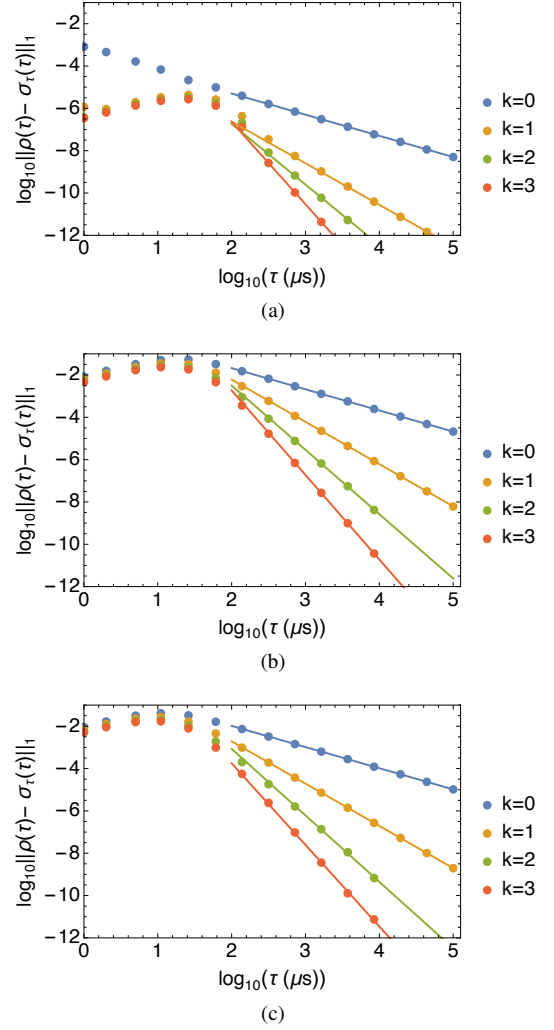

Figure 2. (Color online) Adiabatic error $\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1$ as a function of annealing time τ using the boundary cancellation method for different k's and different temperatures, for the Davies-Lindblad adiabatic master equation with an Ohmic bath. (a) $T = 1$mK, (b) $T = 12$mK, (c) $T = 20$mK. Parameters are: $g = 10^{-5/2}$GHz $= 3.16$MHz, $\omega_c = 8\pi$GHZ$= 25.13$GHz and $\eta = 1(\text{ns})^2$. These parameters can describe experiments with flux qubits [28, 29]. The continuous lines are best fits of the form $\sim \tau^{-\alpha_k}$. The resulting exponents for $k = (0,1,2,3)$ are given by (a) $\alpha = (1.00, 1.96, 2.86, 3.89)$, (b) $\alpha = (0.99, 1.99, 3.03, 3.99)$, (c) $\alpha = (0.99, 1.99, 3.14, 3.85)$.

from Eq. (11a) to Eq. (11b). Since $\mathcal{L}(s)$ is independent of τ, the right hand side of Eq. (11b) is (bounded and) independent of τ and the result follows. $\square$

Results of numerical simulations for a single qubit evolving according to Eq. (17) are shown in Fig. 2. The Hamiltonian is taken to be $H_S(t) = \omega_x\sigma^x[1 - \vartheta_k(t/\tau)] + \omega_z\sigma^z\vartheta_k(t/\tau)$. The schedule is given by $\vartheta_k(s) = 2B_{(s+1)/2}(k+1,k+1)/B_1(k+1,k+1)$ where $B_s(a,b)$ is the incomplete Beta function [30]. It has the property of having vanishing derivatives at $s = 1$ up to order k but not for $k + 1$. The system-bath operator is

$A = \sigma^y$, and the bath correlation function is Ohmic, i.e.,

$$\hat{G}(\omega) := \int_{-\infty}^{+\infty} e^{i\omega t} G(t) dt = g^2 \eta 2\pi \frac{\omega e^{-|\omega|/\omega_c}}{1 - e^{-\beta\omega}}, \quad (29)$$

where η is a constant with dimension of time squared. The simulations are carried out for an annealing time τ that is sufficiently large for the asymptotic region to be reached, where $\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1 \sim \tau^{-\alpha_k}$, where $\alpha_k \approx k + 1$ (fits in Fig. 2). Note that for the DLAME, the instantaneous steady state is given by the thermal Gibbs state: $\sigma_\tau(t) = \rho_G(t) := \exp(-\beta H_S(t))/Z$.

