

Ultrastrongly coupled open systems and fine grained time

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Abstract

We study the dynamics of a d -level quantum system coupled to a bosonic reservoir when the coupling constant is large. It is known that in the limit of infinite coupling strength, the system undergoes an instantaneous nonselective measurement, resulting in the immediate decoherence in the measurement basis, followed by a unitary Zeno dynamics. Here we resolve this dynamical process by introducing a fine grained scaling regime of short times proportional to the inverse coupling. We provide a rigorous derivation of the open system dynamics in this regime of ultrastrong coupling and demonstrate how decoherence unfolds continuously in the new time scale. We show that Markovian dynamics which are not given by semigroups arise naturally, in contrast to what happens in the weak coupling theory.

1 Introduction

An open quantum system is a (typically small) quantum system S interacting with another system (much larger and typically infinite) called the reservoir R . The compound SR evolves

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arbitrary values of the coupling constant λ , by a so-called polaron transformation. This gives rise to the strategy of splitting the dynamics into an exactly solvable part for arbitrary λ and times t , which is then perturbed by the non commuting part of the system Hamiltonian. Rigorous results in this regime have been obtained in [11, 17]; see also the recent analysis of [26, 10]. A different approach is the so-called reaction-coordinate mapping, that amounts to incorporating some degrees of freedom of the reservoir into the system and treating the remaining ones perturbatively as an effective bath [1, 2, 25]. Despite these advances, so far the methods are tailored to specific models and a general mathematical treatment is not available for the regime of strong coupling [27], in contrast to the ultraweak and weak coupling regimes.

The *Zeno coupling* limit is $t > 0$ fixed and $\lambda \rightarrow \infty$. It is shown in [14] that the system undergoes the *Zeno effect* in this limit, namely, it experiences instantaneous nonselective measurement in the eigenbasis of the coupling operator, followed by a residual dynamics generated by a Zeno Hamiltonian. The effect of the nonselective measurement on the system density matrix, is to delete (set to zero) all non-diagonal density matrix elements while leaving the diagonal unchanged. This means that the system undergoes instantaneous decoherence in the given basis due to the Zeno, “ $\lambda = \infty$ ” coupling limit. This causes a discontinuity in the system state at time $t = 0_+$. Of course one expects that if λ is large but finite, then the system decoherence due to the coupling to the reservoir, would proceed at a finite speed and in a continuous fashion. Therefore, in an attempt to temporally resolve the decoherence process, we investigate here the regime of large but finite λ , and small but nonzero times t , such that $\tau = \lambda t$ is an arbitrary but fixed number,

$$\lambda \rightarrow \infty, \quad t \rightarrow 0_+, \quad \tau = \lambda t \in (0, \infty). \quad (1)$$

We call (1) the ultrastrong coupling regime¹ (see also Figure 1) and τ is the *fine grained* time. It is akin to the coarse grained $\tau' = \lambda^2 t$ with $\lambda \rightarrow 0$ and $t \rightarrow \infty$ appearing in the ultraweak coupling theory.

We show in Section 3 that in the ultrastrong coupling limit (1), the system density matrix $\rho_S(\tau)$ varies continuously in the fine grained time τ , and connects continuously to the initial system state for $\tau \rightarrow 0_+$ and to the fully decohered (measured) density matrix at $\tau \rightarrow \infty$. The decoherence process is determined by a decoherence function which depends on the properties of the reservoir initial state and the reservoir part of the interaction. For a typical SR model with a bosonic reservoir (of the ‘spin-boson’ type) in a thermal equilibrium state (at any temperature — or more generally for any Gaussian reservoir state), the decoherence function behaves as $e^{-\alpha\tau^2}$ for some $\alpha > 0$.

In Section 4 we analyze the Markovianity properties of the dynamics $\rho_S(\tau) = \Lambda(\tau)\rho_S(0)$. We show in particular that for a large group of models (including all Gaussian reservoir states) the dynamics is Markovian, but it is not given by a semigroup. The introduction of the fine grained time scaling regime and the analysis of the resulting open system evolution, is the main novelty of this work. Here we deal with finite dimensional systems S . The question of decoherence in continuous variable systems, in particular spatial decoherence, is of great interest in the context of open many-body systems. We study this in [15].

