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Abstract. We develop from first principles Markovian master equations suited for studying the time evolution of a system evolving adiabatically while coupled weakly to a thermal bath. We derive two sets of equations in the adiabatic limit, one using the rotating wave (secular) approximation that results in a master equation in Lindblad form, the other without the rotating wave approximation but not in Lindblad form. The two equations make markedly different predictions depending on whether or not the Lamb shift is included. Our analysis keeps track of the various time and energy scales associated with the various approximations we make, and thus allows for a systematic inclusion of higher order corrections, in particular beyond the adiabatic limit. We use our formalism to study the evolution of an Ising spin chain in a transverse field and coupled to a thermal bosonic bath, for which we identify four distinct evolution phases. While we do not expect this to be a generic feature, in one of these phases dissipation acts to increase the fidelity of the system state relative to the adiabatic ground state.

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Contents

1. Introduction

Recent developments in quantum information processing, in particular theoretical [1] and experimental [2] proposals for adiabatic quantum computation, have generated considerable renewed interest in the old topic of quantum adiabatic dynamics [3, 4]. While much work has been done on rigorous formulations of adiabatic approximations for closed quantum systems, e.g. [5–12], adiabatic evolution in open quantum systems is still a relatively unexplored topic.

In this regard master equations governing the evolution of a quantum system with a time-dependent Hamiltonian coupled to an external environment or bath are an important tool.

The study of master equations with time-dependent Hamiltonians is certainly not a new topic, going back at least as far as the pioneering work of Davies and Spohn [13], who derived an exact master equation for an adiabatic but infinitesimally weak system–bath interaction. Other, more recent approaches have been attempted, but in each case certain limitations apply. For example, Childs *et al* [14] used the Lindblad equation with a time-independent Hamiltonian at each time step as an approximation to the adiabatic evolution of a system with a time-dependent Hamiltonian. Sarandy and Lidar [15] derived a phenomenological adiabatic master equation, based on the idea that in the adiabatic limit the dynamical superoperator can be decomposed in terms of independently evolving Jordan blocks. This approach is phenomenological in the sense that it does not allow one to derive the various parameters appearing in the final master equation from underlying system and bath Hamiltonians. Approaches based on non-Hermitian effective Hamiltonians, e.g. [16–18], are necessarily also phenomenological. A rigorous phenomenological master equation derivation was given by Joye [19]. Oreshkov and Calsamiglia [20] connected open system adiabaticity to the theory of noiseless subsystems. Thunström *et al* [21] derived a master equation from first principles in the physically reasonable joint limit of slow change and weak open system disturbances, but did not elucidate the relative time and energy scales involved in their approximations. Various authors provided derivations for slow periodic Hamiltonians [22–24]. Such derivations are valuable and can be made rigorous, but the assumption of periodicity can be excessive, especially in the context of adiabatic quantum computation. Bounds on the validity of the adiabatic approximation for open systems, but without master equations, were presented in [25] (see also [10]). Various authors derived or studied adiabatic master equations limited to the case of a single qubit, where detailed physical considerations are possible [26–28].

Our goal in this work is to derive master equations for adiabatic open system dynamics from first principles, while keeping track of all physical approximations, time and energy scales. In this manner we hope to fill a gap in the earlier literature on this topic, and to provide tools allowing for detailed comparisons with experiments satisfying the explicit assumptions behind our approximations. In particular, we derive several Markovian master equations, distinguished by different levels of adiabatic perturbation theory. When we add the rotating wave approximation (RWA) (sometimes called the secular approximation) we arrive at master equations in Lindblad form [29], for which positivity of the state is guaranteed at all times [30]. Our formalism allows for the calculation of non-adiabatic corrections, which we also discuss. We apply our master equations to numerically study the evolution of a transverse field Ising chain coupled to a thermal bath, and discuss generic features of the evolution.

Our basic starting point is the observation that the Markovian and adiabatic limits are fundamentally compatible, in the sense that a Markovian bath is ‘fast’, while an adiabatically evolving system is ‘slow’. As long as the corresponding timescales are appropriately matched, it is possible to derive an adiabatic master equation which is internally consistent. Somewhat more technically, we observe that in the interaction picture with respect to the unperturbed system and bath evolutions, where the bath is evolving ‘fast’ while the system is evolving ‘slowly’, and for sufficiently weak system–bath coupling, it is possible to consistently apply adiabatic perturbation theory to the time-dependent system operators. This insight allows us to derive our adiabatic Markovian master equations. Our work is conceptually similar in its starting point to that of Amin *et al* [31] (see also the supplementary information of [2]), but is significantly more

general. Some of our results are also conceptually similar to those found by Kamleitner and Shnirman [24], by de Vega *et al* [32] and by Yung [33], but are again more general. The master equations we derive are a natural generalization of standard time-independent Hamiltonian results [30, 35], and our master equations reduce to the standard results after freezing the time dependence of the system Hamiltonian.

The structure of this paper is the following. We set the stage in section 2, where we define the system–bath model, perform the Born–Markov approximation and introduce the bath correlation functions and spectral-density. We pay special attention to constraints imposed (via the Kubo–Martin–Schwinger (KMS) condition) by baths in thermal equilibrium, and single out the case of the Ohmic oscillator bath. We interrupt the formal development in section 3, where we provide a summary of all the time and energy scales appearing in our various approximations, and the inequalities they must mutually satisfy. We then proceed to derive our adiabatic master equations in section 4. We proceed in several steps. First, in section 4.1 we find the adiabatic limit of the time-dependent system operators. Next, in section 4.2 we find two pairs of master equations in the adiabatic limit, one pair in the interaction picture, the other in the Schrödinger picture. The master equations within a given picture are distinguished by whether we apply the adiabatic approximation once or twice. Next, in section 4.3, we introduce the RWA, which allows us to reduce the Schrödinger picture master equations into Lindblad form. We conclude the formal development by discussing non-adiabatic corrections to our master equations in section 4.4. We move on to a detailed numerical study of an example in section 5, of a ferromagnetic chain in a transverse field, coupled to an Ohmic oscillator bath at finite temperature. We apply two of our Schrödinger picture master equations, with and without the RWA, and show that without inclusion of the Lamb shift term they yield similar predictions. When the Lamb shift is included, however, substantial differences emerge. We discern four distinct phases in the evolution from the transverse field to the ferromagnetic Ising model, which we discuss and analyze. Concluding remarks are presented in section 6. The paper is supplemented with detailed appendixes where many of the technical details of the derivations and required background are provided, both for ease of flow of the general presentation and for completeness.

2. Preliminaries

2.1. Model

We consider a general system–bath Hamiltonian

$$H(t) = H_{\mathrm{S}}(t) + H_{\mathrm{B}} + H_{\mathrm{I}}, \tag{1}$$

where $H_{\mathrm{S}}(t)$ is the time-dependent, adiabatic system Hamiltonian, H_{B} is the bath Hamiltonian and H_{I} is the interaction Hamiltonian. Without loss of generality the interaction Hamiltonian can be written in the form:

$$H_{\mathrm{I}} = g \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}, \tag{2}$$

where the operators A_{α} and B_{α} are Hermitian and dimensionless with unit operator norm, and g is the (weak) system–bath coupling. The joint system–bath density matrix $\rho(t)$ satisfies the Schrödinger equation $\dot{\rho} = -\mathrm{i}[H, \rho(t)]$, where we have assumed units such that $\hbar = 1$.

Let $U_S(t,t') = T_+ \exp[-i\int_{t'}^{t} d\tau \;\; H_S(\tau)]$ and $U_B(t,t') = \exp(-i(t-t')H_B)$ denote the free system and bath unitary evolution operators (T_+ denotes time ordering), and define $U_0(t,t') = U_S(t,t') \otimes U_B(t,t')$. Likewise, let $U(t,t') = T_+ \exp[-i\int_{t'}^{t} d\tau \; H(\tau)]$ denote the joint Schrödinger picture system–bath unitary evolution operator. We transform to the interaction picture with respect to $H_S(t)$ and H_B, by defining $\tilde{U}(t,0) = U_0^\dagger(t,0)U(t,0)$, which, together with the interaction picture density matrix $\tilde{\rho}(t) = U_0^\dagger(t,0)\rho(t)U_0(t,0)$, satisfies

$$\frac{d}{dt}\tilde{U}(t,0) = -i\tilde{H}_I(t)\tilde{U}(t,0), \quad \tilde{U}(0,0) = \mathbb{1}, \tag{3a}$$

$$\frac{d}{dt}\tilde{\rho}(t) = -i[\tilde{H}_I(t), \tilde{\rho}(t)], \quad \tilde{\rho}(0) = \rho(0). \tag{3b}$$

We restrict the use of tilde variables to refer to variables in the interaction picture. The time-dependent interaction picture Hamiltonian $\tilde{H}_I(t)$ is related to its Schrödinger picture counterpart via:

$$\tilde{H}_I(t) = U_0^\dagger(t,0)H_I U_0(t,0) = g\sum_\alpha A_\alpha(t) \otimes B_\alpha(t), \tag{4}$$

where we have defined the time-dependent system and bath operators:

$$A_\alpha(t) = U_S^\dagger(t,0)A_\alpha U_S(t,0), \tag{5a}$$

$$B_\alpha(t) = U_B^\dagger(t,0)B_\alpha U_B(t,0). \tag{5b}$$

We are interested in deriving a master equation for the system-only state,

$$\tilde{\rho}_S(t) \equiv \mathrm{Tr}_B[\tilde{\rho}(t)] = U_S^\dagger(t,0)\mathrm{Tr}_B(U_B^\dagger(t,0)\rho(t)U_B(t,0))U_S(t,0) \tag{6a}$$

$$= U_S^\dagger(t,0)\mathrm{Tr}_B(U_B(t,0)U_B^\dagger(t,0)\rho(t))U_S(t,0) = U_S^\dagger(t,0)\rho_S(t)U_S(t,0), \tag{6b}$$

where in the second line we used the fact that U_B acts only on the bath.

2.2. *Born–Markov approximation*

Writing the formal solution of equation (3*b*) as

$$\tilde{\rho}(t) = \tilde{\rho}(0) - i\int_0^t d\tau \; [\tilde{H}_I(\tau), \tilde{\rho}(\tau)], \tag{7}$$

and substituting this solution back into equation (3*b*), we obtain, after tracing over the bath degrees of freedom, the equation of motion for the system density matrix $\tilde{\rho}_S(t) = \mathrm{Tr}_B\tilde{\rho}(t)$

$$\frac{d}{dt}\tilde{\rho}_S(t) = -i\,\mathrm{Tr}_B[\tilde{H}_I(t), \tilde{\rho}(0)] - \mathrm{Tr}_B\left[\tilde{H}_I(t), \int_0^t d\tau \; [\tilde{H}_I(t-\tau), \tilde{\rho}(t-\tau)]\right], \tag{8}$$

We make the standard Born approximation assumption, that we can decompose the density matrix as $\tilde{\rho}(t) = \tilde{\rho}_S(t) \otimes \rho_B + \chi(t)$ where $\chi(t)$, which expresses correlations between the

system and the bath, is small in an appropriate sense and can hence be neglected from now on [30, 34].[7] Thus the equation of motion reduces to:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_{\mathrm{S}}(t) = g^2 \sum_{\alpha,\beta} \int_0^t \mathrm{d}\tau \left(A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t-\tau)A_\alpha(t) - A_\alpha(t)A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t-\tau) \right) \mathcal{B}_{\alpha\beta}(t, t-\tau) + \mathrm{h.c.}, \tag{9}$$

where we defined the two-point correlation functions:

$$\mathcal{B}_{\alpha\beta}(t, t-\tau) \equiv \langle B_\alpha(t) B_\beta(t-\tau) \rangle = \mathrm{Tr}\left[B_\alpha(t) B_\beta(t-\tau) \rho_{\mathrm{B}} \right]. \tag{10}$$

In equation (9), we have assumed for simplicity (but without loss of generality) that $\langle B_\alpha \rangle_0 = \mathrm{Tr}[B_\alpha(t)\tilde{\rho}_{\mathrm{B}}(0)] = 0$, so that the inhomogeneous term in equation (8) vanishes. Since we assumed that the bath state ρ_{B} is stationary, the correlation function is homogeneous in time:

$$\mathcal{B}_{\alpha\beta}(t, t-\tau) = \langle B_\alpha(t) B_\beta(t-\tau) \rangle = \langle B_\alpha(\tau) B_\beta(0) \rangle = \langle B_\beta(0) B_\alpha(\tau) \rangle^* = \mathcal{B}_{\alpha\beta}(\tau, 0). \tag{11}$$

For notational simplicity we will denote $\mathcal{B}_{\alpha\beta}(\tau, 0)$ by $\mathcal{B}_{\alpha\beta}(\tau)$ when this does not lead to confusion. Let us denote the time scale over which the two-point correlations of the bath decay by τ_{B}, e.g. $|\mathcal{B}_{\alpha\beta}(\tau)| \sim \exp(-\tau/\tau_{\mathrm{B}})$. More precisely, we shall require throughout that

$$\int_0^\infty \mathrm{d}\tau \ \tau^n |B_{\alpha\beta}(\tau)| \sim \tau_{\mathrm{B}}^{n+1}, \qquad n \in \{0, 1, 2\}. \tag{12}$$

As we show in appendix B, if $\tau_{\mathrm{B}} \ll 1/g$, then we can apply the Markov approximation to each of the four summands in equation (9), i.e., replace $\tilde{\rho}_{\mathrm{S}}(t-\tau)$ by $\tilde{\rho}_{\mathrm{S}}(t)$:

$$\int_0^t \mathrm{d}\tau \ (\cdots \tilde{\rho}_{\mathrm{S}}(t-\tau) \cdots) \, \mathcal{B}_{\alpha\beta}(\tau) \approx \int_0^\infty \mathrm{d}\tau \ (\cdots \tilde{\rho}_{\mathrm{S}}(t) \cdots) \, \mathcal{B}_{\alpha\beta}(\tau) + O(\tau_{\mathrm{B}}^3 g^2), \tag{13}$$

where $(\cdots)$ refers to the products of A_α and A_β operators in equation (9), and where we have also assumed that $t \gg \tau_{\mathrm{B}}$ and the integrand vanishes sufficiently fast for $\tau \gg \tau_{\mathrm{B}}$, so that the upper limit can be taken to infinity. Note that by equation (12) the integral on the rhs of equation (13) is of $O(\tau_{\mathrm{B}})$, so that the *relative* magnitude of the two terms is $O[(g\tau_{\mathrm{B}})^2]$. An explicit derivation of the upper bound on the error due to this approximation can be found in appendix B. The resulting Markovian equation cannot resolve the dynamics over a time scale shorter than τ_{B}.

2.3. Correlation functions, the Kubo–Martin–Schwinger condition, and the spectral-density matrix

In computing the terms appearing in equation (13) we are faced with integrals of the form $\int_0^\infty \mathrm{d}\tau A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau)$ and $\int_0^\infty \mathrm{d}\tau A_\alpha(t)A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)\mathcal{B}_{\alpha\beta}(\tau)$. Our goal is to express these integrals in terms of the *spectral-density matrix*

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau} \mathcal{B}_{\alpha\beta}(\tau), \tag{14}$$

[7] When this term is not neglected it can be shown to give rise to an inhomogeneous contribution to the master equation [30, 34] and also to restrict the set of system states for which the master equation can be used, due to the requirement of positivity of $\rho_{\mathrm{S}}(t)$ [34]. The smallness of $\chi(t)$ is consistent with any correlations decaying very rapidly, in our case on the timescale τ_{B} of the bath correlation functions. It is also consistent with our goal of developing a master equation for an adiabatically evolving system, whose state at all times is close to the ground state and hence very nearly pure; clearly if $\rho_{\mathrm{S}}(t)$ is pure then $\chi(t)$ must vanish.

the standard quantity in master equations. It is convenient to replace the one-sided Fourier transform in the spectral-density matrix by a complete Fourier transform. Thus we split it into a sum of Hermitian matrices,

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + \mathrm{i}\, S_{\alpha\beta}(\omega), \tag{15}$$

where we show in appendix C that γ and S are given by

$$\gamma_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau} \mathcal{B}_{\alpha\beta}(\tau) = \gamma^*_{\beta\alpha}(\omega), \tag{16a}$$

$$S_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \gamma_{\alpha\beta}(\omega') \mathcal{P}\left(\frac{1}{\omega - \omega'}\right) = S^*_{\beta\alpha}(\omega). \tag{16b}$$

If we assume not only that the bath state is stationary, but that it is also in thermal equilibrium at inverse temperature β, i.e. $\rho_{\mathrm{B}} = \mathrm{e}^{-\beta H_{\mathrm{B}}}/\mathcal{Z}$, then it follows that the correlation function satisfies the KMS condition [30]

$$\langle B_a(\tau) B_b(0)\rangle = \langle B_b(0) B_a(\tau + \mathrm{i}\beta)\rangle. \tag{17}$$

If in addition the correlation function is analytic in the strip between $\tau = -\mathrm{i}\,\beta$ and 0, then it follows that the Fourier transform of the bath correlation function satisfies the detailed balance condition

$$\gamma_{ab}(-\omega) = \mathrm{e}^{-\beta\omega}\gamma_{ba}(\omega). \tag{18}$$

For a proof see appendix D.

It is important to note that the KMS detailed balance condition imposes a restriction on the decay of the correlation function. To see this, note first that $|\mathcal{B}_{ab}(-\tau)| = |\mathrm{Tr}[\rho_{\mathrm{B}} U_{\mathrm{B}}(\tau) B_a U_{\mathrm{B}}^{\dagger}(\tau) B_b]| = |\mathrm{Tr}[B_a U_{\mathrm{B}}^{\dagger}(\tau) B_b U_{\mathrm{B}}(\tau)\rho_{\mathrm{B}}]| = |\langle B_a(0) B_b(\tau)\rangle| = |\langle B_b(\tau) B_a(0)\rangle| = |\mathcal{B}_{ba}(\tau)|$, where we used equation (11). Now assume that equation (12) would have to hold for all n. It would follow that

$$\begin{aligned}\left|\frac{\mathrm{d}^n}{\mathrm{d}\omega^n}\gamma_{ab}(\omega)\right|_{\omega=0} &= \left|\int_{-\infty}^{\infty} \tau^n \mathrm{e}^{\mathrm{i}\omega\tau}\mathcal{B}_{ab}(\tau)\mathrm{d}\tau\big|_{\omega=0}\right| = \left|\int_{-\infty}^{\infty} \tau^n \mathcal{B}_{ab}(\tau)\mathrm{d}\tau\right| \\ &\leqslant \int_0^{\infty} \tau^n \left(|\mathcal{B}_{ba}(\tau)| + |\mathcal{B}_{ab}(\tau)|\right)\mathrm{d}\tau \sim 2\tau_{\mathrm{B}}^{n+1} \quad \forall n \in \{0, 1, \ldots\}.\end{aligned} \tag{19}$$

Thus all derivatives of $\gamma_{ab}(\omega)$ would have to be finite at $\omega = 0$.