2. The Redfield master equations

We now turn our attention to the two types of Redfield master equations. We first consider the ARME.

Proposition 5. *Assume the adiabatic Redfield master equation [Eq. (23)] holds. Moreover, assume that the system Hamiltonian $H_S(t)$ is smooth and $\partial_t^{(j)}[H_S(t)]_{t=\tau} = 0$ for $j = 1, 2, \ldots, k$. Then $\partial_t^{(j)}[\mathcal{L}_\tau(t)]_{t=\tau} = 0$ for $j = 1, 2, \ldots, k$. As a consequence, the adiabatic expansion (4a) holds with $b_n(s) = 0$ for $n = 1, 2, \ldots, k$.*

Proof. The result follows simply by repeatedly taking the derivative of $A_\beta(-r, t)$ with respect to t at $t = \tau$ using the Duhamel formula, exactly as in the proof of Proposition 4. □

In contrast to the DLAME case [Eq. (17)], we cannot prove that the bound (7) generally holds in the present case. The reason is that this requires bounding the error $r_k(\zeta, 1)$ by a constant independent of τ. However, since the ARME does not always generate a contraction, this is not always possible for all initial states and parameter values. We do not report numerical simulations for the ARME case since for the parameters chosen here the evolutions it generates turn out to be completely-positive and trace-preserving (CPTP), and hence the results will agree with Proposition 4.

We next consider the SPRME [Eq. (22)]. In this case even Proposition 5 does not apply. For example, even if $\partial_t H_S(\tau) = 0$, if we differentiate the non-adiabatic generator once at $t = \tau$ with $\partial_t H_s(\tau) = 0$ we obtain a term proportional to $G_{\alpha,\beta}(\tau)$ and a term proportional to $\int_0^\tau r^2 G_{\alpha,\beta}(\tau) dr = O(\tau_B^3 g^2)$ under the assumption of a fast bath. However, both these terms are supposed to be small and so one may hope that the conclusions of Proposition 4 are qualitatively valid at least in some range of parameters.

In order to check the latter conjecture we performed numerical simulations using Eq. (22) for the same Hamiltonian $H_S(t)$ and system-bath operator used for the DLAME simulations of Fig. 2. The results are shown in Fig. 3, where we see that boundary cancellation improves the adiabatic error for sufficiently large annealing times. The slope seems to roughly track the $k + 1$ rule expected if the assumptions of Proposition 4 were to hold, but we caution that the asymptotic regime was not reached due to the heavy computational cost of these
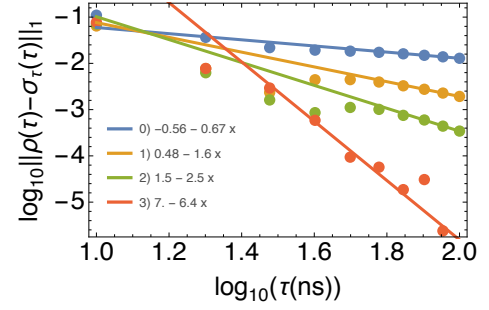

Figure 3. (Color online) Adiabatic error $\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1$ as a function of annealing time τ using the boundary cancellation method for $k = 0, 1, 2, 3$ for the Schrödinger picture Redfield master equation (22). The parameters are: $g = 0.1$GHz, $\omega_c = 16$GHz, $T = 12$mK. For $k = 0, 1, 2$ the fit is obtained using the last four most significant points, for $k = 3$ the penultimate point has been excluded from the fit. Note that the total annealing times here are much shorter than in Fig. 2 and the asymptotic region where $\|\rho_\tau(\tau) - \sigma_\tau(\tau)\|_1 \sim \tau^{-(k+1)}$ has not yet been reached. Boundary cancellation is seen to provide a consistent advantage for $\tau \gtrsim 20$ns.
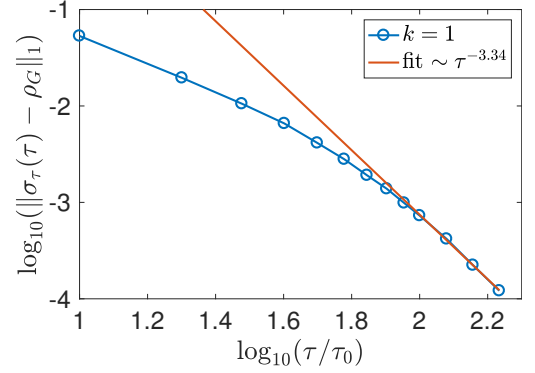

Figure 4. Distance of the instantaneous steady state of the generator (22) from the corresponding Gibbs state $\rho_G(\tau)$. The timescale is $\tau_0 = 1$ns. Other parameters are the same as in Fig. 3. The same plot is obtained for different values of k.

simulations. In fact, the numerical computation of the integral appearing in Eq. (22) constitutes its own challenge; more details are given in Appendix D.

Note that the generator in Eq. (22) reduces to $-i[H_S(0), \bullet]$ at $t = 0$. As such the instantaneous steady state is degenerate at $t = 0$. We fixed the initial state by taking $\sigma_\tau(0) := \lim_{t\to 0^+} \sigma_\tau(t)$. It turns out that $\sigma_\tau(0) = \mathbb{1}/2$ in all of our simulations. At the other boundary $t = \tau$, the steady state approaches the thermal state $\rho_G(\tau)$. In fact we have numerically checked that $\|\sigma_\tau(\tau) - e^{-\beta H_S(\tau)}/Z\|_1 \sim \tau^{-\alpha}$; see Fig. 4.

Let us also comment on complete positivity. The precise, general characterization of the region of parameters that ensure this condition is beyond the scope of this work. However, as shown in Fig. 5 for an Ohmic bath, complete positivity is violated at very low temperatures and large values of ω_c. This (counterintuitive) fact seems to be due to the presence of fast oscillations appearing for large ω_c.
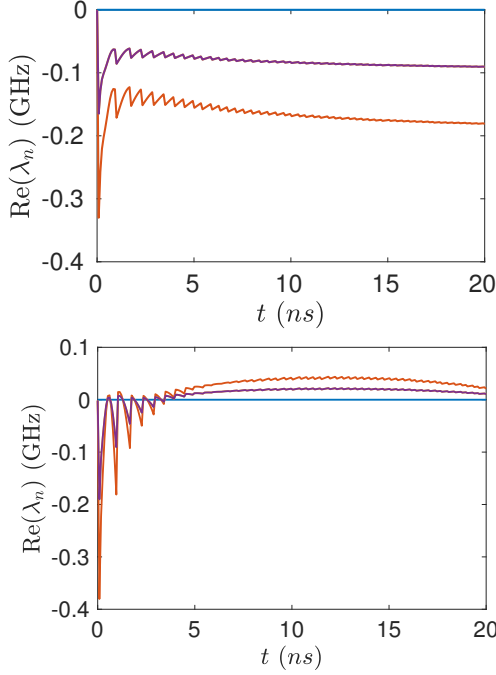
Figure 5. (Color online) Real part of instantaneous eigenvalues of the generator (22), for $\tau = 20$ns and $k = 0$. Top panel: $g = 0.1$GHz , $\omega_c = 16$GHz, $T = 12$mK (as in Fig. 3). Bottom panel: $g = 0.1$GHz, $\omega_c = 25.13$GHZ, $T = 1$mK. In the bottom panel the instantaneous eigenvalues of the generator $\mathcal{L}_\tau(t)$ acquire a positive real part in some range $t \in [0, \tau]$, which means that the propagator is not completely positive.

3. The Hamiltonian case

The next result (analogous to Theorem 4 of [16]) shows that the boundary cancellation result is stable with respect to non-Markovianity, and at the same time that the lack of boundedness that can in principle emerge from the Redfield master equation is unphysical. This requires that we assume vanishing derivatives at both the initial and final times.