On the other hand, it follows from the KMS condition (18) that

$$\left[\frac{\mathrm{d}}{\mathrm{d}(-\omega)}\gamma_{ab}(-\omega)\right]_{\omega\geqslant 0} = \left[\beta\mathrm{e}^{-\beta\omega}\gamma_{ba}(\omega) - \mathrm{e}^{-\beta\omega}\frac{\mathrm{d}}{\mathrm{d}\omega}\gamma_{ba}(\omega)\right]\Big|_{\omega\geqslant 0}, \tag{20}$$

so that in the limit as ω approaches zero from below or above,

$$\gamma'_{ab}(0_-) = \beta\gamma_{ba}(0) - \gamma'_{ba}(0_+). \tag{21}$$

This shows that in principle $\gamma'_{aa}(\omega)$ may be discontinuous at $\omega = 0$. Indeed, the continuity condition $\gamma'_{aa}(0_-) = \gamma'_{aa}(0_+)$ implies, from the KMS condition recast as equation (21), that

$$2\gamma'_{aa}(0) = \beta\gamma_{aa}(0). \tag{22}$$

This conclusion can be extended to the entire γ matrix by diagonalizing it first. When equation (22) is not satisfied $\gamma''_{aa}(0)$ diverges, so that equation (19) does not hold except for $n \in \{0, 1\}$. A simple example of this is $\gamma_{ab}(\omega) = c > 0$ (constant) for $\omega \geqslant 0$. Another example is a super-Ohmic spectral density $\gamma_{ab}(\omega) = \omega^2/(1 - \mathrm{e}^{-\beta\omega})$ for $\omega \geqslant 0$ and $\gamma_{ab}(\omega) = \omega^2/(\mathrm{e}^{-\beta\omega} - 1)$ for $\omega \leqslant 0$. Both examples violate equation (19) for $n \geqslant 2$. Note, moreover, that when this happens, it follows from equation (19) that $\int_0^\infty \tau^2 \left(|\mathcal{B}_{ab}(-\tau)| + |\mathcal{B}_{ab}(\tau)|\right) \mathrm{d}\tau$ is divergent, so that we must conclude that $|\mathcal{B}_{ab}(\tau)| \gtrsim 1/\tau^3$ for sufficiently large $|\tau|$, meaning that the correlation function has a power-law tail and, in particular, cannot be exponentially decaying.

On the other hand, equation (22) tells us that continuity and a lack of divergence at $\omega = 0$ require $\gamma'_{aa}(0)$ to satisfy a condition which prohibits it from being arbitrary. This is indeed the case for the Ohmic oscillator bath discussed in section 5.1, which satisfies equation (22) with finite $\gamma_{aa}(0)$. For this case the bath correlation function is exponentially decaying assuming the oscillator bath has an infinite cutoff. However, as we show in section 5.2 the Ohmic bath transitions from exponential decay to a power-law tail for any finite value of the cutoff, at some finite transition time τ_{tr}. In this case we find $|B_{\alpha\beta}(\tau)| \sim (\tau/\tau_{\mathrm{M}})^{-2}$, where τ_{M} is a time-scale associated with the onset of non-Markovian effects, and hence we have to relax equation (12), and replace it with

$$\int_0^{\tau_{\mathrm{tr}}} \mathrm{d}\tau\ \tau^n |B_{\alpha\beta}(\tau)| \sim \tau_{\mathrm{B}}^{n+1}, \quad n \in \{0, 1, \ldots\}, \tag{23a}$$

$$\int_{\tau_{\mathrm{tr}}}^{\infty} \mathrm{d}\tau\ |B_{\alpha\beta}(\tau)| \sim \int_{\tau_{\mathrm{tr}}}^{\infty} \mathrm{d}\tau\ (\tau/\tau_{\mathrm{M}})^{-2} = \tau_{\mathrm{M}}^2/\tau_{\mathrm{tr}}. \tag{23b}$$

3. Timescales

In this subsection we summarize, for convenience, the relations between the different timescales which shall arise in our derivation. The total evolution time is denoted t_{f} and the minimum ground state energy gap of H_{S} is Δ, i.e.

$$\Delta \equiv \min_{t\in[0,t_{\mathrm{f}}]} \varepsilon_1(t) - \varepsilon_0(t), \tag{24}$$

where $\varepsilon_0(t)$ and $\varepsilon_1(t)$ are the ground and first excited state energies of $H_{\mathrm{S}}(t)$. We shall arrive at master equations of the following general form:

$$\dot{\rho}_{\mathrm{S}}(t) = [\mathcal{L}_{\mathrm{uni}}(t) + \mathcal{L}^{\mathrm{ad}}_{\mathrm{diss}}(t) + \mathcal{L}^{\mathrm{non-ad}}_{\mathrm{diss}}(t)]\rho_{\mathrm{S}}(t). \tag{25}$$

Here $\mathcal{L}_{\mathrm{uni}} = -\mathrm{i}[H_{\mathrm{S}}(t) + H_{\mathrm{LS}}, \cdot]$ is the unitary evolution superoperator including the Lamb shift correction, $\mathcal{L}^{\mathrm{ad}}_{\mathrm{diss}}$ is the dissipative superoperator in the fully adiabatic limit and $\mathcal{L}^{\mathrm{non-ad}}_{\mathrm{diss}}$ is the dissipative superoperator with leading order non-adiabatic corrections.

Let

$$h \equiv \max_{s\in[0,1];a,b} |\langle\varepsilon_a(s)|\partial_s H_{\mathrm{S}}(s)|\varepsilon_b(s)\rangle|, \tag{26}$$

where $s \equiv t/t_{\mathrm{f}}$ is the dimensionless time. To ensure that $\mathcal{L}_{\mathrm{uni}}$ generates adiabatic evolution to leading order we shall require the standard adiabatic condition

$$\frac{h}{\Delta^2 t_{\mathrm{f}}} \ll 1. \tag{27}$$

In order to derive equation (25), the three superoperators are ordered in perturbation theory, in the sense that

$$\|\mathcal{L}_{\rm uni}\| \gg \|\mathcal{L}_{\rm diss}^{\rm ad}\| \gg \|\mathcal{L}_{\rm diss}^{\rm non-ad}\|, \tag{28}$$

where the norm could be chosen as the supoperator norm, i.e. the largest singular value (see appendix A). We may then assume that

$$\|\mathcal{L}_{\rm uni}\| \gg \Delta \gg \|\mathcal{L}_{\rm diss}^{\rm ad}\|. \tag{29}$$

Combining the $O(\tau_{\rm B})$ due to the integral on the rhs of equation (13) (as already remarked there) with the g^2 prefactor from equation (9), we have

$$\|\mathcal{L}_{\rm diss}^{\rm ad}\| \sim g^2\tau_{\rm B}. \tag{30}$$

To ensure the first inequality in equation (28) we thus require

$$\frac{g^2\tau_{\rm B}}{\Delta} \ll 1. \tag{31}$$

The non-adiabatic correction is of order $\frac{h}{\Delta^2 t_{\rm f}}$, and when it appears in $\mathcal{L}_{\rm diss}^{\rm non-ad}$ it is multiplied by the same factor as $\mathcal{L}_{\rm diss}^{\rm ad}$, i.e. we have

$$\|\mathcal{L}_{\rm diss}^{\rm non\text{-}ad}\| \sim g^2\tau_{\rm B}\frac{h}{\Delta^2 t_{\rm f}}. \tag{32}$$

To ensure the second inequality in equation (28) thus amounts to the adiabatic condition, equation (27). All this is added to the condition

$$g\tau_{\rm B} \ll 1, \tag{33}$$

for the validity of the Markovian approximation, mentioned in the context of equation (13) and justified rigorously in appendix B.

There is one additional, independent time scale we have to concern ourselves with. This is the time scale associated with changes in the instantaneous energy eigenbasis relative to $\tau_{\rm B}$. If we require the change in the basis to be small on the time scale of the bath $\tau_{\rm B}$, we must have:

$$\frac{h\tau_{\rm B}^2}{t_{\rm f}} \ll 1. \tag{34}$$

We justify this claim in section 4.1 and appendix F.

Note that the adiabatic condition, equation (27), implies $\frac{h\tau_{\rm B}}{\Delta t_{\rm f}} \ll \Delta\tau_{\rm B}$, while equation (34) can be written as $\frac{h\tau_{\rm B}}{\Delta t_{\rm f}} \ll \frac{1}{\Delta\tau_{\rm B}}$. Putting this together thus yields

$$\frac{h\tau_{\rm B}}{\Delta t_{\rm f}} \ll \min\left(\Delta\tau_{\rm B}, \frac{1}{\Delta\tau_{\rm B}}\right). \tag{35}$$

Our other inequalities (equations (31) and (33)) can be summarized as

$$g\tau_{\rm B} \ll \min(1, \Delta/g). \tag{36}$$

4. Derivation of adiabatic master equations

4.1. Adiabatic limit of the time-dependent system operators

Let us first work in the strict adiabatic limit. We will discuss non-adiabatic corrections in section 4.4. We denote the instantaneous eigenbasis of $H_S(t)$ by $\{|\varepsilon_a(t)\rangle\}$, with corresponding real eigenvalues (energies) $\{\varepsilon_a(t)\}$, i.e. $H_S(t)|\varepsilon_a(t)\rangle = \varepsilon_a(t)|\varepsilon_a(t)\rangle$, and Bohr frequencies $\omega_{ba}(t) \equiv \varepsilon_b(t) - \varepsilon_a(t)$. As shown in appendix E.1 we can then write the system time evolution operator as:

$$U_S(t,t') = U_S^{\mathrm{ad}}(t,t') + O\left(\frac{h}{\Delta^2 t_f}\right), \tag{37a}$$

$$U_S^{\mathrm{ad}}(t,t') = \sum_a |\varepsilon_a(t)\rangle\langle\varepsilon_a(t')|e^{-i\mu_a(t,t')}, \tag{37b}$$

where $U_S^{\mathrm{ad}}(t,t')$ is the 'ideal' adiabatic evolution operator. It represents a transformation of instantaneous eigenstate $|\varepsilon_a(t')\rangle$ into the later eigenstate $|\varepsilon_a(t)\rangle$, along with a phase

$$\mu_a(t,t') = \int_{t'}^{t} d\tau\, [\varepsilon_a(\tau) - \phi_a(\tau)], \tag{38}$$

where $\phi_a(t) = i\langle\varepsilon_a(t)|\dot{\varepsilon}_a(t)\rangle$ is the Berry connection. The correction term $O\left(\frac{h}{\Delta^2 t_f}\right)$ is derived in appendix E.2.

To achieve our goal of arriving at a master equation expressed in terms of the spectral-density matrix, our basic strategy is to replace the system operator $A_\beta(t-\tau) = U_S^\dagger(t-\tau,0)A_\beta U_S(t-\tau,0)$ with an appropriate adiabatic approximation, which will allow us to take this operator outside the integral. To see how, note first that

$$U_S(t-\tau,0) = U_S(t-\tau,t)U_S(t,0) = U_S^\dagger(t,t-\tau)U_S(t,0). \tag{39}$$

We now make two approximations: firstly, as per equation (37*a*) we replace $U_S(t,0)$ by $U_S^{\mathrm{ad}}(t,0)$; secondly, we replace $U_S^\dagger(t,t-\tau)$ by $e^{i\tau H_S(t)}$, an approximation justified by the appearance of the short-lived bath correlation function $\mathcal{B}_{\alpha\beta}(\tau)$ inside the integrals we are concerned with. Thus, we write

$$U_S(t-\tau,0) = e^{i\tau H_S(t)}U_S^{\mathrm{ad}}(t,0) + \Theta(t,\tau), \tag{40}$$

and find the bound on the error due to dropping $\Theta(t,\tau)$ in appendix F. Let

$$\mu_{ba}(t,t') \equiv \mu_b(t,t') - \mu_a(t,t'), \tag{41a}$$

$$\Pi_{ab}(t) \equiv |\varepsilon_a(t)\rangle\langle\varepsilon_b(t)|. \tag{41b}$$

Neglecting the operator-valued correction term $\Theta(t,\tau)$ entirely, we have, upon substituting equation (37*b*) and using $e^{i\tau H_S(t)}|\varepsilon_a(t)\rangle = e^{i\tau\varepsilon_a(t)}|\varepsilon_a(t)\rangle$, that

$$\int_0^\infty d\tau\, A_\beta(t-\tau)\tilde{\rho}_S(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) \tag{42a}$$

$$\approx \int_0^\infty d\tau\, U_S^{\mathrm{ad}\dagger}(t,0)e^{-i\tau H_S(t)}A_\beta\, e^{i\tau H_S(t)}U_S^{\mathrm{ad}}(t,0)\tilde{\rho}_S(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) \tag{42b}$$

$$= \int_0^\infty \mathrm{d}\tau \sum_{ab} \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} |\varepsilon_a(0)\rangle\langle\varepsilon_a(t)|\mathrm{e}^{-\mathrm{i}\tau H_\mathrm{S}(t)} A_\beta \mathrm{e}^{\mathrm{i}\tau H_\mathrm{S}(t)} |\varepsilon_b(t)\rangle\langle\varepsilon_b(0)|\tilde{\rho}_\mathrm{S}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \quad (42c)$$

$$= \sum_{ab} \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} |\varepsilon_a(0)\rangle\langle\varepsilon_a(t)|A_\beta|\varepsilon_b(t)\rangle\langle\varepsilon_b(0)|\tilde{\rho}_\mathrm{S}(t) A_\alpha(t) \int_0^\infty \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\tau[\varepsilon_b(t)-\varepsilon_a(t)]} \mathcal{B}_{\alpha\beta}(\tau), \quad (42d)$$

where the approximation in (42*a*) is shown in appendix F to be $O[\tau_\mathrm{B} \min\{1, \frac{h}{\Delta^2 t_\mathrm{f}} + \frac{\tau_\mathrm{B}^2 h}{t_\mathrm{f}}\}]$. The first term, $\frac{h}{\Delta^2 t_\mathrm{f}}$, is the smallness parameter of the adiabatic approximation, which we have already assumed to be small. The second term, $\frac{\tau_\mathrm{B}^2 h}{t_\mathrm{f}}$ (mentioned in equation (34)), is new, and its smallness is associated with changes in the instantaneous energy eigenbasis relative to τ_B. We are interested in the regime where both terms are small.

Thus, to the same level of approximation

$$\int_0^\infty \mathrm{d}\tau A_\beta(t-\tau)\tilde{\rho}_\mathrm{S}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \approx \sum_{ab} \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} A_{\beta ab}(t) \Pi_{ab}(0) \tilde{\rho}_\mathrm{S}(t) A_\alpha(t) \Gamma_{\alpha\beta}(\omega_{ba}(t)), \quad (43)$$

where

$$A_{\alpha ab}(t) \equiv \langle\varepsilon_a(t)|A_\alpha|\varepsilon_b(t)\rangle = A^*_{\alpha ba}(t), \quad (44)$$

and $\Gamma_{\alpha\beta}(\omega_{ba}(t))$ is the spectral-density matrix defined in equation (14). Similarly, we have for the other term

$$\int_0^\infty \mathrm{d}\tau A_\alpha(t) A_\beta(t-\tau)\tilde{\rho}_\mathrm{S}(t) \mathcal{B}_{\alpha\beta}(\tau) \approx \sum_{ab} \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} A_{\beta ab}(t) A_\alpha(t) \Pi_{ab}(0) \tilde{\rho}_\mathrm{S}(t) \Gamma_{\alpha\beta}(\omega_{ba}(t)). \quad (45)$$

4.2. Master equations in the adiabatic limit

We are now ready to put everything together. Starting from the Born–Markov master equation constructed from equations (9) and (13), and using the approximations (43) and (45), we arrive at the following *one-sided adiabatic interaction picture master equation*:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_\mathrm{S}(t) = g^2 \sum_{ab} \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} \sum_{\alpha\beta} \Gamma_{\alpha\beta}(\omega_{ba}(t)) A_{\beta ab}(t) \left[\Pi_{ab}(0)\tilde{\rho}_\mathrm{S}(t), A_\alpha(t)\right] + \mathrm{h.c.} \quad (46)$$

Since we used an adiabatic approximation for $A_\beta(t-\tau)$, it makes sense to do the same for $A_\alpha(t)$, i.e. to replace the latter with $U_\mathrm{S}^{\mathrm{ad}\dagger}(t,0) A_\alpha U_\mathrm{S}^\mathrm{ad}(t,0)$. If this is done, we obtain the *double-sided adiabatic interaction picture master equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_\mathrm{S}(t) = g^2 \sum_{abcd} \mathrm{e}^{-\mathrm{i}[\mu_{dc}(t,0)+\mu_{ba}(t,0)]} \sum_{\alpha\beta} \Gamma_{\alpha\beta}(\omega_{ba}(t)) A_{\alpha cd}(t) A_{\beta ab}(t) \left[\Pi_{ab}(0)\tilde{\rho}_\mathrm{S}(t), \Pi_{cd}(0)\right] + \mathrm{h.c.} \quad (47)$$

It is convenient to transform back into the Schrödinger picture. Using $\tilde{\rho}_\mathrm{S}(t) = U_\mathrm{S}^\dagger(t,0)\rho_\mathrm{S}(t)U_\mathrm{S}(t,0)$ (equation (6)) implies that $\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_\mathrm{S}(t) = U_\mathrm{S}^\dagger(t,0)\left(\mathrm{i}[H_\mathrm{S}(t), \rho_\mathrm{S}(t)] + \frac{\mathrm{d}}{\mathrm{d}t}\rho_\mathrm{S}(t)\right) U_\mathrm{S}(t,0)$. Hence, using equation (46), we find the *one-sided adiabatic Schrödinger picture master equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_\mathrm{S}(t) = -\mathrm{i}[H_\mathrm{S}(t), \rho_\mathrm{S}(t)] + g^2 \sum_{ab}\sum_{\alpha\beta} \Gamma_{\alpha\beta}(\omega_{ba}(t)) \left[L'_{ab,\beta}(t)\rho_\mathrm{S}(t), A_\alpha\right] + \mathrm{h.c.}, \quad (48)$$

where

$$L'_{ab,\beta}(t) = \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,0)} A_{\beta ab}(t) U_{\mathrm{S}}(t,0) \Pi_{ab}(0) U_{\mathrm{S}}^{\dagger}(t,0). \tag{49}$$

This form of the master equation has not appeared in previous studies of adiabatic master equations. If we again use the adiabatic approximation for $U_{\mathrm{S}}(t,0)$, i.e. replace $U_{\mathrm{S}}(t,0)\Pi_{ab}(0)U_{\mathrm{S}}^{\dagger}(t,0)$ by $U_{\mathrm{S}}^{\mathrm{ad}\dagger}(t,0)\Pi_{ab}(0)U_{\mathrm{S}}^{\mathrm{ad}}(t,0)$, we obtain the *double-sided adiabatic Schrödinger picture master equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -\mathrm{i}\,[H_{\mathrm{S}}(t), \rho_{\mathrm{S}}(t)] + g^2 \sum_{\alpha\beta}\sum_{ab} \Gamma_{\alpha\beta}(\omega_{ba}(t)) \left[L_{ab,\beta}(t)\rho_{\mathrm{S}}(t), A_{\alpha}\right] + \mathrm{h.c.}, \tag{50}$$

where

$$L_{ab,\alpha}(t) \equiv A_{\alpha ab}(t)|\varepsilon_a(t)\rangle\langle\varepsilon_b(t)| = L_{ba,\alpha}^{\dagger}(t). \tag{51}$$

Comparing to equation (25), the first term in equations (48) and (50) is $\mathcal{L}_{\mathrm{uni}}(t)$, while the second is $\mathcal{L}_{\mathrm{diss}}^{\mathrm{ad}}(t)$.

The master equations we have found so far are not in Lindblad form, and hence do not guarantee the preservation of positivity of ρ_{S}. We thus introduce an additional approximation, which will transform the master equations into completely positive form.

4.3. Master equation in the adiabatic limit with rotating wave approximation: Lindblad form

In order to arrive at a master equation in Lindblad form, we can perform a RWA. To do so, let us revisit the $t \to \infty$ limit taken in the Markov approximation in equation (13). Supposing we do not take this limit quite yet, we can follow the same arguments leading to equation (42*c*), which we rewrite, along with the adiabatic approximation $A_{\alpha}(t) \approx U_{\mathrm{S}}^{\mathrm{ad}\dagger}(t,0)A_{\alpha}U_{\mathrm{S}}^{\mathrm{ad}}(t,0)$. This yields

$$\int_0^t \mathrm{d}\tau\, A_{\beta}(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)A_{\alpha}(t)\mathcal{B}_{\alpha\beta}(\tau) \tag{52a}$$

$$\approx \int_0^t \mathrm{d}\tau \sum_{abcd} \mathrm{e}^{-\mathrm{i}[\mu_{ba}(t,0)+\mu_{dc}(t,0)]} |\varepsilon_a(0)\rangle\langle\varepsilon_a(t)|A_{\beta}|\varepsilon_b(t)\rangle\langle\varepsilon_b(0)|\tilde{\rho}_{\mathrm{S}}(t)|\varepsilon_c(0)\rangle$$

$$\times \langle\varepsilon_c(t)|A_{\alpha}|\varepsilon_d(t)\rangle\langle\varepsilon_d(0)|\mathrm{e}^{\mathrm{i}\tau\omega_{ba}(t)}\mathcal{B}_{\alpha\beta}(\tau). \tag{52b}$$

We note that $\mu_{dc}(t,0) + \mu_{ba}(t,0) = \int_0^t \mathrm{d}\tau\,[\omega_{dc}(\tau) + \omega_{ba}(\tau) - (\phi_d(\tau) - \phi_c(\tau)) + (\phi_b(\tau) - \phi_a(\tau))]$. One can now make the argument that when the $t \to \infty$ limit is taken, terms for which the integrand vanishes will dominate, thus enforcing the 'energy conservation' condition $b = c$ and $a = d$, or $c = d$ and $a = b$ (without over-counting the case $a = b = c = d$). This is a similar RWA as made in the standard time-independent treatment, although here, the approximation of phase cancelation is made along the entire time evolution of the instantaneous energy eigenstates. Clearly, in light of the appearance of other terms involving t in equation (52*b*), this argument is far from rigorous. Nevertheless, we proceed from equation (52*b*) to write, in the $t \to \infty$ limit,

$$\int_0^t \mathrm{d}\tau\, A_{\beta}(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)A_{\alpha}(t)\mathcal{B}_{\alpha\beta}(\tau) \approx \sum_{a\neq b} A_{\beta ab}(t)A_{\alpha ba}(t)\Pi_{ab}(0)\tilde{\rho}_{\mathrm{S}}(t)\Pi_{ba}(0)\Gamma_{\alpha\beta}(\omega_{ba}(t))$$

$$+ \sum_{ab} A_{\beta aa}(t)A_{\alpha bb}(t)\Pi_{aa}(0)\tilde{\rho}_{\mathrm{S}}(t)\Pi_{bb}(0)\Gamma_{\alpha\beta}(0). \tag{53}$$

We show in appendix G how, by performing a transformation back to the Schrödinger picture, along with a double-sided adiabatic approximation, we arrive from equation (53) at the *Schrödinger picture adiabatic master equation in Lindblad form*:

$$\dot{\rho}_{\rm S}(t) = -{\rm i}\,[H_{\rm S}(t) + H_{\rm LS}(t),\, \rho_{\rm S}(t)] \tag{54a}$$

$$+\sum_{\alpha\beta}\sum_{a\neq b}\gamma_{\alpha\beta}(\omega_{ba}(t))\left[L_{ab,\beta}(t)\rho_{\rm S}(t)L^{\dagger}_{ab,\alpha}(t) - \frac{1}{2}\left\{L^{\dagger}_{ab,\alpha}(t)L_{ab,\beta}(t),\, \rho_{\rm S}(t)\right\}\right] \tag{54b}$$

$$+\sum_{\alpha\beta}\sum_{ab}\gamma_{\alpha\beta}(0)\left[L_{aa,\beta}(t)\rho_{\rm S}(t)L^{\dagger}_{bb,\alpha}(t) - \frac{1}{2}\left\{L^{\dagger}_{aa,\alpha}(t)L_{bb,\beta}(t),\, \rho_{\rm S}(t)\right\}\right], \tag{54c}$$

where the Hermitian Lamb shift term is

$$H_{\rm LS}(t) = \sum_{\alpha\beta}\left[\sum_{a\neq b}L^{\dagger}_{ab,\alpha}(t)L_{ab,\beta}(t)S_{\alpha\beta}(\omega_{ba}(t)) + \sum_{ab}L^{\dagger}_{aa,\alpha}(t)L_{bb,\beta}(t)S_{\alpha\beta}(0)\right]. \tag{55}$$

Since the bath correlations are of positive type, it follows from Bochner's theorem that the matrix γ—the Fourier transform of the bath correlation functions—is also positive [30]. Therefore, this Lindblad form for our master equation guarantees the positivity of the density matrix.

We emphasize that equations (48), (50) and (54) all generalize both the standard Redfield and Lindblad time-independent Hamiltonian results to the case of a time-dependent Hamiltonian in the adiabatic limit[8]. The time-independent result can easily be recovered by simply freezing the time dependence of the Hamiltonian, energy eigenvalues and eigenvectors. To see this explicitly, let us restrict ourselves to the Lindblad case. The sum over the energy eigenvalues can be replaced by the sum over their differences, such that:

$$\sum_{a,b}\to\sum_{\omega},\quad L_{ab,\alpha}\to A_{\omega,\alpha} = \sum_{\varepsilon_b-\varepsilon_a=\omega}|\varepsilon_a\rangle\langle\varepsilon_a|A_\alpha|\varepsilon_b\rangle\langle\varepsilon_b|,\quad \omega_{ba}\to\omega. \tag{56}$$

The resulting equation becomes:

$$\dot{\rho}_{\rm S}(t) = -{\rm i}\,[H_{\rm S}+H_{\rm LS},\,\rho(t)] + \sum_{\alpha\beta}\sum_{\omega}\gamma_{\alpha\beta}(\omega)\left(A_{\omega,\beta}\rho_{\rm S}(t)A^{\dagger}_{\omega,\alpha} - \frac{1}{2}\left\{A^{\dagger}_{\omega,\alpha}A_{\omega,\beta},\,\rho_{\rm S}(t)\right\}\right), \tag{57}$$

which is the standard form for the time-independent Lindblad master equation. This should make the physical meaning of our derivation evident. We have systematically generalized the time-independent result such that the Lindblad operators now rotate with the (adiabatically) changing energy eigenstates, which makes them time-dependent. This is a non-trivial difference, as it encodes an important physical effect: *the dissipation/decoherence of the system occurs in the instantaneous energy eigenbasis*.

Equations (50) and (54) are the two master equations we use for numerical simulations presented later in this paper. We note that equation (54) appears similar to the Markovian adiabatic master equation found in [24], but is more general and did not require the assumption of periodic driving.

[8] See for example equation (3.143) in [30] and equation (8.1.33) in [35].

4.4. Non-adiabatic corrections to the master equations

So far, we assumed the adiabatic limit of evolution of the system (see equation (37*a*)). The adiabatic perturbation theory we review in appendix E.1 allows us to compute systematic non-adiabatic corrections to the master equations we have derived. This perturbation theory is essentially an expansion in powers of $1/t_{\rm f}$, and we rederive in appendix E.1 the well known result [5] that to first order

$$U_{\rm S}(t,t') = U_{\rm S}^{\rm ad}(t,t')\left[\mathbb{I} + V_1(t,t')\right], \tag{58}$$

where

$$V_1(t,t') = -\sum_{a\neq b} |\varepsilon_a(t')\rangle\langle\varepsilon_b(t')| \int_{t'}^{t} {\rm d}\tau {\rm e}^{-{\rm i}\mu_{ba}(\tau,t')}\langle\varepsilon_a(\tau)|\dot{\varepsilon}_b(\tau)\rangle. \tag{59}$$

Thus, to derive the lowest order non-adiabatic corrections to our master equations is a matter of repeating our calculations of sections 4.1 and 4.3 with $U_{\rm S}^{\rm ad}(t,t')$ replaced everywhere by the first order term $U_{\rm S}^{\rm ad}(t,t')V_1(t,t')$, and adding the result to the zeroth order master equations we have already derived. Rather than actually computing these corrections, let us estimate when they are important.

The condition under which the zeroth order adiabatic approximation is accurate is equation (27), which is now replaced by

$$\frac{h}{t_{\rm f}} \lesssim \Delta^2, \tag{60}$$

i.e. with the $\ll$ replaced by a mere $\lesssim$. However, we would still like to perform the approximation of equation (40), in the sense that $U_{\rm S}(t-\tau,0) \approx {\rm e}^{{\rm i}\tau H_{\rm S}(t)} U_{\rm S}^{\rm ad}(t,t')\left[\mathbb{I} + V_1(t,t')\right]$. This still requires

$$\frac{h}{t_{\rm f}} \ll \frac{1}{\tau_{\rm B}^2}, \tag{61}$$

which is what allows the use of ${\rm e}^{{\rm i}\tau H_{\rm S}(t)}$ in this approximation (as shown in appendix F). Taken together, these two conditions are weaker than equation (35), which we can rewrite as $\frac{h}{t_{\rm f}} \ll \min(\Delta^2, \frac{1}{\tau_{\rm B}^2})$.

Recall that to ensure the validity of the Markov approximation and $\|\mathcal{L}_{\rm uni}\| \gg \|\mathcal{L}_{\rm diss}^{\rm ad}\|$, we also had to demand the inequalities in equations (31) and (33); these can be now summarized as $\max\left(g, \frac{g^2}{\Delta}\right) \ll \frac{1}{\tau_{\rm B}}$, to be compared with equation (61).

5. An illustrative example: transverse field Ising chain coupled to a boson bath

5.1. The model

We proceed to use our master equations to study the evolution of the Ising Hamiltonian with transverse field

$$H_{\rm S}(t) = A(t)H_{\rm S}^X + B(t)H_{\rm S}^Z, \tag{62a}$$

$$H_{\rm S}^X \equiv \sum_{i=1}^{N} \sigma_i^x, \tag{62b}$$

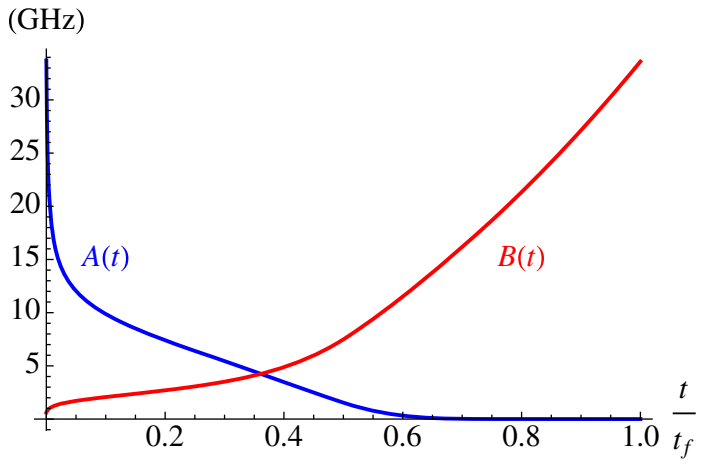

Figure 1. The $A(t)$ and $B(t)$ functions in equation (62*a*). $A(0) = 33.7\,\text{GHz}$.

$$H_S^Z \equiv -\sum_{i=1}^{N} h_i \sigma_i^z + \sum_{i,j=1}^{N} J_{ij} \sigma_i^z \sigma_j^z, \tag{62c}$$

where the functions $A(t)$ and $B(t)$ are shown in figure 1, and were chosen for concreteness to describe the interpolation between the transverse field and Ising term in the D-Wave Rainier chip [2]. This is a system which begins with the transverse magnetic field H_S^X turned on while the Ising term H_S^Z is turned off, and then slowly switches between the two.

We couple this spin-system to a bath of harmonic oscillators, with bath and interaction Hamiltonian

$$H_B = \sum_{k=1}^{\infty} \omega_k b_k^\dagger b_k, \quad H_I = \sum_{i=1}^{N} \sigma_i^z \otimes B_i, \quad B_i = \sum_k g_k^i \left(b_k^\dagger + b_k \right), \tag{63}$$

where $b_k^\dagger$ and b_k are, respectively, raising and lowering operators for the kth oscillator with natural frequency ω_k, and g_k^j is the corresponding coupling strength to spin j. This is the standard pure dephasing spin-boson model [36], except that our system is time-dependent. The resulting form for our operator L (equation (51)) is

$$L_{ab,i} = |\varepsilon_a(t)\rangle\langle\varepsilon_a(t)|\sigma_i^z|\varepsilon_b(t)\rangle\langle\varepsilon_b(t)| = A_{iab}(t)|\varepsilon_a(t)\rangle\langle\varepsilon_b(t)|. \tag{64}$$

Recall that our analysis assumed that the bath is in thermal equilibrium at inverse temperature $\beta = 1/(k_B T)$, and hence is described by a thermal Gibbs state $\rho_B = \exp(-\beta H_B)/\mathcal{Z}$. We show in appendix H that this yields

$$\gamma_{ij}(\omega) = \frac{2\pi J(|\omega|)}{1 - e^{-\beta|\omega|}} g^i_{|\omega|} g^j_{|\omega|} (\Theta(\omega) + e^{-\beta|\omega|}\Theta(-\omega)) \tag{65a}$$

$$S_{ij}(\omega_{ba}(t)) = \int_0^\infty d\omega \frac{J(\omega)}{1 - e^{-\beta\omega}} g^i_\omega g^j_\omega \left(\mathcal{P}\left(\frac{1}{\omega_{ba}(t) - \omega} \right) + e^{-\beta\omega} \mathcal{P}\left(\frac{1}{\omega_{ba}(t) + \omega} \right) \right), \tag{65b}$$

where only one of the Heaviside functions is non-zero at $\omega = 0$. To complete the model specification, we assume an Ohmic bath spectral function

$$J(\omega) = \eta\omega\, \mathrm{e}^{-\omega/\omega_\mathrm{c}}, \tag{66}$$

where ω_c is a high-frequency cutoff and η is a positive constant with dimensions of time squared.

It is often stated that the terms associated with the Lamb shift H_LS (equation (55)), i.e. equation (65*b*), can be neglected, since the relative order of S and H_S is $g^2\tau_\mathrm{B}/\Delta$, and indeed we have assumed $g^2\tau_\mathrm{B}/\Delta \ll 1$ (equation (31)). However, this argument is misleading for two reasons. Firstly, S can be divergent, as is easy to see in the limit $\omega_\mathrm{c} = \infty$ for the Ohmic model (66), where for $\omega \gg \max_{ba} \omega_{ba}(t)$, the integrand tends to a constant. Secondly, S should be compared to γ, as both are of the same order $g^2\tau_\mathrm{B}$, and both result in changes to the system relative to its unperturbed state. Indeed, in the interaction picture with respect to $H_\mathrm{S} + H_\mathrm{LS}$ (recall equation (54*a*)), the overall transition rates between states with quantum numbers a and b will depend on the dressed (i.e. shifted) energy gaps $\omega_{ba} + \omega_{ba}^\mathrm{LS}$. The importance of this Lamb shift effect was also stressed by de Vega *et al* [32]. We analyze the Lamb shift effect in section 5.3.

Finally, we note that although the harmonic oscillators bath with linear coupling to the system provides a γ matrix that satisfies the KMS condition, it is important to note that this model has infrared singularities that destroy the ground state of the total system [37]. The KMS condition assumes a stable ground state and stable thermal states, which our underlying spin-boson model violates. However, for the purposes of our work, a γ matrix that satisfies the KMS condition will suffice without too much concern about how it is derived.

5.2. *Correlation function analysis*

In light of the subtleties alluded to in section 2.3 associated with satisfying the KMS condition, we analyze the different timescales determining the behavior of the Ohmic correlation function in this subsection. Removing the ω dependence from the g's in equation (65*a*) and substituting $J(\omega)$ from equation (66), it is possible to compute the bath correlation function analytically for the resulting

$$\gamma_{ab}(\omega) = \frac{2\pi\omega\, \mathrm{e}^{-|\omega|/\omega_\mathrm{c}}}{1 - \mathrm{e}^{-\beta\omega}} g^a g^b, \tag{67}$$

by inverse Fourier transform of equation (16*a*). The result is

$$\mathcal{B}_{ab}(\tau) = \frac{\eta}{\beta^2} g^a g^b \left(\psi^{(1)}\left(\frac{1}{\beta\omega_\mathrm{c}} + \frac{\mathrm{i}\,\tau}{\beta} \right) + \psi^{(1)}\left(1 + \frac{1}{\beta\omega_\mathrm{c}} - \frac{\mathrm{i}\,\tau}{\beta} \right) \right), \tag{68}$$

where $\psi^{(m)}$ is the mth Polygamma function (see appendix I for the derivation). We first assume

$$\beta\omega_\mathrm{c} \gg 1, \tag{69}$$

and consider an expansion in large $\beta\omega_\mathrm{c}$:

$$\mathcal{B}_{ab}(\tau) = \frac{\eta}{\beta^2} g^a g^b \left(-\pi^2 \mathrm{csch}^2\left(\frac{\pi\tau}{\beta} \right) + \sum_{n=1}^{\infty} \frac{\psi^{(n)}\left(1 - \frac{\mathrm{i}\,\tau}{\beta}\right) + \psi^{(n)}\left(\frac{\mathrm{i}\,\tau}{\beta}\right)}{(n-1)!\,(\beta\omega_\mathrm{c})^n} \right), \tag{70}$$

followed by an expansion in large τ/β:

$$\mathcal{B}_{ab}(\tau) = \frac{\eta}{\beta^2} g^a g^b \left(-4\pi^2 \mathrm{e}^{-\tau/\tau_\mathrm{B}} + \frac{1}{(\tau/\tau_M)^2} + O\left(\mathrm{e}^{-2\tau/\tau_\mathrm{B}}, \tau^{-3} \right) \right). \tag{71}$$

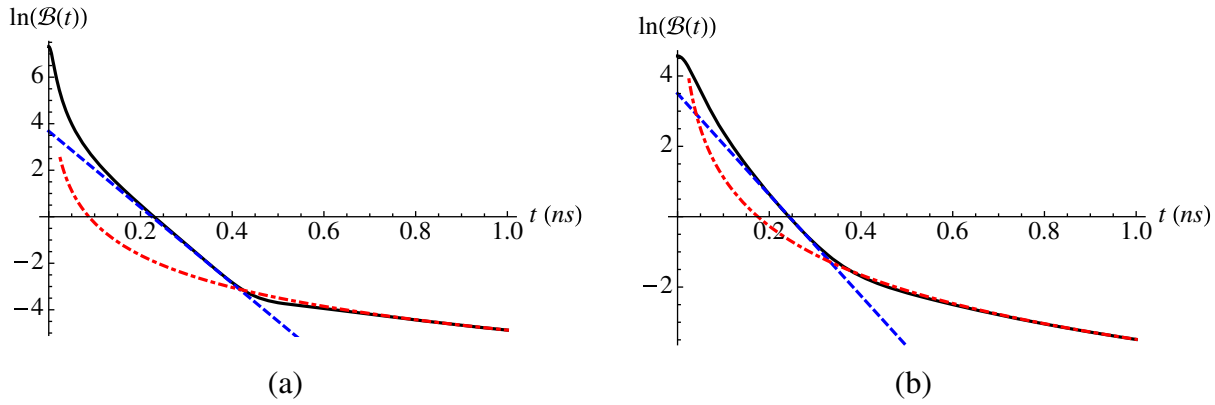

Figure 2. (a) An example of the bath correlation function $\mathcal{B}_{ab}(\tau)$ for $\beta = 2.6^{-1}$ ns and $\omega_c = 32\pi$ GHz. The solid black curve is the function $\ln|\mathcal{B}_{ab}(\tau)|$. The blue dashed curve is the function $\ln 4\pi^2 \exp(-2\pi\tau/\beta)$ and the red dot-dashed curve is the function $\ln 2\beta\tau^{-2}/\omega_c$. (b) Same as in (a), but $\omega_c = 8\pi$ GHz, and the blue dashed curve is the function $\ln d_0 \exp(-(2\pi/\beta + c_1\omega_c + c_2\omega_c^2\beta)\tau)$ with $c_1 \approx -0.039$, $c_2 \approx -0.004$, $d_0 \approx 33.13$. (a) $\omega_c = 32\pi$ GHz, (b) $\omega_c = 8\pi$ GHz.