Proposition 6. *Assume that the total Hamiltonian has the form $H_{\text{tot}}(s) = H_S(s) + H_B + H_I$, where only H_S depends on the rescaled time s. Let $|\phi(s)\rangle$ denote the instantaneous eigenstate of $H_{\text{tot}}(s)$ related to some total energy level and $|\psi(s)\rangle$ the Schrödinger-evolved state starting from $|\phi(0)\rangle$. Also assume that this level is separated by a finite gap from the rest of the spectrum for all $s \in [0,1]$. Let $\rho(s) = \text{Tr}_B |\psi(s)\rangle\langle\psi(s)|$ and $\sigma(s) = \text{Tr}_B |\phi(s)\rangle\langle\phi(s)|$. If $H_S^{(j)}(0) = H_S^{(j)}(1)$ for $j = 1, 2, \ldots, k$ then*

$$\|\rho(1) - \sigma(1)\|_1 \leq \frac{C_k}{\tau^{k+1}}. \tag{30}$$

Proof. Obviously, if $H_S^{(j)}(1) = 0$ then also $H^{(j)}(1) = 0$. We now apply the analogous result of Proposition 2 for unitary dynamics, which requires the derivatives of the generator (the Hamiltonian) to vanish also at $s = 0$ [13]. So we have $\||\psi(s)\rangle\langle\psi(s)| - |\phi(s)\rangle\langle\phi(s)|\|_1 \leq C_k \tau^{-(k+1)}$. Since

CPTP maps are contractions for the trace norm distance (i.e., $\|\mathcal{E}\rho_1 - \mathcal{E}\rho_2\|_1 \leq \|\rho_1 - \rho_2\|_1$), the result follows from the fact that the partial trace is a CPTP map:

$$\|\rho(s) - \sigma(s)\|_1 \leq \||\psi(s)\rangle\langle\psi(s)| - |\phi(s)\rangle\langle\phi(s)|\|_1$$
$$\leq \frac{C_k}{\tau^{k+1}}. \tag{31}$$

$\square$

IV. SUMMARY AND CONCLUSIONS

We have generalized the boundary cancellation method to open systems described by a time-dependent Liouvillian $\mathcal{L}_\tau(t)$. If $\mathcal{L}_\tau(t)$ is ergodic (i.e., its instantaneous steady state is unique), generates a completely positive quantum map, and has vanishing derivatives up to order k at the end of the evolution, then the adiabatic steady-state preparation error is upper bounded by C_k/τ^{k+1}. Next, we performed a detailed analysis to investigate whether the assumptions underlying this result can be satisfied in a realistic setting, where one controls only the system Hamiltonian. For the time-dependent Davies-Lindblad adiabatic master equation derived in [20] the boundary cancellation result can indeed by achieved by requiring that the system Hamiltonian has vanishing derivatives up to order k only at the end of the evolution. To go beyond this setting we derived two time-dependent master equations of the Redfield type, one in the Schrödinger picture with a general time-dependent system Hamiltonian and the other under an additional adiabatic approximation. In this case the lack of complete positivity prevents the rigorous applicability of our result. However our numerical simulations shows that boundary cancellation still holds for the Schrödinger picture Redfield master equation, for the range of parameters where the evolution is positive. We have also shown analytically that the boundary cancellation result exhibits a degree of robustness in the sense that even if the derivatives do not exactly vanish but instead are upper bounded, then the adiabatic error can still be reduced, with the reduction being more pronounced for longer annealing times.

Boundary cancellation is a relatively straightforward method that can be applied to experimental quantum annealers used to prepare steady states such as thermal Gibbs states. It allows for a smaller error at a given preparation time, or equivalently a shorter preparation time at a given error, and should hence be used when possible.

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Appendix A: Proof of Proposition 1

Proposition 1 is a special case of Theorem 6 of [22] and all we need to prove is that the terms $a_n(s)$ of Eq. (15) in that reference satisfy $a_0(s) = T(s,0)a_0(0) = \sigma(s)$ and $a_n(s) = 0$ for $n \geq 1$, where $T(s,s')$ denotes the parallel transport (perfect adiabatic evolution) operator, which satisfies $P(s)T(s,s') = T(s,s')P(s')$.