This expansion reveals the two independent time-scales that are relevant for us. First, there is the time scale τ_B associated with the exponential decay (corresponding to the true Markovian bath), given by:

$$\tau_B \overset{\omega_c\to\infty}{\longrightarrow} \tau'_B = \frac{\beta}{2\pi}, \tag{72}$$

then the time scale associated with non-Markovian corrections (the power-law tail):

$$\tau_M = \sqrt{\frac{2\beta}{\omega_c}}. \tag{73}$$

For sufficiently large ω_c, these two time scales capture the two types of behavior found in $\mathcal{B}_{ab}(\tau)$, as illustrated in figure 2(a).

The transition between the exponential decay and the power-law tail occurs at a time τ_{tr} given by $4\pi^2 e^{-\tau_{tr}/\tau'_B} = (\frac{\tau_M}{\tau_{tr}})^2$, or equivalently by

$$\frac{\exp(\theta)}{\theta^2} = \frac{1}{2}\beta\omega_c, \qquad \theta \equiv 2\pi\frac{\tau_{tr}}{\beta}. \tag{74}$$

This transcendental equation has a formal solution in terms of the Lambert-W function [38], i.e. the inverse function of $f(W) = We^W$, as can be seen by changing variables to $y = -\theta/n$, and rewriting $\theta^n e^{-\theta} = a \equiv 2/(\beta\omega_c)$ as $ye^y = -a^{1/n}/n$, whose solution is $\theta = -ny = -nW(-\frac{1}{n}a^{1/n})$. However, for our purposes the following observations will suffice. We seek a Markovian-like solution, where τ_{tr} is large compared to the thermal timescale set by β, i.e. we are interested in the regime where $\theta \gg 1$. In this case we can neglect θ^2 compared to e^θ, and approximate the solution to equation (74) by $\theta \sim \ln(\beta\omega_c/2)$. Thus

$$\tau_{tr} \sim \beta \ln(\beta\omega_c). \tag{75}$$

This agrees with the first term of the asymptotic expansion $W(x) = \ln(x) - \ln\ln(x) + \frac{\ln\ln(x)}{\ln(x)} + \cdots$, which is accurate for $x \gtrsim 3$ [38].

When $\beta\omega_c \gg 1$ is not strictly satisfied, the exponential regime is less pronounced, and τ_B' is corrected by powers of ω_c. By dimensional analysis, the corrections must be of the form:

$$\tau_B = \tau_B' + \sum_{n=1}^{\infty} \frac{c_n}{\omega_c^n \beta^{n-1}}, \tag{76}$$

where c_n are constants of order one that must be fitted (see figure 2(b)).

The implications of this cutoff-induced transition for our perturbation theory inequalities are explored in appendix F, where we show that a sufficient condition for the theory to hold is

$$\frac{1}{\omega_c \ln(\beta\omega_c)} < \min\left\{2\tau_B, \frac{\tau_B h}{\Delta^2 t_f} + \frac{\tau_B^3 h}{t_f}\right\}, \tag{77}$$

which can be interpreted as saying that the cutoff should be the largest energy scale. Equation (77) joins the list of inequalities given in section 3 as an additional special condition that applies in the Ohmic case, along with $\beta\omega_c \gg 1$.

5.3. Numerical results

For concreteness, we take $g_\omega^i = g$, $\omega_c = 8\pi$ GHz and $T = 20\,\text{mK} \approx 2.6\,\text{GHz}$ (in units such that $\hbar = 1$; this is the operating temperature of the D-Wave Rainier chip [2]), corresponding to $\tau_B = 0.06\,\text{ns}$ for the Ohmic model with infinite cutoff, equation (72), and $\tau_B \approx 0.07\,\text{ns}$ for $\omega_c = 8\pi$ using equation (76). For this value of ω_c the transition between the exponential and power-law regimes is still sharp (see figure 2(b)) and occurs at approximately $\tau_{tr} = 0.33\,\text{ns}$. For these values, we satisfy at least one of the cases from equation (77), including numerical prefactors: $\frac{1}{\omega_c \ln(\beta\omega_c)} < 2\tau_B$.

We focus on the $N = 8$ site ferromagnetic chain with parameters:

$$h_0 = \frac{1}{4}, \quad h_{i>0} = 0, \quad J_{i,i+1} = -1, \quad i = 0, \ldots, 7, \tag{78}$$

where we pin the first spin in order to break the degeneracy in the ground state of the classical Ising Hamiltonian. The system is initialized in the Gibbs state:

$$\rho_S(t=0) = \frac{e^{-\beta H_S(0)}}{\mathcal{Z}}. \tag{79}$$

To help the numerics, we truncate our system to the lowest $n = 18$ levels (out of 256), rotating the density matrix into the instantaneous energy eigenbasis at each time step. The error associated with this is small as long as our evolution does not cause scattering into higher n states, as we have checked. The forward propagation algorithm used is an implicit second order Runge–Kutte method called TR-BDF2 with an adaptive time step [39, 40].

Figure 3 presents our results for the evolution of the system described in the previous subsection. We computed the overlap between the instantaneous ground state of $H_S(t)$ and the instantaneous density matrix predicted by our two master equations (50) (non-RWA) and (54) (RWA). Although our two master equations predict different numerical values for this overlap, the qualitative features of the evolution are the same. We observe a generic feature of four distinct regions of the evolution: a gapped phase (labeled '1' in figure 3), an excitation phase (labeled '2'), a relaxation phase (labeled '3'), and finally a frozen phase (labeled '4'). We elaborate on these regions in the following subsection. Furthermore, we observe that the larger t_f (therefore more adiabatic) evolution shows a smaller difference between the two master

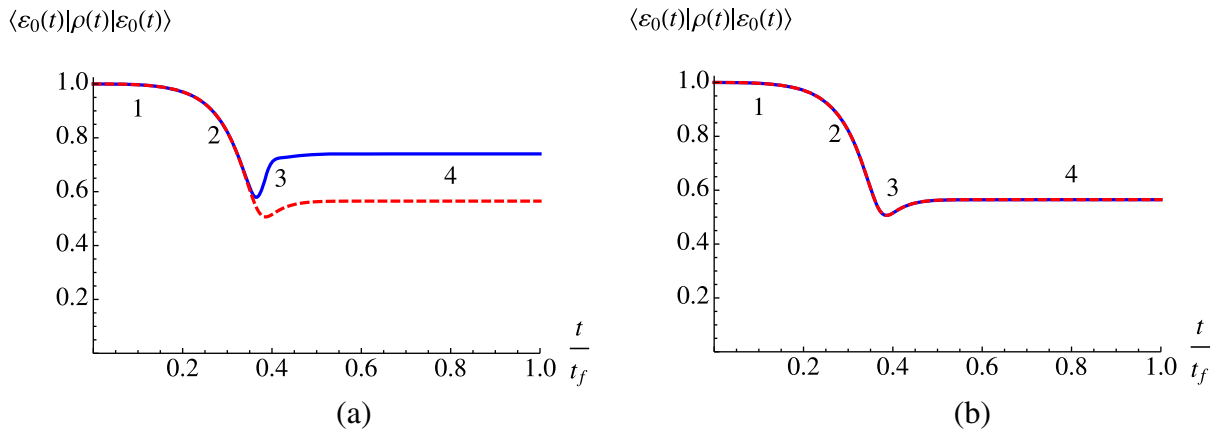

Figure 3. Fidelity, or overlap of the system density matrix with the instantaneous ground state along the time evolution for $t_f = 10\,\mu$s and $\eta g^2/(\hbar^2) = 1.2 \times 10^{-4}/(2\pi)$. The solid blue curve was calculated using equation (50) (no RWA), while the dashed red curve was calculated using equation (54) (Lindblad form, after the RWA). Four phases are indicated: thermal (1), excitation (2), relaxation (3) and frozen (4). Panel (a) includes the Lamb shift terms, while (b) excludes them.

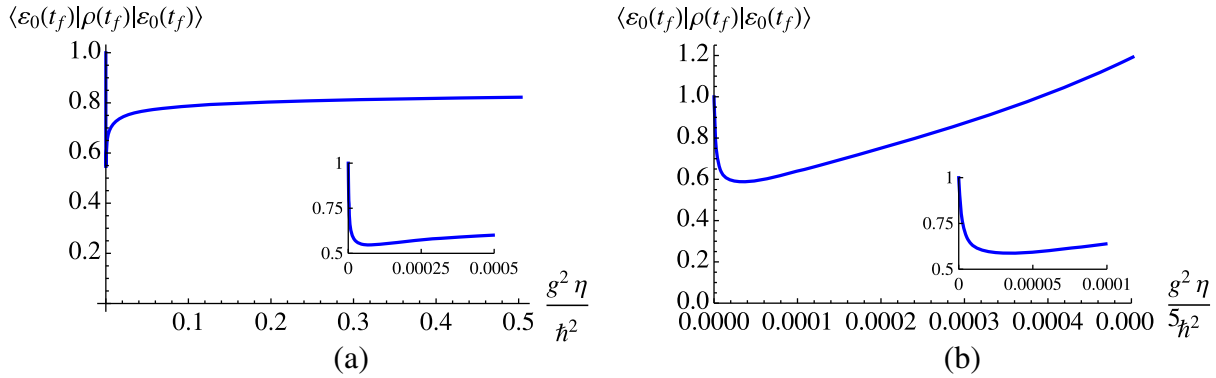

Figure 4. Dependence of the fidelity at $t_f = 10\,\mu$s on the coupling strength to the thermal bath is varied using our two master equations. The insets are closeups of the behavior near zero coupling. (a) RWA, (b) non-RWA.

equations for the final fidelity. The results in figure 3 illustrate the importance of the Lamb shift. We find that while its effect is small in the RWA, its effect is relatively large in the non-RWA.

In order to study the importance of the relaxation phase, we can study the behavior of the fidelity at $t = t_f$ as we change the coupling strength g. We observe (see figure 4) that there is a rapid drop in fidelity from the closed system result as soon as the coupling to the thermal bath is turned on, but there is a subsequent steady increase in the fidelity as the coupling strength is further increased. This increase in fidelity is a direct consequence of the higher importance of the relaxation phase (made possible by the increasing coupling strength) in restoring the probability of being in the ground state. However, we also observe that there is a very pronounced difference between the behavior of the results from the two master equations as the coupling is increased.

In the case of the Lindblad equation, the fidelity saturates, whereas for the non-RWA equation, we see an increase in fidelity and a subsequent violation of positivity. These results bring to light the relative advantages and disadvantages of both master equations. For the Lindblad equation, positivity of the density matrix is guaranteed, but it clearly is not capturing the physics associated with the increasing importance of the thermal relaxation that the non-RWA equation captures. However, the non-RWA equation fails to preserve positivity of the density matrix so it is unable to reliably describe the system at higher coupling strength. Others have also noted that the RWA and non-RWA can lead to physically different conclusions, e.g. in the context of Berry phases in cavity QED [41].

5.4. The four different phases

5.4.1. Phase 1—the gapped phase. For times sufficiently close to the initial time, the ground state of $H_S(t)$ is the ground state of H_S^X, i.e. the state $|0\rangle \equiv \otimes_{j=1}^N |-\rangle_j$, where $|\pm\rangle_j = (|\downarrow\rangle_j \pm |\uparrow\rangle_j)/\sqrt{2}$ with energy $\varepsilon_0(0) = -NA(0)$, and where $|\downarrow\rangle_j, |\uparrow\rangle_j$ are the $+1, -1$ eigenstates of σ_j^z (computational basis states of the jth spin or qubit). The lowest lying energy states are then the N-fold degenerate states with a single flip of one of the spins in the x-direction, i.e. $|i\rangle \equiv \otimes_{j=1}^{i-1} |-\rangle_j |+\rangle_i \otimes_{j=i+1}^N |-\rangle_j$, with energy $\varepsilon_1(0) = -(N-2)A(0)$. Therefore the gap between the ground state and the first excited states is:

$$\Delta(t) = \varepsilon_1(t) - \varepsilon_0(t) \overset{t \ll t_f}{\approx} [-(N-2)A(t)] - [-NA(t)] = 2A(t), \tag{80}$$

which is at least twice as large as our $k_B T \approx 2.6\,\text{GHz}$, almost until $A(t_c) = B(t_c) \approx 5\,\text{GHz}$ at $t_c \approx 0.35 t_f$ (see figure 1). Noting that $\sigma_i^z |\pm\rangle_i = |\pm\rangle_i$, we can write the following relations in terms of the ground and first excited states:

$$\omega_{i0} = \Delta = -\omega_{0i}, \quad \sigma_i^z |i\rangle = |0\rangle. \tag{81}$$

Noting that $\sigma_i^z |j\rangle$ is a doubly excited state $\forall j \neq i \in \{1, \ldots, N\}$, we truncate the problem to the ground and first excited states only, so that there are just three types of values of $\gamma(\omega)$ we need to consider: $\gamma(0)$, $\gamma(\omega_{i0})$, $\gamma(\omega_{0i})$. Recalling the KMS condition, equation (18), we have

$$\gamma(\omega_{0i}) = \mathrm{e}^{-\beta\omega_{i0}} \gamma(\omega_{i0}), \tag{82}$$

which shows that upward transitions are exponentially suppressed relative to downward transitions, by a factor ranging between $\mathrm{e}^{-2A(0)/(k_B T)} \approx \mathrm{e}^{-67.4/2.6} \approx 7 \times 10^{-12}$ and $\mathrm{e}^{-2A(0.3t_f)/2.6} \approx \mathrm{e}^{-3.8} \approx 0.02$. This explains why for early times (Phase 1) the system hardly deviates from the ground state, which in turn is very close to the thermal state (79).

To make this argument more precise, denoting $\rho_{00} = \langle 0|\rho|0\rangle$ and $\rho_{ii} = \langle i|\rho|i\rangle$, we can write the effective (truncated to the ground and first excited states) Lindblad equation (54) as the simplified rate equations

$$\dot{\rho}_{ii} \approx \gamma_{ii}(\omega_{i0}) \left(-\rho_{ii} + \mathrm{e}^{-\beta\omega_{i0}} \rho_{00}\right), \tag{83a}$$

$$\rho_{00} \approx 1 - N\rho_{ii}, \tag{83b}$$

where we have assumed that the system is initially in the thermal state (79) and the gap is large (relative to $k_B T$). A derivation of equation (83) can be found in appendix J. We compare our simulation results with the results from the above equations in figure 5 and find very good agreement for early times.

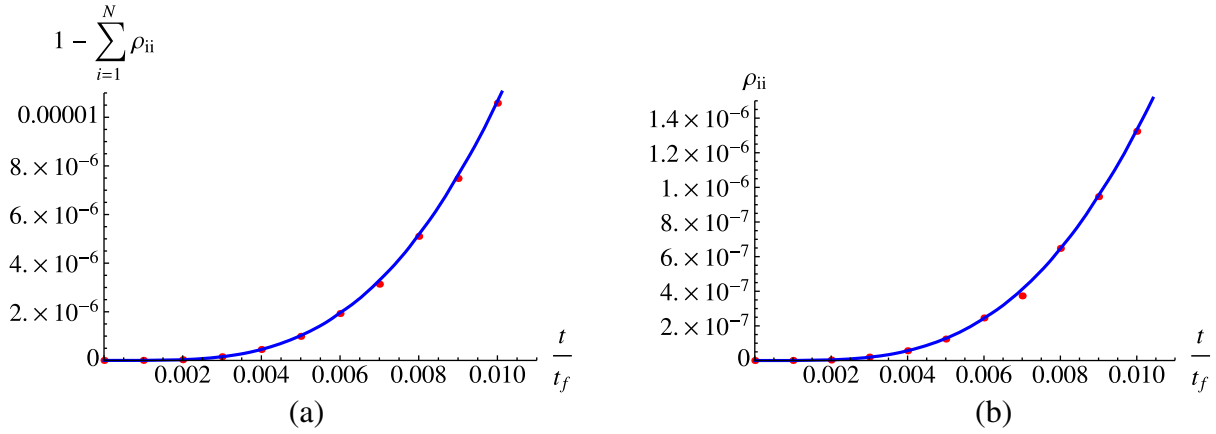

Figure 5. Early evolution of diagonal elements of the system density matrix in the thermal regime. Red dots are from using the Lindblad equation (54), while the solid blue curve is from the solution of equation (83). (a) Ground state, (b) excited states.

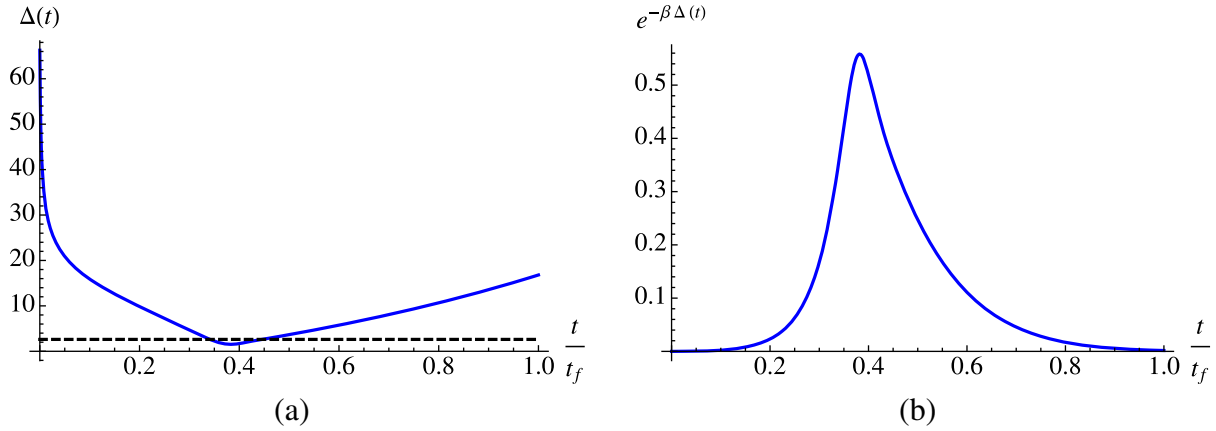

Figure 6. The behavior of the gap and the exponential suppression factor along the time evolution. The dashed line is $k_{\mathrm{B}}T \approx 2.6\,\mathrm{GHz}$. (a) The gap, (b) suppression factor.