Proof. We use the adiabatic series in [22] and follow the same notation therein with the only modification being that we replace $\mathcal{L}^{-1}$ by S. The terms $a_n(s)$ in Theorem 6 of [22] satisfy $P(s)a_n(s) = a_n(s)$ while $Q(s)b_n(s) = b_n(s)$. The initial condition implies that $\rho(0) = a_0(0) = \sigma(0)$ (and $a_n(0) = 0$ for $n \geq 1$). The assumption that $\mathcal{L}(s)$ is TPHP together with uniqueness implies that $\dot{P}(s)b_n(s) = \dot{P}(s)Q(s)b_n(s) = 0$. In fact, using Hilbert-Schmidt scalar product notation, $P = |\sigma\rangle\langle\mathbb{1}|$, so $\dot{P} = |\dot{\sigma}\rangle\langle\mathbb{1}|$ and $\dot{P}Q = 0$ follows. Since $S = SQ = QS$ we also have $\dot{P}S = S\dot{P} = 0$. This implies, from Eq. (15) of [22], that that $a_0(s) = T(s,0)a_0(0) = \sigma(s)$ and $a_n(s) = 0$ for $n \geq 1$. Our Eq. (4a) then follows from Eq. (14) of [22]. In addition, Eq. (6) is a special case of Eq. (17) of [22] under our additional initial condition assumption $\rho(0) = \sigma(0)$, which implies that $r_k(\zeta,0) = 0$. $\square$

Note that Eq. (4a) can be written as

$$\rho(s) = \sum_{n=0}^{k} \left(\zeta S(s)\frac{d}{ds}\right)^n \sigma(s) + \zeta^{k+1} r_k(\zeta, s). \quad \text{(A1)}$$

Appendix B: Explicit Constants for the Adiabatic Error

By the assumption of ergodicity $\dot{\sigma} = \dot{P}\sigma = -S\dot{\mathcal{L}}\sigma$. We use some results from [7]. We have

$$b_1 = -S^2\dot{\mathcal{L}}\sigma \quad \text{(B1a)}$$
$$\dot{b}_1 = \left(2S^2\dot{\mathcal{L}}S\dot{\mathcal{L}} - 2S^3\dot{\mathcal{L}}P\dot{\mathcal{L}} - S^2\ddot{\mathcal{L}} - P\dot{\mathcal{L}}S^3\dot{\mathcal{L}} + S\dot{\mathcal{L}}S^2\dot{\mathcal{L}}\right)\sigma \quad \text{(B1b)}$$
$$b_2 = S\left(2S^2\dot{\mathcal{L}}S\dot{\mathcal{L}} - 2S^3\dot{\mathcal{L}}P\dot{\mathcal{L}} - S^2\ddot{\mathcal{L}} + S\dot{\mathcal{L}}S^2\dot{\mathcal{L}}\right)\sigma. \quad \text{(B1c)}$$

So

$$\|b_1\| \leq \|S\|^2 \left\|\dot{\mathcal{L}}\right\| \quad \text{(B2a)}$$
$$\left\|\dot{b}_1\right\| \leq 6\|S\|^3 \left\|\dot{\mathcal{L}}\right\|^2 + \|S\|^2 \left\|\ddot{\mathcal{L}}\right\| \quad \text{(B2b)}$$
$$\|b_2\| \leq 5\|S\|^4 \left\|\dot{\mathcal{L}}\right\|^2 + \|S\|^3 \left\|\ddot{\mathcal{L}}\right\|. \quad \text{(B2c)}$$

Moreover, one can show that

$$\left\|\dot{b}_2\right\| \leq 60\|S\|^5 \left\|\dot{\mathcal{L}}\right\|^3 + 19\|S\|^4 \left\|\dot{\mathcal{L}}\right\| \left\|\ddot{\mathcal{L}}\right\| + \|S\|^3 \left\|\dddot{\mathcal{L}}\right\|. \quad \text{(B3)}$$

Let us now use Proposition 1 with $k = 0$:

$$\|\rho(1) - \sigma(1)\| \leq \frac{1}{\tau}\|r_0(\tau,1)\|$$
$$\leq \frac{1}{\tau}\left(\|b_1(1)\| + \|b_1(0)\| + \sup_{s\in[0,1]}\left\|\dot{b}_1(s)\right\|\right)$$
$$= \frac{B_0}{\tau}, \quad \text{(B4)}$$

where one can take B_0 as in Eq. (15a). Similarly we can use Proposition 1 with $k = 1$ and obtain:

$$\|\rho(1) - \sigma(1)\| \leq \frac{1}{\tau}\|b_1(1)\| + \frac{1}{\tau^2}\|r_1(\tau,1)\|, \quad \text{(B5)}$$

implying

$$\|\rho(1) - \sigma(1)\| \leq \frac{A_1}{\tau} + \frac{B_1}{\tau^2}, \quad \text{(B6)}$$

with A_1 and B_1 as in Eqs. (15b) and (15c), respectively.