5.4.2. Phase 2—the excitation phase. When $A(t)$ becomes small enough such that $\beta\Delta(t) \sim O(1)$, then the KMS condition no longer suppresses excitations from the ground state to higher excited states (see figure 6). If we interpret the master equation as a set of rate equations for the matrix elements of ρ, we can identify the rate of scattering into the ith state from the jth state as being the term in the $\dot{\rho}_{ii}$ equation with coefficient ρ_{jj}. Therefore, we find that the rate of scattering from the ground state to excited states is given by

$$\text{Excitation rate} \propto \gamma(\Delta(t))\mathrm{e}^{-\beta\Delta(t)}\rho_{00}, \tag{84}$$

whereas the relaxation rate is given by

$$\text{Relaxation rate} \propto \gamma(\Delta(t))\rho_{ii}. \tag{85}$$

Therefore, as we emerge from the gapped phase, we have $\rho_{00} \gg \rho_{ii}$, so scattering into excited states dominates over relaxation into the ground state. This explains the loss of fidelity in phase 2.

5.4.3. Phase 3—the relaxation phase. As the gap begins to grow again and the suppression factor shrinks (see figure 6), the KMS condition begins to suppress scattering into higher excited states while allowing relaxation to occur. In our model this causes a resurgence in the overlap with the ground state. Therefore, in this phase, the presence of the thermal bath can actually help to increase the fidelity, as was also observed in [26, 32, 42].

The excitation and relaxation phases reveal the two competing processes for a successful adiabatic computation. If we spend too long in the excitation phase (or if the gap shrinks too fast relative to t_f and the evolution is not adiabatic), the system loses almost all fidelity with the ground state, and the system would have to spend a very long time in the relaxation phase to recover some of that fidelity.

However, we stress that fidelity recovery will not be observed if the population becomes distributed over a large number of excited states in the excitation phase. This would happen, e.g., if when the gap closes there is an exponential number of states close to the ground state, such as in the quantum Ising chain with alternating sector interaction defects [43]. To see this more explicitly in the context of our analysis, note from equation (83*b*) that if there is an exponential number N of ρ_{ii} coupled to ρ_{00} (i.e. N is an exponentially large fraction of the dimension of the system Hilbert space), then ρ_{00} decreases exponentially. By equation (84) this means that all ρ_{ii} become exponentially small, but not zero. In phase 3, by equation (85), the relaxation is suppressed as long as the gap is not very large, because the relaxation is proportional to ρ_{ii}, which is exponentially small. This analysis presumes that the system–bath Hamiltonian has non-negligible coupling between the ground and excited states, i.e. that $|\langle 0|\sigma_\beta^z|i\rangle| > 0$ in our model (see equation (J.6*a*)). This suggests another mechanism that can suppress relaxation: the ground state in phase 1 might have a large Hamming distance from the ground state in phase 3. Relaxation is then suppressed simply because the coupling is small.

We might expect that there exists an optimum t_f for which the fidelity is maximized by the end of the relaxation phase. However, for the simple case of the spin-chain we considered, we did not observe such an optimum t_f. The fidelity continues to grow (albeit slowly) for sufficiently high t_f. This is illustrated in figure 7.

5.4.4. Phase 4—the frozen phase. As the gap continues to grow, the relaxation phase ends (notice that the tail in figure 6(b) is longer than the actual relaxation phase) and the system's dynamics are frozen in the ground state. This is because H_S becomes almost entirely diagonal in the σ^z basis, and so the off-diagonal components of the $L_{ab,i}$ operators vanish (or become very small), i.e. $A_{iab}(t) = \langle \varepsilon_a(t)|\sigma_i^z|\varepsilon_b(t)\rangle \propto \delta_{ab}$ (equation (64)) leaving only the diagonal ones. At this point, while off-diagonal elements may continue to decay, the system ground state is no longer affected by the bath; this is the onset of the frozen phase.

5.5. Thermal equilibration

An interesting question is whether the system reaches thermal equilibrium throughout the evolution. To answer this we computed the trace-norm distance (defined in equation (A.1))

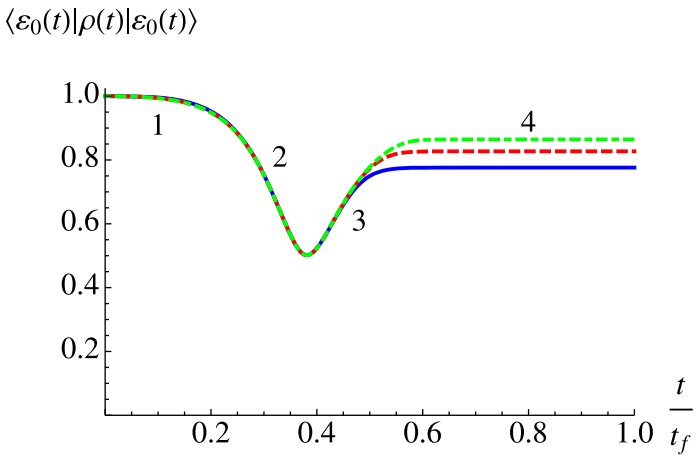

Figure 7. Time evolution of the system density matrix using the RWA equation with $\eta g^2/(\hbar^2) = 0.4/(2\pi)$ for different t_f's. Solid blue curve is for $t_f = 10\,\mu$s, dashed red curve is for $t_f = 100\,\mu$s and dot-dashed green curve is for $t_f = 1$ ms.

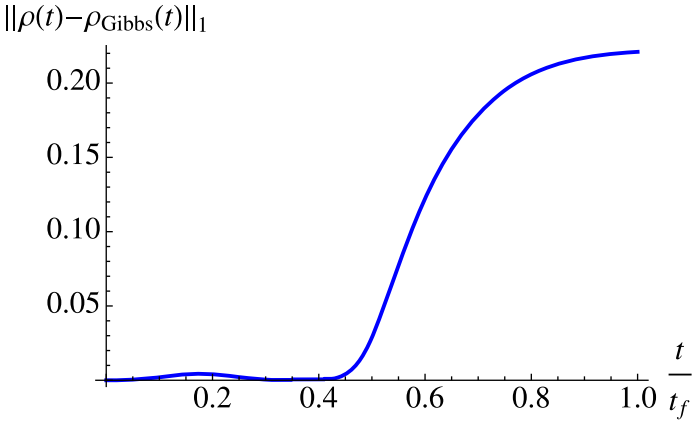

Figure 8. Trace-norm distance between the evolving system density matrix (using the Lindblad equation) and the Gibbs state for an annealing time of $t_f = 10\,\mu$s and $\eta g^2/(\hbar^2) = 0.4/(2\pi)$.

between the instantaneous system density matrix and the instantaneous Gibbs state $\rho_{\text{Gibbs}}(t) = \exp[-\beta H_S(t)]/\mathcal{Z}$, where $\mathcal{Z} = \text{Tr}\left[\exp\left(-\beta H_S(t)\right)\right]$ is the partition function, for the Ising chain discussed above. The result is shown in figure 8. The distance is zero at $t = 0$ since the system is initialized in the Gibbs state, and then begins to grow slowly as the system transitions from the gapped phase to the excitation phase. Though not generic, the distance decreases as the gap shrinks while the excitation phase becomes the relaxation phase, and the system returns to a near Gibbs state where the gap is minimum (at $t/t_f \sim 0.4$). As the gap opens up again in the transition from the relaxation phase to the frozen phase, the distance begins to grow and continues to grow throughout the frozen phase. As such, the system is quite far from the Gibbs state at the final time. This feature is significant for adiabatic quantum computation, since it shows the potential for preparation of states which are biased away from thermal equilibrium towards preferential occupation of the ground state. However, we note that on sufficiently long timescales one

should expect (from general thermodynamic arguments) terms proportional to σ^x and σ^y in the system–bath interaction, which we neglected in writing the interaction Hamiltonian H_I in equation (63), to become important, and to disrupt the frozen phase, allowing the system to fully equilibrate into the Gibbs state.

6. Conclusions

Using a bottom-up, first principles approach, we have developed a number of Markovian master equations to describe the adiabatic evolution of a system with a time-dependent Hamiltonian, coupled to a bath in thermal equilibrium. Our master equations systematically incorporate both time-dependent perturbation theory in the (weak) system–bath coupling g, and adiabatic perturbation theory in the inverse of the total evolution time t_f. Since we have kept track of the various time and energy scales involved in our approximations, higher order corrections (starting at third order in g and second order in $1/t_f$) can be incorporated if desired, a problem we leave for a future publication. Using two of our master equations, we studied generic features of the adiabatic evolution of a spin chain in the presence of a transverse magnetic field, and coupled to a bosonic heat bath. We identified four phases in this evolution, including a phase where thermal relaxation aids the fidelity of the adiabatic evolution. We hope that this work will prove useful in guiding ongoing experiments on adiabatic quantum information processing, and will serve to inspire the development of increasingly more accurate adiabatic master equations, going beyond the Markovian limit.

Acknowledgments

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Appendix A. Norms and inequalities

We provide a brief summary of norms and inequalities between them, as pertinent to our work. For more details see, e.g., [44–46]. Let $|A| \equiv \sqrt{A^\dagger A}$. Unitarily invariant norms are norms that satisfy, for all unitary U, V, and for any operator A: $\| UAV \|_{\rm ui} = \| A \|_{\rm ui}$. Examples of unitarily invariant norms are the trace norm

$$\|A\|_1 \equiv \mathrm{Tr}|A| = \sum_i s_i(A), \tag{A.1}$$

where $s_i(A)$ are the singular values (eigenvalues of $|A|$), and the supoperator norm, which is the largest eigenvalue of $|A|$:

$$\|A\|_\infty \equiv \sup_{|\psi\rangle:\langle\psi|\psi\rangle=1} \sqrt{\langle\psi|A^\dagger A|\psi\rangle} = \max_i s_i(A). \tag{A.2}$$

Therefore $\| A|\psi\rangle \| \leqslant \| A \|_\infty$ for all normalized states $|\psi\rangle$, and $\| A \|_\infty \leqslant \| A \|_1$.

All unitarily invariant norms satisfy submultiplicativity:

$$\|AB\|_{\mathrm{ui}} \leqslant \|A\|_{\mathrm{ui}}\|B\|_{\mathrm{ui}}. \tag{A.3}$$

The norms of interest to us are also multiplicative over tensor products and obey an ordering:

$$\|A \otimes B\|_i = \|A\|_i \|B\|_i \quad i = 1, \infty, \tag{A.4a}$$

$$\|AB\|_{\mathrm{ui}} \leqslant \|A\|_\infty \|B\|_{\mathrm{ui}}. \tag{A.4b}$$

In particular, $\| AB \|_1 \leqslant \| A \|_\infty \| B \|_1$.

Another useful fact is that the partial trace is contractive, i.e.

$$\|\mathrm{Tr}_B(X)\|_1, \|\mathrm{Tr}_A(X)\|_1 \leqslant \|X\|_1, \tag{A.5}$$

for any operator X acting on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Actually this result extends to other unitarily invariant norms, with a prefactor depending on the dimension of the traced-out Hilbert space [46].

Appendix B. Markov approximation bound

We wish to derive an upper bound associated with the error from the approximation made in equation (13), which involves the replacement of $\tilde{\rho}_{\mathrm{S}}(t-\tau)$ by $\tilde{\rho}_{\mathrm{S}}(t)$ and the extension of the upper integration limit to infinity, i.e.

$$\begin{aligned}\mathcal{I} &:= \int_0^t \mathrm{d}\tau \left\{A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t-\tau)A_\alpha(t) + \cdots\right\} \mathcal{B}_{\alpha\beta}(\tau) \\ &\mapsto \int_0^\infty \mathrm{d}\tau \left\{A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)A_\alpha(t) + \cdots\right\} \mathcal{B}_{\alpha\beta}(\tau) = \mathcal{I} + \Delta_1 + \Delta_2,\end{aligned} \tag{B.1}$$

where

$$\begin{aligned}\Delta_1 &:= \int_0^\infty \mathrm{d}\tau \left\{A_\beta(t-\tau)\left[\tilde{\rho}_{\mathrm{S}}(t) - \tilde{\rho}_{\mathrm{S}}(t-\tau)\right]A_\alpha(t) + \cdots\right\} \mathcal{B}_{\alpha\beta}(\tau) \\ \Delta_2 &:= \int_t^\infty \mathrm{d}\tau \left\{A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t-\tau)A_\alpha(t) + \cdots\right\} \mathcal{B}_{\alpha\beta}(\tau),\end{aligned} \tag{B.2}$$

and where the ellipsis denotes the three other summands appearing in equation (13). The Markov approximation is more accurate the smaller the error terms Δ_1 and Δ_2.

Consider first the Δ_1 term. We shall show that it is of order $g^2\tau_{\mathrm{B}}^3$. For simplicity we consider only the first of its four summands (the bounds for the other three are identical to that for the first):

$$\begin{aligned}&\left\| \int_0^\infty \mathrm{d}\tau A_\beta(t-\tau)\left[\tilde{\rho}_{\mathrm{S}}(t) - \tilde{\rho}_{\mathrm{S}}(t-\tau)\right]A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau)\right\|_1 \\ &\quad\leqslant \int_0^\infty \mathrm{d}\tau \|A_\beta(t-\tau)\|_\infty \tau \max_{t'\in[t-\tau,t]} \left\|\frac{\mathrm{d}\tilde{\rho}_{\mathrm{S}}(t')}{\mathrm{d}t'}\right\|_1 \|A_\alpha(t)\|_\infty |\mathcal{B}_{\alpha\beta}(\tau)| \\ &\quad= \int_0^\infty \mathrm{d}\tau\ \tau \max_{t'\in[t-\tau,t]} \left\|\frac{\mathrm{d}\tilde{\rho}_{\mathrm{S}}(t')}{\mathrm{d}t'}\right\|_1 |\mathcal{B}_{\alpha\beta}(\tau)|,\end{aligned} \tag{B.3}$$

where we used the triangle inequality, $\|A_\alpha(t)\|_\infty = \|A\| = 1$ and $\|XY\|_1 \leqslant \|X\|_\infty \|Y\|_1$ (see appendix A). We can now use equation (9) to upper-bound the time derivative:

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t}\tilde{\rho}_{\mathrm{S}}(t) \right\|_1 \leqslant g^2 \sum_{\alpha,\beta} \int_0^t \mathrm{d}\tau \left(\|A_\beta(t-\tau)\|_\infty \|\tilde{\rho}_{\mathrm{S}}(t-\tau)\|_1 \|A_\alpha(t)\|_\infty + \cdots \right) |\mathcal{B}_{\alpha\beta}(\tau)|$$

$$= 4g^2 \sum_{\alpha,\beta} \int_0^t \mathrm{d}\tau |\mathcal{B}_{\alpha\beta}(\tau)|, \tag{B.4}$$

where the factor of 4 is due to the same number of summands appearing in equation (9). Substituting this bound back into equation (B.3) we have

$$\int_0^\infty \mathrm{d}\tau\ \tau \max_{t' \in [t-\tau,t]} \left\| \frac{\mathrm{d}\tilde{\rho}_{\mathrm{S}}(t')}{\mathrm{d}t'} \right\|_1 |\mathcal{B}_{\alpha\beta}(\tau)| \leqslant 4g^2 \sum_{\alpha\beta} \int_0^\infty \mathrm{d}\tau\ \tau\ |\mathcal{B}_{\alpha\beta}(\tau)| \max_{t' \in [t-\tau,t]} \int_0^{t'} \mathrm{d}\tau' |\mathcal{B}_{\alpha\beta}(\tau')|$$

$$\lesssim 4g^2 \sum_{\alpha\beta} \int_0^\infty \mathrm{d}\tau\ \tau\ |\mathcal{B}_{\alpha\beta}(\tau)| \tau_{\mathrm{B}} \leqslant 4g^2 \tau_{\mathrm{B}}^3 \sum_{\alpha\beta} 1, \tag{B.5}$$

where we used $\int_0^{t'} \mathrm{d}\tau' |\mathcal{B}_{\alpha\beta}(\tau')| \leqslant \int_0^\infty \mathrm{d}\tau' |\mathcal{B}_{\alpha\beta}(\tau')|$ and equation (12).

This is to be compared to the term we use after the Markov approximation:

$$\left\| \int_0^\infty \mathrm{d}\tau A_\beta(t-\tau)_\beta \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_1 \leqslant \int_0^\infty \mathrm{d}\tau |\mathcal{B}_{\alpha\beta}(\tau)| \sim \tau_{\mathrm{B}}. \tag{B.6}$$

Comparing equations (B.5) and (B.6), we see that the relative error is $O[(g\tau_{\mathrm{B}})^2]$.

Next consider the Δ_2 term. We have

$$\left\| \int_t^\infty \mathrm{d}\tau A_\beta(t-\tau) \tilde{\rho}_{\mathrm{S}}(t-\tau) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_1$$

$$\leqslant \int_t^\infty \mathrm{d}\tau \|A_\beta(t-\tau)\|_\infty \|\tilde{\rho}_{\mathrm{S}}(t-\tau)\|_1 \|A_\alpha(t)\|_\infty |\mathcal{B}_{\alpha\beta}(\tau)| = \int_t^\infty \mathrm{d}\tau\ |\mathcal{B}_{\alpha\beta}(\tau)|. \tag{B.7}$$

The last integral converges provided $|\mathcal{B}_{\alpha\beta}(\tau)| \sim 1/\tau^x$ with $x > 1$. This is typically the case. For example, for the Ohmic spin-boson model discussed in section 5.2 we show that for $t > \tau_{\mathrm{tr}} \sim \beta \ln(\beta\omega_{\mathrm{c}})$, the bath correlation function $|\mathcal{B}_{\alpha\beta}(\tau)| \sim \frac{\eta g^2}{\beta\omega_{\mathrm{c}}} \frac{1}{\tau^2}$. In this case, then, we can set $t = \tau_{\mathrm{tr}}$ and bound

$$\|\Delta_2\|_1 \lesssim \frac{\eta g^2}{\beta\omega_{\mathrm{c}}} \int_{\tau_{\mathrm{tr}}}^\infty \mathrm{d}\tau\ \frac{1}{\tau^2} \sim \frac{\eta g^2}{\beta^2 \omega_{\mathrm{c}} \ln(\beta\omega_{\mathrm{c}})}, \tag{B.8}$$

which tends to zero as the cutoff tends to infinity at a fixed finite temperature (even if the lower integration limit is replaced by a constant), as expected in the weak coupling limit assumed in our work. Note that the infinite temperature limit, where equation (B.8) diverges, is incompatible with weak coupling, and requires the so-called singular coupling limit [22, 30].

Appendix C. Properties of the spectral-density matrix $\boldsymbol{\Gamma_{\alpha\beta}(\omega)}$

Introducing the Fourier transform pair

$$\mathcal{B}_{\alpha\beta}(\tau, 0) = \int_{-\infty}^\infty \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega\tau} \gamma_{\alpha\beta}(\omega), \quad \gamma_{\alpha\beta}(\omega) = \int_{-\infty}^\infty \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau} \mathcal{B}_{\alpha\beta}(\tau, 0), \tag{C.1}$$

and using the property that

$$\int_0^\infty \mathrm{d}\tau \mathrm{e}^{\mathrm{i}(\omega-\omega')\tau} = \pi\delta(\omega-\omega') + \mathrm{i}\mathcal{P}\left(\frac{1}{\omega-\omega'}\right), \tag{C.2}$$

where $\mathcal{P}$ denotes the Cauchy principal value[9], we have, using equation (14),

$$\begin{aligned}\Gamma_{\alpha\beta}(\omega) &= \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega\tau}\int_{-\infty}^\infty \frac{\mathrm{d}\omega'}{2\pi}\mathrm{e}^{-\mathrm{i}\omega'\tau}\gamma_{\alpha\beta}(\omega') \\ &= \int_{-\infty}^\infty \frac{\mathrm{d}\omega'}{2\pi}\gamma_{\alpha\beta}(\omega')\int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}(\omega-\omega')\tau} = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + \mathrm{i}S_{\alpha\beta}(\omega),\end{aligned} \tag{C.3}$$

in agreement with equation (15), where

$$S_{\alpha\beta}(\omega) = \int_{-\infty}^\infty \frac{\mathrm{d}\omega'}{2\pi}\gamma_{\alpha\beta}(\omega')\mathcal{P}\left(\frac{1}{\omega-\omega'}\right), \tag{C.4}$$

in agreement with equation (16).

Note that:

$$\mathcal{B}^*_{\alpha\beta}(\tau,0) = \langle B_\alpha(\tau)B_\beta(0)\rangle^* = \mathrm{Tr}\left[B_\alpha(\tau)B_\beta(0)\rho_\mathrm{B}\right]^* = \mathrm{Tr}\left[B_\beta(0)B_\alpha(\tau)\rho_\mathrm{B}\right] = \mathcal{B}_{\beta\alpha}(0,\tau). \tag{C.5}$$

When ρ_B commutes with H_B (which we have assumed), we further have

$$\begin{aligned}\mathcal{B}_{\beta\alpha}(0,\tau) &= \mathrm{Tr}\left[B_\beta(0)U_\mathrm{B}^\dagger(\tau)B_\alpha(0)U_\mathrm{B}(\tau)\rho_\mathrm{B}\right] = \mathrm{Tr}\left[\rho_\mathrm{B}U_\mathrm{B}(\tau)B_\beta(0)U_\mathrm{B}^\dagger(\tau)B_\alpha(0)\right] \\ &= \mathcal{B}_{\beta\alpha}(-\tau,0).\end{aligned} \tag{C.6}$$

Thus the spectral-density matrix satisfies:

$$\begin{aligned}\Gamma^*_{\alpha\beta}(\omega) &= \int_0^\infty \mathrm{d}\tau\mathrm{e}^{-\mathrm{i}\omega\tau}\mathcal{B}^*_{\alpha\beta}(\tau,0) = \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{-\mathrm{i}\omega\tau}\mathcal{B}_{\beta\alpha}(-\tau,0) = \int_{-\infty}^0 \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega\tau}\mathcal{B}_{\beta\alpha}(\tau,0) \\ &= \frac{1}{2}\gamma_{\beta\alpha}(\omega) - \mathrm{i}S_{\beta\alpha}(\omega).\end{aligned} \tag{C.7}$$

Appendix D. Proof of the Kubo–Martin–Schwinger condition

The proof of the time-domain version of the KMS condition, equation (17), is the following calculation:

$$\langle B_a(\tau)B_b(0)\rangle = \mathrm{Tr}[\rho_\mathrm{B}U_\mathrm{B}^\dagger(\tau,0)B_aU_\mathrm{B}(\tau,0)B_b] = \frac{1}{\mathcal{Z}}\mathrm{Tr}[B_b\mathrm{e}^{-(\beta-\mathrm{i}\tau)H_\mathrm{B}}B_a\mathrm{e}^{-\mathrm{i}\tau H_\mathrm{B}}] \tag{D.1a}$$

$$= \frac{1}{\mathcal{Z}}\mathrm{Tr}[B_b\mathrm{e}^{\mathrm{i}(\tau+\mathrm{i}\beta)H_\mathrm{B}}B_a\mathrm{e}^{-\mathrm{i}(\tau+\mathrm{i}\beta)H_\mathrm{B}}\mathrm{e}^{-\beta H_\mathrm{B}}] \tag{D.1b}$$

$$= \mathrm{Tr}[\rho_\mathrm{B}B_bU_\mathrm{B}^\dagger(\tau+\mathrm{i}\beta,0)B_aU_\mathrm{B}(\tau+\mathrm{i}\beta,0)] \tag{D.1c}$$

$$= \langle B_b(0)B_a(\tau+\mathrm{i}\beta)\rangle. \tag{D.1d}$$

[9] By definition, $\mathcal{P}\left(\frac{1}{x}\right)[f] = \lim_{\epsilon\to0}\int_{\mathbb{R}\setminus[-\epsilon,\epsilon]}\frac{f(x)}{x}\,\mathrm{d}x$, where f belongs to the set of smooth functions with compact support on the real line $\mathbb{R}$.

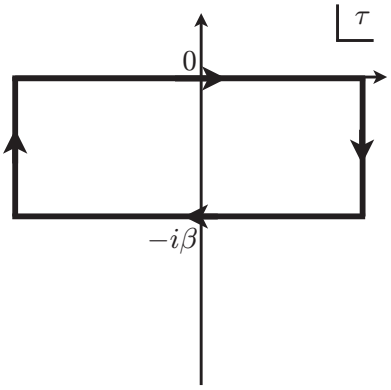

Figure D.1. Contour used in proof of the KMS condition.

Note that using the same technique it also follows that

$$\langle B_a(\tau)B_b(0)\rangle = \langle B_b(-\tau - \mathrm{i}\,\beta)B_a(0)\rangle. \tag{D.2}$$

To prove that this implies the frequency domain condition, equation (18), we compute the Fourier transform:

$$\gamma_{ab}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau}\langle B_a(\tau)B_b(0)\rangle = \int_{-\infty}^{\infty} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau}\langle B_b(-\tau - \mathrm{i}\,\beta)B_a(0)\rangle. \tag{D.3}$$

To perform this integral we replace it with a contour integral in the complex plane, $\oint_C \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau}\langle B_b(-\tau - \mathrm{i}\,\beta)B_a(0)\rangle$, with the contour C as shown in figure D.1. This contour integral vanishes by the Cauchy–Goursat theorem [47] since the closed contour encloses no poles (the correlation function $\langle B_b(\tau)B_a(0)\rangle$ is analytic in the open strip $(0, -\mathrm{i}\,\beta)$ and is continuous at the boundary of the strip [48]), so that

$$\oint_C (\cdots) = 0 = \int_{\uparrow} (\cdots) + \int_{\downarrow} (\cdots) + \int_{\rightarrow} (\cdots) + \int_{\leftarrow} (\cdots), \tag{D.4}$$

where $(\cdots)$ is the integrand of equation (D.3), and the integral $\int_{\rightarrow}$ is the same as in equation (D.3). After making the variable transformation $\tau = -x - \mathrm{i}\,\beta$, where x is real, we have

$$\int_{\leftarrow} (\cdots) = -\mathrm{e}^{\beta\omega} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega x}\langle B_b(x)B_a(0)\rangle. \tag{D.5}$$

Assuming that $\langle B_a(\pm\infty - \mathrm{i}\beta)B_b(0)\rangle = 0$ (i.e. the correlation function vanishes at infinite time), we further have $\int_{\uparrow} (\cdots) = \int_{\downarrow} (\cdots) = 0$, and hence we find the result:

$$\int_{-\infty}^{\infty} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\omega\tau}\langle B_b(-\tau - \mathrm{i}\,\beta)B_a(0)\rangle = \mathrm{e}^{\beta\omega} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega\tau}\langle B_b(\tau)B_a(0)\rangle = \mathrm{e}^{\beta\omega}\gamma_{ba}(-\omega), \tag{D.6}$$

which, together with equation (D.3), proves equation (18).

Appendix E. Non-adiabatic corrections

For completeness we provide a brief review of pertinent aspects of adiabatic perturbation theory, and the derivation of the adiabatic condition relating the total evolution time to the ground state gap. See, e.g., [5] for additional details.

E.1. Adiabatic perturbation theory

To consider adiabatic corrections, we recall that U_S satisfies

$$\mathrm{i}\partial_t U_S(t,t') = H_S(t)U_S(t,t'), \tag{E.1}$$

where

$$H_S(t) = \sum_a \varepsilon_a(t)|\varepsilon_a(t)\rangle\langle\varepsilon_a(t)|. \tag{E.2}$$

Define the 'adiabatic intertwiner' $W(t,t')$:

$$W(t,t') \equiv \sum_a |\varepsilon_a(t)\rangle\langle\varepsilon_a(t')| = T_+ \exp\left[-\mathrm{i}\int_{t'}^{t} \mathrm{d}\tau\ K(\tau)\right], \tag{E.3}$$

where the 'intertwiner Hamiltonian' is

$$K(t) \equiv \mathrm{i}[\partial_t W(t,t')]W^\dagger(t,t') = \mathrm{i}\sum_a |\dot{\varepsilon}_a(t)\rangle\langle\varepsilon_a(t)| \tag{E.4a}$$

$$= \mathrm{i}[\dot{P}_0(t), P_0(t)], \tag{E.4b}$$

and where $P_0(t) \equiv |\varepsilon_0(t)\rangle\langle\varepsilon_0(t)|$ is the projection onto the ground state of $H_S(t)$. The result (E.4*b*) is by no means obvious and is proven in section E.3.

To extract the geometric phase we define

$$H_G(t) \equiv \sum_a \phi_a(t)|\varepsilon_a(t)\rangle\langle\varepsilon_a(t)|, \tag{E.5a}$$

$$\phi_a(t) = \mathrm{i}\langle\varepsilon_a(t)|\dot{\varepsilon}_a(t)\rangle, \tag{E.5b}$$

$$H'_S(t) \equiv H_S(t) - H_G(t). \tag{E.5c}$$

Now define V via the 'adiabatic interaction picture' transformation:

$$V(t,t') = W^\dagger(t,t')U_S(t,t'), \tag{E.6}$$

along with

$$\tilde{H}_S(t,t') = W^\dagger(t,t')H_S(t)W(t,t') = \sum_a \varepsilon_a(t)|\varepsilon_a(t')\rangle\langle\varepsilon_a(t')|, \tag{E.7a}$$

$$\tilde{H}_G(t,t') = W^\dagger(t,t')H_G(t)W(t,t') = \sum_a \phi_a(t)|\varepsilon_a(t')\rangle\langle\varepsilon_a(t')|, \tag{E.7b}$$

$$\tilde{H}'_S(t,t') \equiv \tilde{H}_S(t,t') - \tilde{H}_G(t,t'), \tag{E.7c}$$

$$\tilde{K}(t,t') = W^\dagger(t,t')K(t)W(t,t') = \mathrm{i}W^\dagger(t,t')\partial_t W(t,t'). \tag{E.7d}$$

Note that the time dependence of $\tilde{H}_S$ and $\tilde{H}'_S(t)$ is entirely in the energy eigenvalue and not in the eigenstates. Then V obeys the Schrödinger equation:

$$\mathrm{i}\,\partial_t V(t,t') = \tilde{H}_S^{\mathrm{ad}}(t,t')V(t,t'). \tag{E.8}$$

where

$$\tilde{H}_S^{\mathrm{ad}}(t,t') \equiv \tilde{H}_S(t,t') - \tilde{K}(t,t') = W^\dagger(t,t')[H_S(t) - K(t)]W(t,t'). \tag{E.9}$$

When the evolution is nearly adiabatic $\tilde{H}_{\rm S}^{\rm ad}(t,t')$ is a perturbation, so that we consider a solution of equation (E.8) for V of the form:

$$V(t,t') = V_0(t,t')\left(\mathbb{1} + V_1(t,t') + \cdots\right), \tag{E.10}$$

with the zeroth order solution associated with the purely adiabatic evolution, including the geometric phase:

$$V_0(t,t') \equiv T_+ \exp\left[-\mathrm{i}\int_{t'}^{t} \mathrm{d}\tau\, \tilde{H}'_{\rm S}(\tau,t')\right] \tag{E.11a}$$

$$U_{\rm S}^{\rm ad}(t,t') \equiv W(t,t')V_0(t,t') = \sum_a |\varepsilon_a(t)\rangle\langle\varepsilon_a(t')|\mathrm{e}^{-\mathrm{i}\int_{t'}^{t}\mathrm{d}\tau[\varepsilon_a(\tau)-\phi_a(\tau)]}. \tag{E.11b}$$

Differentiating with respect to t, we have

$$\dot{U}_S^{\rm ad}(t,t') = \dot{W}(t,t')V_0(t,t') + W(t,t')\dot{V}_0(t,t') \tag{E.12a}$$

$$= -\mathrm{i}\,K(t)W(t,t')V_0(t,t') - \mathrm{i}\,W(t,t')\tilde{H}'_{\rm S}(t,t')V_0(t,t') \tag{E.12b}$$

$$= -\mathrm{i}\left[H_{\rm S}^{\rm ad}(t) - H_{\rm G}(t)\right]U_{\rm S}^{\rm ad}(t,t'), \tag{E.12c}$$

where

$$H_{\rm S}^{\rm ad}(t) \equiv K(t) + H_{\rm S}(t). \tag{E.13}$$

Plugging the equation (E.10) expansion into equation (E.8), we obtain, to first order in $1/t_{\rm f}$:[10]

$$\mathrm{i}\partial_t V_1(t,t') = -V_0^{\dagger}(t,t')[\tilde{K}(t,t') - \tilde{H}_{\rm G}(t,t')]V_0(t,t') \tag{E.14a}$$

$$= -\mathrm{i}U_{\rm S}^{\rm ad\dagger}(t,t')\partial_t W(t,t')V_0(t,t') + U_{\rm S}^{\rm ad\dagger}(t,t')H_{\rm G}(t)U_{\rm S}^{\rm ad}(t,t'). \tag{E.14b}$$

Note that $U_{\rm S}^{\rm ad\dagger}(t,t')H_{\rm G}(t)U_{\rm S}^{\rm ad}(t,t') = \sum_a \phi_a(t)|\varepsilon_a(t')\rangle\langle\varepsilon_a(t')|$. Therefore, integrating, and using

$$\mu_{ba}(t,t') = \int_{t'}^{t}\mathrm{d}\tau\,\omega_{ba}(\tau), \quad \omega_{ba}(\tau) = [\varepsilon_b(\tau) - \phi_b(t)] - [\varepsilon_a(\tau) - \phi_a(t)], \tag{E.15}$$

we can write the solution as:

$$V_1(t,t') = -\int_{t'}^{t}\mathrm{d}\tau\left[U_S^{\rm ad\dagger}(\tau,t')\partial_\tau W(\tau,t')V_0(\tau,t') - \sum_a \phi_a(\tau)|\varepsilon_a(t')\rangle\langle\varepsilon_a(t')|\right]$$

$$= -\sum_{a\neq b}\int_{t'}^{t}\mathrm{d}\tau\mathrm{e}^{-\mathrm{i}\mu_{ba}(\tau,t')}|\varepsilon_a(t')\rangle\langle\varepsilon_b(t')|\langle\varepsilon_a(\tau)|\dot{\varepsilon}_b(\tau)\rangle. \tag{E.16}$$

Therefore, the system evolution operator can be written as:

$$U_{\rm S}(t,t') = U_{\rm S}^{\rm ad}(t,t') + Q(t,t')U_{\rm S}^{\rm ad}(t,t') + O\left(t_{\rm f}^{-2}\right), \tag{E.17}$$

where the correction term can be made appropriately dimensionless in a more careful second order analysis, and where

$$Q(t,t') \equiv U_{\rm S}^{\rm ad}(t,t')V_1(t,t')U_{\rm S}^{\rm ad\dagger}(t,t')$$

$$= \sum_{a\neq b}\mathrm{e}^{-\mathrm{i}\mu_{ba}(t,t')}\left(-\int_{t'}^{t}\mathrm{d}\tau\mathrm{e}^{\mathrm{i}\mu_{ba}(\tau,t')}\langle\varepsilon_a(\tau)|\dot{\varepsilon}_b(\tau)\rangle\right)|\varepsilon_a(t)\rangle\langle\varepsilon_b(t)|. \tag{E.18}$$

[10] To see that this is an expansion in powers of $1/t_{\rm f}$, transform to the dimensionless time variable $s = t/t_{\rm f}$.

E.2. Adiabatic timescale analysis

Equation (E.17) shows that the first order correction to the purely adiabatic evolution is given by Q. Thus the adiabatic timescale is found by ensuring that the matrix elements of Q are all small. Let us show that a sufficient condition for this is $\frac{h}{\Delta^2 t_\mathrm{f}} \ll 1$ (equation (27)). More rigorous analyses replace the $\ll$ condition with an inequality relating the same parameters to the fidelity between the ground state of $H_\mathrm{S}(t_\mathrm{f})$ and the solution of the Schrödinger equation at t_f, e.g. [6, 10–12].