Appendix C: Derivation of the Schrödinger picture and adiabatic Redfield master equations

1. SPRME

The first few steps are customary. In the interaction picture, after the Born approximation (see Eq. (3.116) of [23] and additional details therein) the dynamics of the system's density matrix in the interaction picture ρ_I are given by

$$\dot{\rho}_I(t) = -\int_0^t dt' \text{Tr}_B\left[H_I(t),[H_I(t'),\rho_I(t')\otimes\rho_B]\right]. \quad \text{(C1)}$$

After substituting the interaction Hamiltonian $H_I = g\sum_\alpha A_\alpha \otimes B_\alpha$ and a change of integration variable, we obtain:

$$\dot{\rho}_I(t) = \sum_{\alpha,\beta}\int_0^t dt' G_{\alpha,\beta}(t-t')\left[A_\beta(t')\rho_I(t'),A_\alpha(t)\right] + \text{h.c.}, \quad \text{(C2)}$$

which is the same as Eq. (9) of [20]. This equation is non-local in time because on the right-hand-side the unknown $\rho_I(t)$ appears also for times $t' \neq t$. In order to make it time-local we use the Markov approximation $\rho_I(t') \approx \rho_I(t)$. When this substitution is made in Eq. (C1) the resulting equation is called the Redfield master equation (RME) according to [23] [see Eq. (3.117) therein], though in our case the system Hamiltonian is explicitly time-dependent, in contrast to standard Redfield theory.

We now estimate the error made with this Markov approximation. We use the same techniques utilized in Appendix B of

Ref. [20] but note that we do not extend the upper integration limit to ∞ as done there. One can then show that the relative error of this approximation is of the order of magnitude of the following integral:

$$\sum_{\alpha,\beta} \int_0^\tau dt'\, t'|G_{\alpha,\beta}(t')|. \tag{C3}$$

If $G_{\alpha,\beta}(t)$ is an exponentially decaying function of t with time decay constant τ_B ("fast bath"), the integral in Eq. (C3) is of the order of $O(\tau_B^2 g^2)$, in agreement with Ref. [20].

Consider now the case where $G_{\alpha,\beta}(t)$ decays algebraically. I.e., assume that for times $t > t_0$,

$$|G_{\alpha,\beta}(t)| \sim g^2 \left(\frac{\tau_M}{t}\right)^\theta, \tag{C4}$$

where we neglected the (unimportant) dependence on the labels α, β. For $\theta \neq 2$ the relative error is then of the order of

$$\int_{t_0}^\tau dt'\, t'|G_{\alpha,\beta}(t')| = \frac{g^2 \tau_M^\theta}{\theta - 2}\left(\frac{1}{t_0^{\theta-2}} - \frac{1}{\tau^{\theta-2}}\right). \tag{C5}$$

For the case $\theta = 2$ we obtain instead

$$\int_{t_0}^\tau dt'\, t'|G_{\alpha,\beta}(t')| \sim (g\tau_M)^2 \ln(\tau/t_0). \tag{C6}$$

Note that for $\theta < 2$ the relative error Eq. (C5) increases as τ grows larger and in fact diverges as $\tau \to \infty$. The same is true for $\theta = 2$ although in this case the growth is only logarithmic. Keeping the upper integration limit in Eq. (C2), finite and bounded by τ, circumvents this problem in case of an insufficiently fast bath.

Neglecting this error, we obtain:

$$\dot{\rho}_I(t) = \sum_{\alpha,\beta} \int_0^t dt' G_{\alpha,\beta}(t')\left[A_\beta(t-t')\rho_I(t), A_\alpha(t)\right] + \text{h.c.} \tag{C7}$$

This is still the RME, in somewhat more explicit form. After transforming back to the Schrödinger picture via $\rho(t) = U_0(t,0)\rho_I(t)U_0(0,t)$, we directly obtain the SPRME given in Eq. (22).

2. ARME

At this point, since the bath correlation function is peaked in a small time-window we can expand $U_0(t,t-t')$ in powers of t'. This is effectively an expansion in powers of t'/τ, and we can use

$$U_0(t,t-t') = e^{-isH_S(t)} + O\left((t'/\tau)^2\right). \tag{C8}$$

If $G_{\alpha,\beta}(r)$ decays exponentially the error of this latter approximation is then of order of

$$\int_0^\infty dt' \left(\frac{t'}{\tau}\right)^2 |G_{\alpha,\beta}(t')| = \tau_B^3 \left(\frac{g}{\tau}\right)^2, \tag{C9}$$

while the leading term [Eq. (C7) after substituting Eq. (C8)] is $O\left(\tau_B g^2\right)$. Dividing, the relative error is

$$\left(\frac{\tau_B}{\tau}\right)^2 \ll 1. \tag{C10}$$

In this sense this approximation is adiabatic as it requires τ large, i.e., $\tau \gg \tau_B$.

For an algebraic bath, the order of magnitude of the (absolute) error is:

$$\int_{t_0}^\tau dt' \left(\frac{t'}{\tau}\right)^2 |G_{\alpha,\beta}(t')| = \frac{g^2 \tau_M^\vartheta}{\tau^2(\vartheta - 3)}\left(t_0^{-(\vartheta-3)} - \tau^{-(\vartheta-3)}\right), \tag{C11}$$

while the order of magnitude of the leading term is:

$$\int_{t_0}^\tau dt' |G_{\alpha,\beta}(t')| = \frac{g^2 \tau_M^\vartheta}{(\vartheta - 1)}\left(t_0^{-(\vartheta-1)} - \tau^{-(\vartheta-1)}\right). \tag{C12}$$

For $\vartheta > 3$ the relative error becomes, assuming $\tau \gg t_0$, $O\left((t_0/\tau)^2\right)$ and is small in the adiabatic limit (here $\tau \gg t_0$). Instead, e.g., for $\vartheta = 2$ one obtains $O\left(\tau/t_0\right)$ and so the error is large.

Finally, discarding the error term in Eq. (C8) we obtain the ARME given in Eq. (23).

Appendix D: Numerical computation of the integral in Eq. (22)

We consider the case of a single system-bath operator A; generalization is straightforward. The integral that we need to compute is

$$W(t) = \int_0^t dr\, G(r)U_0(t,t-r)AU_0(t-r,t). \tag{D1}$$

Recall that the standard fourth order Runge-Kutta, which is routinely used in many ODE solvers, is equivalent to Simpson's rule for integration. With this in mind we simply implement the integral using Simpson's rule. This means that the integral in Eq. (D1) is replaced by the following sum:

$$\int_0^t dr f(r) \approx \Delta r \sum_{j=0}^n f(r_j)w_j, \tag{D2}$$

where $r_j = j\Delta r$, for $j = 0, 1, \ldots, n$, $\Delta r = t/n$, and $w_0 = w_n = 1/3$ while $w_j = 4/3$ for j odd and $w_j = 2/3$ for j even. The error in the Simpson's rule is $\propto t(\Delta r)^4 = t^5 n^{-4}$. In order to have a constant error we must pick $n \propto t^{5/4} = t^{1.25}$. To be conservative, in our simulations we pick $n \propto t^{1.3}$. Next we need to compute $T_j := U_0(t,t-r_j)$. We use

$$\begin{aligned} T_0 &= U_0(t,t) = \mathbb{1} \\ T_1 &= U_0(t,t-\Delta r) \approx \exp\left(-i\Delta r H_S(t)\right) \\ T_{j+1} &:= T_j \exp\left(-i\Delta r H_S(t-r_j)\right),\; j = 0,1,\ldots,n-1. \end{aligned} \tag{D3}$$

Note that this approximation preserves unitarity, i.e., $T_j T_j^\dagger = \mathbb{1}$ for $j = 0, 1, \ldots, n$.

Finally, the differential equation (22) assumes the form

$$\frac{\partial \rho(t)}{\partial t} = -i \left[H_S(t), \rho(t) \right] + \left([W(t)\rho(t), A] + \text{h.c.} \right). \quad \text{(D4)}$$

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