Starting from equation (E.18) and taking matrix elements we have

$$Q_{ab}(t,t') = \mathrm{e}^{-\mathrm{i}\mu_{ba}(t,t')}\left(-\int_{t'}^{t} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\mu_{ba}(\tau,t')}\langle\varepsilon_a(\tau)|\partial_\tau|\varepsilon_b(\tau)\rangle\right). \tag{E.19}$$

Changing variables to dimensionless time $s = t/t_\mathrm{f}$, $\mu_{ba}(t,t')$ becomes $t_\mathrm{f}\int_{t'/t_\mathrm{f}}^{s}\mathrm{d}s'\,\omega_{ba}(s') = t_\mathrm{f}\tilde{\mu}_{ba}(s,t'/t_\mathrm{f})$, and

$$\int_{t'}^{t} \mathrm{d}\tau \mathrm{e}^{\mathrm{i}\mu_{ba}(\tau,t')}\langle\varepsilon_a(\tau)|\partial_\tau|\varepsilon_b(\tau)\rangle = \int_{t'/t_\mathrm{f}}^{s} \mathrm{d}s'\ \mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ba}(s',t'/t_\mathrm{f})}\langle\varepsilon_a(s')|\partial_{s'}|\varepsilon_b(s')\rangle, \tag{E.20}$$

where $\tilde{\mu}$ now involves a dimensionless time integration. Using the fact that $\mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ba}(s',t'/t_\mathrm{f})} = \frac{\mathrm{i}}{t_\mathrm{f}\omega_{ab}(s')}\frac{\mathrm{d}}{\mathrm{d}s'}\mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ba}(s',t'/t_\mathrm{f})}$, we can integrate equation (E.20) by parts as

$$\begin{aligned}\int_{t'/t_\mathrm{f}}^{s} \mathrm{d}s'\ \mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ba}(s',t'/T)}\langle\varepsilon_a(s')|\partial_{s'}|\varepsilon_b(s')\rangle &= \frac{\mathrm{i}}{t_\mathrm{f}\omega_{ab}(s')}\mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ab}(s',t'/t_\mathrm{f})}\langle\varepsilon_a(s')|\partial_{s'}|\varepsilon_b(s')\rangle\Big|_{t'/t_\mathrm{f}}^{s} \\ &\quad -\frac{\mathrm{i}}{t_\mathrm{f}}\int_{t'/t_\mathrm{f}}^{s}\mathrm{d}s'\ \frac{\mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ab}(s',t'/t_\mathrm{f})}}{\omega_{ab}(s')}\frac{\mathrm{d}}{\mathrm{d}s'}\langle\varepsilon_a(s')|\partial_{s'}|\varepsilon_b(s')\rangle.\end{aligned} \tag{E.21}$$

Now note that for non-degenerate energy eigenstates, differentiation with respect to t of $H_\mathrm{S}(t)|\varepsilon_a(t)\rangle = \varepsilon_a(t)|\varepsilon_a(t)\rangle$, and substitution of $s = t/t_\mathrm{f}$ in equation (26), directly yields the relation:[11]

$$\langle\varepsilon_b(t)|\dot{\varepsilon}_a(t)\rangle = \frac{\langle\varepsilon_b(t)|\dot{H}_\mathrm{S}(t)|\varepsilon_a(t)\rangle}{\omega_{ab}(t)} \sim \frac{h}{\Delta t_\mathrm{f}}. \tag{E.22}$$

Substitution into equation (E.21) yields, with the help of equation (E.22),

$$|Q_{ab}(t,t')| \leqslant \frac{|\langle\varepsilon_a(s)|\partial_s H_\mathrm{S}(s)|\varepsilon_b(s)\rangle|}{\omega_{ab}^2(s)t_\mathrm{f}}\Big|_{t'/t_\mathrm{f}}^{t/t_\mathrm{f}} + \left|\int_{t'/t_\mathrm{f}}^{t/t_\mathrm{f}}\mathrm{d}s'\ \frac{\mathrm{e}^{\mathrm{i}t_\mathrm{f}\tilde{\mu}_{ab}(s',t'/t_\mathrm{f})}}{\omega_{ab}^2(s')t_\mathrm{f}}\frac{\mathrm{d}}{\mathrm{d}s'}\langle\varepsilon_a(s')|\partial_{s'}H_\mathrm{S}(s')|\varepsilon_b(s')\rangle\right|.$$

Continued integration by parts will yield higher powers of the dimensionless quantity $\frac{\langle\varepsilon_a(s)|\partial_\tau H_\mathrm{S}(s)|\varepsilon_b(s)\rangle}{\omega_{ab}^2(s)t_\mathrm{f}}$. Thus a sufficient condition for the smallness of $|Q_{ab}(t,t')|$ for all a, b is that

$$\frac{\max_{s;a,b}|\langle\varepsilon_a(s)|\partial_s H_\mathrm{S}(s)|\varepsilon_b(s)\rangle|}{\min_{s;a,b}\omega_{ab}^2(s)t_\mathrm{f}} \ll 1, \tag{E.23}$$

[11] Differentiating (where $\dot{x} \equiv \partial_t x$), we have $\dot{H}_\mathrm{S}|\varepsilon_a(t)\rangle + H_\mathrm{S}(t)|\dot{\varepsilon}_a(t)\rangle = \dot{\varepsilon}_a(t)|\varepsilon_a(t)\rangle + \varepsilon_a(t)|\dot{\varepsilon}_a(t)\rangle$. Taking matrix elements gives $\langle\varepsilon_b(t)|\dot{H}_\mathrm{S}|\varepsilon_a(t)\rangle + \varepsilon_b(t)\langle\varepsilon_b(t)|\dot{\varepsilon}_a(t)\rangle = \dot{\varepsilon}_a(t)\delta_{ab} + \varepsilon_a(t)\langle\varepsilon_b(t)|\dot{\varepsilon}_a(t)\rangle$, which yields equation (E.22) provided $|\varepsilon_b(t)\rangle$ is an eigenstate non-degenerate with $|\varepsilon_a(t)\rangle$.

namely the condition in equation (27), where we assumed that the minimal Bohr frequency is the ground state gap, $\omega_{1,0}$. Of course, this argument is by no means rigorous, and in fact it has been the subject of considerable discussion, e.g. [49–54]. For rigorous analyses see, e.g., [5–7, 10–12]. For our purposes equation (27) suffices.

E.3. Intertwiner Hamiltonian

Here we provide an explicit proof of equation (E.4*b*), a well-known result due to Avron *et al* [55]. The original proof lacks some detail, so our purpose here is to fill in the gaps, for completeness of our presentation (see also [25] for details of the proof). Define the ground state and orthogonal projectors $P_0(t) \equiv |\varepsilon_0(t)\rangle\langle\varepsilon_0(t)|$ and $Q_0(t) \equiv \mathbb{I} - P_0(t)$. Recalling equation (E.17), we have

$$P_0(t)U_{\rm S}(t,t')P_0(t') = P_0(t)U_{\rm S}^{\rm ad}(t,t')P_0(t') + P_0(t)Q(t,t')U_{\rm S}^{\rm ad}(t,t')P_0(t') + O\left(t_{\rm f}^{-2}\right). \tag{E.24}$$

Using equation (E.11*b*) we find $U_{\rm S}^{\rm ad}(t,t')P_0(t') = P_0(t)\mathrm{e}^{-\mathrm{i}\int_{t'}^{t}\mathrm{d}\tau\varepsilon_0(\tau)}$, so that up to a phase $P_0(t)Q(t,t')U_{\rm S}^{\rm ad}(t,t')P_0(t') = P_0(t)Q(t,t')P_0(t')$. However, $Q(t,t')$ (equation (E.18)) contains only off-diagonal terms (since we subtracted the Berry connection in equation (E.5*c*)), so that $P_0(t)Q(t,t')P_0(t') = 0$. Thus, to first order in $1/t_{\rm f}$ the evolution generated by $H_{\rm S}(t)$ keeps the ground state decoupled from the excited states, i.e.

$$P_0(t)U_{\rm S}(t,t')P_0(t') = U_{\rm S}^{\rm ad}(t,t')P_0(t') + O\left(t_{\rm f}^{-2}\right), \tag{E.25a}$$

$$Q_0(t)U_{\rm S}(t,t')Q_0(t') = U_{\rm S}^{\rm ad}(t,t')Q_0(t') + O\left(t_{\rm f}^{-2}\right). \tag{E.25b}$$

Letting $\tau = t - t' > 0$ and expanding around t, we then have, using equations (E.1) and (E.3),

$$P_0(t)[\mathbb{I} + \mathrm{i}\tau H_{\rm S}(t)][P_0(t) - \tau\dot{P}_0(t)] = [\mathbb{I} + \mathrm{i}\tau H_{\rm S}^{\rm ad}(t)][P_0(t) - \tau\dot{P}_0(t)] + O\left(t_{\rm f}^{-2}\right), \tag{E.26a}$$

$$Q_0(t)[\mathbb{I} + \mathrm{i}\tau H_{\rm S}(t)][Q_0(t) - \tau\dot{Q}_0(t)] = [\mathbb{I} + \mathrm{i}\tau H_{\rm S}^{\rm ad}(t)][Q_0(t) - \tau\dot{Q}_0(t)] + O\left(t_{\rm f}^{-2}\right). \tag{E.26b}$$

Using the projector properties $P_0 = P_0^2 \Longrightarrow \dot{P}_0P_0 + P_0\dot{P}_0 = \dot{P}_0$ and $[H_{\rm S}(t), P_0(t)] = 0$ (similarly for Q_0), this simplifies to

$$-\tau P_0(t)\dot{P}_0(t) + \mathrm{i}\tau H_{\rm S}(t)P_0(t) = -\tau\dot{P}_0(t) + \mathrm{i}\tau H_{\rm S}^{\rm ad}(t)P_0(t) + O\left(t_{\rm f}^{-2}\right), \tag{E.27a}$$

$$-\tau Q_0(t)\dot{Q}_0(t) + \mathrm{i}\tau H_{\rm S}(t)Q_0(t) = -\tau\dot{Q}_0(t) + \mathrm{i}\tau H_{\rm S}^{\rm ad}(t)Q_0(t) + O\left(t_{\rm f}^{-2}\right), \tag{E.27b}$$

and, after dropping the $O(t_{\rm f}^{-2})$ corrections, to

$$\mathrm{i}[H_{\rm S}^{\rm ad}(t) - H_{\rm S}(t)]P_0(t) + \dot{P}_0(t)P_0(t) = 0, \tag{E.28a}$$

$$\mathrm{i}[H_{\rm S}^{\rm ad}(t) - H_{\rm S}(t)]Q_0(t) + \dot{Q}_0(t)Q_0(t) = 0. \tag{E.28b}$$

Inserting $Q_0(t) = \mathbb{I} - P_0(t)$ and $\dot{Q}_0(t) = -\dot{P}_0(t)$ into equation (E.28*b*), and subtracting it from equation (E.28*a*), we find, using $\dot{P}_0P_0 + P_0\dot{P}_0 = \dot{P}_0$ once more, the desired result:

$$H_{\rm S}^{\rm ad}(t) = H_{\rm S}(t) + \mathrm{i}[\dot{P}_0(t), P_0(t)], \tag{E.29}$$

which, together with equation (E.13), proves equation (E.4*b*).

Appendix F. Short time bound

We wish to bound the error associated with neglecting Θ in equation (40), i.e. we wish to bound

$$\begin{aligned}\|\Theta(t,\tau)\|_\infty &= \|U_{\rm S}(t-\tau,0) - {\rm e}^{{\rm i}\,\tau H_{\rm S}(t)} U_{\rm S}^{\rm ad}(t,0)\|_\infty \\ &= \|U_{\rm S}^{\rm ad\dagger}(t,0){\rm e}^{-{\rm i}\,\tau H_{\rm S}(t)} U_{\rm S}^{\dagger}(t,t-\tau)U_{\rm S}(t,0) - \mathbb{I}\|_\infty. \end{aligned} \tag{F.1}$$

Using the fact that the operator $\hat{U}(\tau) = {\rm e}^{-{\rm i}\,\tau H_{\rm S}(t)} U_{\rm S}^{\dagger}(t,t-\tau)$ satisfies:

$$\frac{{\rm d}}{{\rm d}\tau}\hat{U} = -{\rm i}\,[H_{\rm S}(t) - H_{\rm S}(t-\tau)]\,\hat{U}(\tau), \tag{F.2}$$

we can write the formal solution for $\hat{U}$ as:

$$\hat{U}(\tau) = \mathbb{I} - {\rm i}\int_0^\tau {\rm d}t' \left[H_{\rm S}(t) - H_{\rm S}(t-t')\right]\hat{U}(t'). \tag{F.3}$$

Therefore we can bound:

$$\|\Theta(t,\tau)\|_\infty = \left\| U_{\rm S}^{\rm ad\dagger}(t,0)U_{\rm S}(t,0) - {\rm i}\int_0^\tau {\rm d}t' U_{\rm S}^{\rm ad}(t,0)\left[H_{\rm S}(t) - H_{\rm S}(t-t')\right]\hat{U}(t')U_{\rm S}(t,0) - \mathbb{I}\right\|_\infty \tag{F.4a}$$

$$\leqslant \min\left\{2, \|Q(t,0)\|_\infty + \int_0^\tau {\rm d}t' \left\| \left[H_{\rm S}(t) - H_{\rm S}(t-t')\right]\right\|_\infty + O(t_{\rm f}^{-2})\right\} \tag{F.4b}$$

$$\leqslant \min\left\{2, \frac{h}{\Delta^2 t_{\rm f}} + \frac{1}{2}\tau^2 \max_{t'\in[t-\tau,t]} \|\partial_{t'} H_{\rm S}(t')\|_\infty + O(t_{\rm f}^{-2})\right\}, \tag{F.4c}$$

where we used equation (E.17) and the fact that supoperator norm between two unitaries is always upper bounded by 2 in the second line, and the standard adiabatic estimate to bound $\|Q(t,0)\|_\infty$ (recall appendix E.2). While h of equation (26) is expressed in terms of a matrix element, a more careful analysis (e.g., [10]) would replace this with an operator norm. Thus we shall make the plausible assumption that $h \sim t_{\rm f} \max_{t'\in[t-\tau,t]} \|\partial_{t'} H_{\rm S}(t')\|_\infty$, and, dropping the subdominant $O(t_{\rm f}^{-2})$, we can write

$$\|\Theta(t,\tau)\|_\infty \leqslant \min\left\{2, \frac{h}{\Delta^2 t_{\rm f}} + \frac{\tau^2 h}{t_{\rm f}}\right\}. \tag{F.5}$$

We can now bound the error term in equation (42*b*). Let $X(t,\tau) \equiv {\rm e}^{{\rm i}\,\tau H_{\rm S}(t)} U_{\rm S}^{\rm ad}(t,0)$, so that $U_{\rm S}(t-\tau,0) = X(t,\tau) + \Theta(t,\tau)$. We can then write

$$\int_0^\infty {\rm d}\tau\, A_\beta(t-\tau)\tilde{\rho}_{\rm S}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) = \int_0^\infty {\rm d}\tau\, X^\dagger(t,\tau)A_\beta X(t,\tau)\tilde{\rho}_{\rm S}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) \tag{F.6a}$$

$$+ \int_0^\infty {\rm d}\tau\, X^\dagger(t,\tau)A_\beta\Theta(t,\tau)\tilde{\rho}_{\rm S}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) + \int_0^\infty {\rm d}\tau\, X\Theta^\dagger(t,\tau)A_\beta X(t,\tau)\tilde{\rho}_{\rm S}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau) \tag{F.6b}$$

$$+ \int_0^\infty {\rm d}\tau\, \Theta^\dagger(t,\tau)A_\beta\Theta(t,\tau)\tilde{\rho}_{\rm S}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau). \tag{F.6c}$$

The first term on the rhs of (F.6*a*) is the approximation we have used in equation (42*b*). The terms in (F.6*b*) and (F.6*c*) can be bounded as follows, using equation (F.5), the unitarity of X, the fact that $\|\tilde{\rho}_S\|_\infty \leqslant 1$ and recalling that $\|A_\alpha\|_\infty = 1$. First we assume that equation (12) applies. Then:

$$\left\| \int_0^\infty \mathrm{d}\tau X^\dagger(t,\tau) A_\beta \Theta(t,\tau) \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_\infty ,$$

$$\left\| \int_0^\infty \mathrm{d}\tau X \Theta^\dagger(t,\tau) A_\beta X(t,\tau) \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_\infty$$

$$\leqslant \int_0^\infty \mathrm{d}\tau \|\Theta(t,\tau)\|_\infty |\mathcal{B}_{\alpha\beta}(\tau)| \lesssim \min\left\{ 2\tau_{\mathrm{B}}, \frac{\tau_{\mathrm{B}} h}{\Delta^2 t_{\mathrm{f}}} + \frac{\tau_{\mathrm{B}}^3 h}{t_{\mathrm{f}}} \right\}, \tag{F.7a}$$

$$\left\| \int_0^\infty \mathrm{d}\tau \Theta^\dagger(t,\tau) A_\beta \Theta(t,\tau) \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_\infty \leqslant \int_0^\infty \mathrm{d}\tau \|\Theta(t,\tau)\|_\infty^2 |\mathcal{B}_{\alpha\beta}(\tau)|$$

$$\lesssim \min\left\{ 4\tau_{\mathrm{B}}, 2\frac{\tau_{\mathrm{B}} h}{\Delta^2 t_{\mathrm{f}}} + 2\frac{\tau_{\mathrm{B}}^3 h}{t_{\mathrm{f}}} \right\}, \tag{F.7b}$$

where in the last inequality we used the fact that if $x \leqslant 2$ then $[\min(2,x)]^2 = x^2 \leqslant 2x$, and if $x \geqslant 2$ then again $[\min(2,x)]^2 = 2\min(2,x) \leqslant 2x$, with $x = \frac{h}{\Delta^2 t_{\mathrm{f}}} + \frac{\tau^2 h}{t_{\mathrm{f}}}$, in order to avoid having to extend equation (12) to higher values of n. In all, then, the approximation error in equation (42*b*) is $O[\min\{\tau_{\mathrm{B}}, \frac{\tau_{\mathrm{B}} h}{\Delta^2 t_{\mathrm{f}}} + \frac{\tau_{\mathrm{B}}^3 h}{t_{\mathrm{f}}}\}]$.

Next we recall from the discussion in section 2.3 that equation (12) must, in the case of a Markovian bath with a finite cutoff, be replaced by the weaker condition (23), reflecting fast decay up to τ_{tr}, followed by power-law decay. In this case the terms in (F.6*b*) can instead be bounded as follows:

$$\left\| \int_0^\infty \mathrm{d}\tau X^\dagger(t,\tau) A_\beta \Theta(t,\tau) \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_\infty ,$$

$$\left\| \int_0^\infty \mathrm{d}\tau X \Theta^\dagger(t,\tau) A_\beta X(t,\tau) \tilde{\rho}_{\mathrm{S}}(t) A_\alpha(t) \mathcal{B}_{\alpha\beta}(\tau) \right\|_\infty$$

$$\leqslant \int_0^{\tau_{\mathrm{tr}}} \mathrm{d}\tau \|\Theta(t,\tau)\|_\infty |\mathcal{B}_{\alpha\beta}(\tau)| + \int_{\tau_{\mathrm{tr}}}^\infty \mathrm{d}\tau \, \|\Theta(t,\tau)\|_\infty |\mathcal{B}_{\alpha\beta}(\tau)|$$

$$\lesssim \min\left\{ 2\tau_{\mathrm{B}}, \frac{\tau_{\mathrm{B}} h}{\Delta^2 t_{\mathrm{f}}} + \frac{\tau_{\mathrm{B}}^3 h}{t_{\mathrm{f}}} \right\} + 2\frac{\tau_{\mathrm{M}}^2}{\tau_{\mathrm{tr}}}, \tag{F.8}$$

in place of (F.7*b*). A similar modification can be computed for the term in (F.6*c*). To compute the order of $\frac{\tau_{\mathrm{M}}^2}{\tau_{\mathrm{tr}}}$, we recall that $\tau_{\mathrm{tr}} \sim \beta \ln(\beta\omega_{\mathrm{c}}) \gg \beta$ (equation (75)), and that $\tau_{\mathrm{M}} = \sqrt{2\beta/\omega_{\mathrm{c}}}$. Thus $\frac{\tau_M^2}{\tau_{\mathrm{tr}}} \sim [\omega_{\mathrm{c}} \ln(\beta\omega_{\mathrm{c}})]^{-1}$. It follows that we can safely ignore the $\frac{\tau_{\mathrm{M}}^2}{\tau_{\mathrm{tr}}}$ term in equation (F.8) provided equation (77) is satisfied. The analysis of the term in (F.6*c*) does not change this conclusion.

Appendix G. Derivation of the Schrödinger picture adiabatic master equation in Lindblad form

Starting from equation (53) and performing a transformation back to the Schrödinger picture, along with a double-sided adiabatic approximation, yields

$$U_{\mathrm{S}}(t,0)\int_0^t \mathrm{d}\tau\, A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)A_\alpha(t)\mathcal{B}_{\alpha\beta}(\tau)U_{\mathrm{S}}^\dagger(t,0)+\mathrm{h.c.} \tag{G.1a}$$

$$\approx \sum_{a\neq b} A_{\beta ab}(t)A_{\alpha ba}(t)\Pi_{ab}(t)\rho_{\mathrm{S}}(t)\Pi_{ba}(t)\Gamma_{\alpha\beta}(\omega_{ba}(t)) + \sum_{ab} A_{\beta aa}(t)A_{\alpha bb}(t)\Pi_{aa}(t)\rho_{\mathrm{S}}(t)\Pi_{bb}(t)\Gamma_{\alpha\beta}(0)+\mathrm{h.c.} \tag{G.1b}$$

$$= \sum_{a\neq b} L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)L_{ab,\alpha}^\dagger(t)\Gamma_{\alpha\beta}(\omega_{ba}(t)) + \sum_{ab} L_{aa,\beta}(t)\rho_{\mathrm{S}}(t)L_{bb,\alpha}^\dagger(t)\Gamma_{\alpha\beta}(0)+\mathrm{h.c.} \tag{G.1c}$$

Similarly, the other terms yield

$$-U_{\mathrm{S}}(t,0)\int_0^t \mathrm{d}\tau\, A_\alpha(t)A_\beta(t-\tau)\tilde{\rho}_{\mathrm{S}}(t)\mathcal{B}_{\alpha\beta}(\tau)U_{\mathrm{S}}^\dagger(t,0) \tag{G.2a}$$

$$\approx -\sum_{a\neq b} L_{ab,\alpha}^\dagger(t)L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)\Gamma_{\alpha\beta}(\omega_{ba}(t)) - \sum_{ab} L_{bb,\alpha}^\dagger(t)L_{aa,\beta}(t)\rho_{\mathrm{S}}(t)\Gamma_{\alpha\beta}(0)-\mathrm{h.c.} \tag{G.2b}$$

Using equations (15) and (16) for the spectral-density matrix and its complex conjugation, we are able to combine the Hermitian conjugate terms, starting from the terms in equation (G.1*c*):

$$\sum_{\alpha\beta}\Gamma_{\alpha\beta}(\omega_{ba}(t))L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)L_{ab,\alpha}^\dagger(t)+\mathrm{h.c.} \tag{G.3a}$$

$$= \sum_{\alpha\beta}\left[\Gamma_{\alpha\beta}(\omega_{ba}(t))L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)L_{ab,\alpha}^\dagger(t)+\Gamma_{\alpha\beta}^*(\omega_{ba}(t))L_{ab,\alpha}(t)\rho_{\mathrm{S}}(t)L_{ab,\beta}^\dagger(t)\right] \tag{G.3b}$$

$$= \sum_{\alpha\beta}\gamma_{\alpha\beta}(\omega_{ba}(t))L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)L_{ab,\alpha}^\dagger(t), \tag{G.3c}$$

where in the last equality we used the freedom to interchange α and β under the summation sign. Likewise, the terms in equation (G.2*b*) yield

$$\sum_{\alpha\beta}\Gamma_{\alpha\beta}(\omega_{ba}(t))L_{ab,\alpha}^\dagger(t)L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)+\mathrm{h.c.} \tag{G.4a}$$

$$= \sum_{\alpha\beta}[\Gamma_{\alpha\beta}(\omega_{ba}(t))L_{ab,\alpha}^\dagger(t)L_{ab,\beta}(t)\rho_{\mathrm{S}}(t)+\Gamma_{\alpha\beta}^*(\omega_{ba}(t))\rho_{\mathrm{S}}(t)L_{ab,\beta}^\dagger(t)L_{ab,\alpha}(t)] \tag{G.4b}$$

$$= \sum_{\alpha\beta}\gamma_{\alpha\beta}(\omega_{ba}(t))\tfrac{1}{2}\{L_{ab,\alpha}^\dagger(t)L_{ab,\beta}(t),\,\rho_{\mathrm{S}}(t)\}+\mathrm{i}\,S_{\alpha\beta}(\omega_{ba}(t))[L_{ab,\alpha}^\dagger(t)L_{ab,\beta}(t),\,\rho_{\mathrm{S}}(t)], \tag{G.4c}$$

where $\{,\}$ denotes the anticommutator. Combining these results with a similar calculation for the aa and bb terms in equations (G.1*c*) and (G.2*b*), finally results in equations (54) and (55).

Appendix H. Calculations for the spin-boson model

We recall the following basic facts about the bosonic operators appearing in equation (63), where $\{n\} \equiv \{n_k\}_k$ is the set of occupation numbers of all modes:

$$[b_k, b_{k'}^\dagger] = \delta_{kk'}, \quad b_k|\{n\}\rangle = \sqrt{n_k}|\{n_k - 1, n\}\rangle, \quad b_k^\dagger|\{n\}\rangle = \sqrt{n_k + 1}|\{n_k + 1, n\}\rangle, \tag{H.1a}$$

$$H_\mathrm{B}|\{n\}\rangle = E_{\{n\}}|\{n\}\rangle = \left(\sum_k n_k\omega_k\right)|\{n\}\rangle. \tag{H.1b}$$

Recalling that the bath operators $B_i = \sum_k g_k^i(b_k^\dagger + b_k)$, we proceed to calculate $\langle B_i(t)B_j(0)\rangle = \langle B_i^\dagger(t)B_j(0)\rangle$ assuming that the bath is in a thermal Gibbs state $\rho_\mathrm{B} = \exp(-\beta H_\mathrm{B})/\mathcal{Z}$, where $\mathcal{Z} = \mathrm{Tr}(\exp(-\beta H_\mathrm{B}))$ is the partition function. We begin by writing:

$$\begin{aligned}\langle B_i(t)B_j(0)\rangle &= \mathrm{Tr}_\mathrm{B}(U_\mathrm{B}^\dagger(t,0)B_i^\dagger U_\mathrm{B}(t,0)B_j\rho_b)\\ &= \sum_{\{m\},\{n\},\{p\}} \langle\{m\}|U_\mathrm{B}^\dagger(t,0)B_i^\dagger|\{n\}\rangle\langle\{n\}|U_\mathrm{B}(t,0)B_j|\{p\}\rangle\langle\{p\}|\rho_b|\{m\}\rangle.\end{aligned} \tag{H.2}$$

The time evolution operator acting on the eigenstates simply produces a phase, so we focus on the operator B_j's role.

$$\langle\{n\}|B_j|\{p\}\rangle = \sum_k \left(g_k^j\sqrt{p_k+1}\,\delta_{\{n\},\{p_k+1,p\}} + g_k^j\sqrt{p_k}\,\delta_{\{n\},\{p_k-1,p\}}\right). \tag{H.3}$$

Plugging this result in, we find:

$$\begin{aligned}\langle B_i(t)B_j(0)\rangle = \frac{1}{\mathcal{Z}}\sum_{\{m\},\{n\},\{p\}}\sum_{k,k'} &\mathrm{e}^{\mathrm{i}(E_{\{m\}}-E_{\{n\}})t}\mathrm{e}^{-jE_{\{m\}}}\\ &\times\Big(g_k^ig_{k'}^j\sqrt{n_k+1}\sqrt{p_{k'}+1}\,\delta_{\{m\},\{n,n_k+1\}}\delta_{\{n\},\{p,p_{k'}+1\}}\delta_{\{p\}\{m\}}\\ &+ g_k^ig_{k'}^j\sqrt{n_k}\sqrt{p_{k'}+1}\,\delta_{\{m\},\{n,n_k-1\}}\delta_{\{n\},\{p,p_{k'}+1\}}\delta_{\{p\}\{m\}}\\ &+ g_k^ig_{k'}^j\sqrt{n_k+1}\sqrt{p_{k'}}\,\delta_{\{m\},\{n,n_k+1\}}\delta_{\{n\},\{p,p_{k'}-1\}}\delta_{\{p\}\{m\}}\\ &+ g_k^ig_{k'}^j\sqrt{n_k}\sqrt{p_{k'}}\,\delta_{\{m\},\{n,n_k-1\}}\delta_{\{n\},\{p,p_{k'}-1\}}\delta_{\{p\}\{m\}}\Big).\end{aligned} \tag{H.4}$$

The only terms that are non-zero are the middle two, giving us:

$$\langle B_i(t)B_j(0)\rangle = \sum_{\{m\}}\sum_k \frac{g_k^ig_k^j}{\mathcal{Z}}(m_k+1)\left(\mathrm{e}^{-\beta E_{\{m\}}}\mathrm{e}^{\mathrm{i}(E_{\{m\}}-E_{\{m_k+1\}})t} + \mathrm{e}^{-\beta E_{\{m_k+1\}}}\mathrm{e}^{\mathrm{i}(E_{\{m_k+1\}}-E_{\{m\}})t}\right). \tag{H.5}$$

Using the fact that:

$$E_{\{m\}} - E_{\{m_k+1\}} = -\omega_k, \quad \mathcal{Z} = \prod_{k=1}^\infty\sum_{m_k=0}^\infty \mathrm{e}^{-\beta m_k\omega_k} = \prod_{k=1}^\infty \frac{1}{1-\mathrm{e}^{-\beta\omega_k}}, \tag{H.6}$$

we can write:

$$\sum_{\{m\}}(m_k+1)\,\mathrm{e}^{-\beta E_{\{m\}}} = 1 - \frac{1}{\beta}\frac{\partial_{\omega_k}\mathcal{Z}}{\mathcal{Z}} = \frac{1}{1-\mathrm{e}^{-\beta\omega_k}}. \tag{H.7}$$

We can simplify our expression to

$$\langle B_i(t)B_j(0)\rangle = \sum_k \frac{1}{1-\mathrm{e}^{-\beta\omega_k}}\left(\mathrm{e}^{-\mathrm{i}\omega_k t} g_k^i g_k^j + \mathrm{e}^{\mathrm{i}\omega_k t-\beta\omega_k} g_k^i g_k^j\right). \tag{H.8}$$

We can replace the sum with an integral:

$$\sum_k = \sum_{\omega'}\int_0^\infty \mathrm{d}\omega f(\omega)\delta(\omega-\omega') = \int_0^\infty \mathrm{d}\omega J(\omega), \tag{H.9}$$

where $f(\omega)$ is a measure of the number of oscillators at frequency ω and $J(\omega)$ is the bath spectral function. Our final result is then:

$$\langle B_i(t)B_j(0)\rangle = \int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{1-\mathrm{e}^{-\beta\omega}}\left(\mathrm{e}^{-\mathrm{i}\omega t} g_\omega^i g_\omega^j + \mathrm{e}^{\mathrm{i}\omega t-\beta\omega} g_\omega^i g_\omega^j\right), \tag{H.10}$$

where we have assumed that oscillators with the same ω_k value interact with the ith spin with the same interaction strength, i.e.

$$g_k^i = g_{k'}^i, \quad \text{if } \omega_k = \omega_{k'}. \tag{H.11}$$

Plugging our result into equation (16), we find:

$$\gamma_{ij}(\omega_{ba}(t)) = \frac{2\pi J(|\omega_{ba}(t)|)}{1-\mathrm{e}^{-\beta|\omega_{ba}(t)|}}\left(g^i_{|\omega_{ba}(t)|}g^j_{|\omega_{ba}(t)|}\Theta(\omega_{ba}(t)) + \mathrm{e}^{-\beta|\omega_{ba}(t)|}g^i_{|\omega_{ba}(t)|}g^j_{|\omega_{ba}(t)|}\Theta(-\omega_{ba}(t))\right) \tag{H.12a}$$

$$S_{ij}(\omega_{ba}(t)) = \int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{1-\mathrm{e}^{-\beta\omega}}\left(g_\omega^i g_\omega^j \mathcal{P}\left(\frac{1}{\omega_{ba}(t)-\omega}\right) + g_\omega^i g_\omega^j \mathrm{e}^{-\beta\omega}\mathcal{P}\left(\frac{1}{\omega_{ba}(t)+\omega}\right)\right), \tag{H.12b}$$

where Θ denotes the Heaviside step function.

Appendix I. Derivation of the Ohmic bath correlation function

Here we derive the bath correlation function for the Ohmic oscillator bath with a finite frequency cutoff, equation (68). We start from the simplified expression for the spectral density,

$$\gamma(\omega) = 2\pi\eta g^2 \frac{\omega \mathrm{e}^{-|\omega|/\omega_\mathrm{c}}}{1-\mathrm{e}^{-\beta\omega}}, \tag{I.1}$$

and compute the bath correlation function by inverse Fourier transform of equation (16*a*):

$$\begin{aligned}\mathcal{B}(\tau) &= \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}\omega\, \mathrm{e}^{-\mathrm{i}\omega\tau}\gamma(\omega)\\ &= \frac{\eta g^2}{\beta^2}\left(\int_{-\infty}^0 \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}x\tau/\beta}\frac{x\mathrm{e}^{x/(\beta\omega_\mathrm{c})}}{1-\mathrm{e}^{-x}} + \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}x\tau/\beta}\frac{x\mathrm{e}^{-x/(\beta\omega_\mathrm{c})}}{1-\mathrm{e}^{-x}}\right),\end{aligned} \tag{I.2}$$

where we changed variables to $x = \beta\omega$.

The Polygamma function is defined as $\psi^{(m)}(z) \equiv \frac{\mathrm{d}^{m+1}}{\mathrm{d}z^{m+1}}\ln\Gamma(z)$, where $\Gamma(z) = \int_0^\infty \mathrm{e}^{-x}x^{z-1}\mathrm{d}x$ is the Gamma function. The Polygamma function may be represented for $\Re(z) > 0$ and $m > 0$ as $\psi^{(m)}(z) = (-1)^{m+1}\int_0^\infty \frac{x^m \mathrm{e}^{-xz}}{1-\mathrm{e}^{-x}}\,\mathrm{d}x$, so that in particular, for $m = 1$, we have

$$\psi^{(1)}(z) = \int_0^\infty \frac{x\mathrm{e}^{-xz}}{1-\mathrm{e}^{-x}}\mathrm{d}x. \tag{I.3}$$

We can rewrite equation (I.2)

$$\mathcal{B}(\tau) = \frac{\eta g^2}{\beta^2}\left(\int_0^\infty \mathrm{d}x\ \frac{x\mathrm{e}^{-x[-\mathrm{i}\,\tau/\beta+1+1/(\beta\omega_\mathrm{c})]}}{1-\mathrm{e}^{-x}} + \int_0^\infty \mathrm{d}x\ \frac{x\mathrm{e}^{-x[\mathrm{i}\,\tau/\beta+1/(\beta\omega_\mathrm{c})]}}{1-\mathrm{e}^{-x}}\right) \tag{I.4a}$$

$$= \frac{\eta g^2}{\beta^2}\left(\psi^{(1)}(-\mathrm{i}\,\tau/\beta+1+1/(\beta\omega_\mathrm{c})) + \psi^{(1)}(\mathrm{i}\,\tau/\beta+1/(\beta\omega_\mathrm{c}))\right), \tag{I.4b}$$

which is the desired result.

Appendix J. Derivation of the effective rate equations in the thermal phase

Here we derive the rate equation (83).

J.1. Single qubit

For illustration, let us consider a single qubit such that the Hamiltonian is given by

$$H_\mathrm{S}(t) = A(t)\sigma^x - B(t)h_z\sigma^z. \tag{J.1}$$

The gap at any given time in the evolution is

$$\Delta(t) = 2\sqrt{A(t)^2 + B(t)^2 h_z^2}. \tag{J.2}$$

Since there are only two states, there are only three $\gamma(\omega)$ terms to calculate (assuming $g_\omega = g$):

$$\gamma(0) = \frac{2\pi g^2}{\beta}, \quad \gamma(+\Delta(t)) = 2\pi g^2 \frac{\Delta(t)}{1-\mathrm{e}^{-\beta\Delta(t)}}, \quad \gamma(-\Delta(t)) = 2\pi g^2 \frac{\Delta(t)\mathrm{e}^{-\beta\Delta(t)}}{1-\mathrm{e}^{-\beta\Delta(t)}}, \tag{J.3}$$

where we have taken the limit $\omega_\mathrm{c} \to \infty$ for simplicity. Let us consider the gapped phase of our evolution where t/t_f is small. In this phase, $B(t) \approx 0$, so we can safely assume that the energy eigenstates remain diagonal in the σ^x basis, with ground state $|-\rangle$ and excited state $|+\rangle$, and do not change such that:

$$\langle \pm|\dot{\rho}|\pm\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(\langle \pm|\rho|\pm\rangle) \equiv \dot{\rho}_{\pm\pm}. \tag{J.4}$$

The resulting equations for the density matrix elements for small times are then

$$\dot{\rho}_{++}(t) = |\langle +|\sigma^z|-\rangle|^2\left(\gamma(-\Delta(t))\rho_{--} - \gamma(\Delta(t))\rho_{++}\right) = \gamma_0(\Delta(t))\left(\mathrm{e}^{-\beta\Delta(t)}\rho_{--} - \rho_{++}\right), \tag{J.5a}$$

$$\rho_{--}(t) = 1 - \rho_{++}(t), \tag{J.5b}$$

where we have used that $\langle +|\sigma^z|+\rangle = \langle -|\sigma^z|-\rangle = 0$, $\langle +|\sigma^z|-\rangle = 1$ and $[H_\mathrm{S}, \rho_\mathrm{S}] \approx 0$. Interpreting equation (J.5) as a rate equation, we see that $\gamma(+\Delta)$ is associated with relaxation from the higher energy state to the lower energy state, and $\gamma(-\Delta(t))$ is associated with the excitation from the lower energy state to the higher energy state. Note that at $t = 0$, we assume that the system is initialized in a thermal state such that $\rho_{++}/\rho_{--} = \mathrm{e}^{-\beta\Delta(0)} \approx 10^{-11}$. Since the gap remains relatively large during the gapped phase, the change in the initial thermal state is minimal.

J.2. N qubits

For the N-qubit case, we can simply generalize our arguments for the single qubit case. For sufficiently small times the system is diagonal in the σ^x basis, and the lowest lying energy states can be considered to be single spin flips in the x-direction. Furthermore, the gap between the ground state and the first excited states is $\Delta(t) = 2A(t)$ (equation (80)), which is large in our case. We can restrict ourselves to only these low lying energy states since higher excited states will have twice the gap to the ground state, and so their contribution will be further suppressed at short times.

Now, using equation (81) and the KMS condition (equation (82)) we find a similar set of equations as in the single qubit case:

$$\dot{\rho}_{ii} \approx \sum_{\alpha\beta} \gamma_{\alpha\beta}(\omega_{i0}) \langle 0|\sigma_\beta^z|i\rangle \langle i|\sigma_\alpha^z|0\rangle \left(-\rho_{ii} + \mathrm{e}^{-\beta\omega_{i0}}\rho_{00}\right) = \gamma_{ii}(\omega_{i0}) \left(\mathrm{e}^{-\beta\omega_{i0}}\rho_{00} - \rho_{ii}\right) \tag{J.6a}$$

$$\rho_{00} \approx 1 - N\rho_{ii}, \tag{J.6b}$$

where we have again assumed that the initial state is the thermal state and the gap is large.

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