Structure of the paper. In Section 2 we recall the setting and main result of [14] on the Zeno dynamics in the limit of infinite coupling. In Section 3 we introduce the new scaling (fine

¹In [14] ultrastrong coupling refers to the limit $\lambda \rightarrow \infty$ with fixed t . We propose to call this the Zeno regime while ultrastrong is reserved for (1). This seems more natural by analogy with the ultraweak coupling regime.

graining of time) that allows to resolve the decoherence process. We derive the open system dynamics in this ultrastrong coupling regime for arbitrary coupling operators. In Section 4 we discuss the characterization of Markovianity for the mentioned dynamics, building on results already available in the literature for pure dephasing processes. We analyze the case of spin-boson models in Section 5.

2 Zeno effect for spin-boson systems as $\lambda \rightarrow \infty$

In this section we present the model of an open system which was used in [14] to derive the Zeno measurement effect on a system S caused by infinitely large coupling to an environment R. The main result of [14] is Theorem 1 below.

A d -level quantum system is coupled to a reservoir with a continuum of modes labeled by $k \in \mathbb{R}^3$, with Bosonic creation and annihilation operators $a^\dagger(k), a(k)$, satisfying the canonical commutation relation $[a(k), a^\dagger(l)] = \delta(k - l)$. The total Hamiltonian is given by

$$H = H_S + H_R + \lambda G \otimes \varphi(g), \quad (2)$$

where H_S is the system Hamiltonian, that is a $d \times d$ hermitian matrix and

$$H_R = \int_{\mathbb{R}^3} \omega(k) a^\dagger(k) a(k) d^3k \quad (3)$$

is the reservoir Hamiltonian. In (3), $\omega(k) \geq 0$ is the energy of the mode k ('dispersion relation'). One may think of the photon dispersion relation $\omega(k) = |k|$, but this is not necessary for our analysis. The interaction term in (2) carries a *coupling constant* $\lambda \in \mathbb{R}$, a system coupling operator

$$G = \sum_{l=1}^{\nu} \gamma_l P_l \quad (4)$$

with distinct (possibly degenerate) eigenvalues γ_j and spectral projections P_l ($\dim P_l \geq 1$), and the field operator

$$\varphi(g) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}^3} (g(k) a^\dagger(k) + \text{h.c.}) d^3k, \quad (5)$$

where $g(k)$ is a complex valued function, called the form factor.

As is known (and discussed in [14]), because H_R has absolutely continuous spectrum one cannot define the reservoir equilibrium state as a density matrix $\propto e^{-\beta H_R}$ (this operator is not trace class, $\text{tr} e^{-\beta H_R} = \infty$). Rather, the construction of the continuous mode equilibrium state is done by taking a limit of discrete mode equilibrium states (the 'thermodynamic limit'). It results in an expectation functional $\omega_{R,\beta}$ for reservoir observables (built from functions of $a^\dagger(k), a(l)$), which can be expressed entirely by the *characteristic function*

$$\omega_{R,\beta}(W(f)) = e^{-\frac{1}{4} \langle f, \coth(\beta\omega/2) f \rangle}. \quad (6)$$

Here, $\langle f, h \rangle = \int_{\mathbb{R}^3} \overline{f(k)} g(k) d^3k$ is the inner product of $L^2(\mathbb{R}^3, d^3k)$ and $W(f)$ is the unitary *Weyl operator*,

$$W(f) = e^{i\varphi(f)} \quad (7)$$

with $\varphi(f)$ as in (5). The characteristic function (6) is also called the generating function, as it can be used to express the expectation for any observable by using the relation $\varphi(f) = -i\partial_\alpha|_{\alpha=0}W(\alpha f)$. One then finds that the two-point function of the reservoir equilibrium state is given by

$$\omega_{\text{R},\beta}(a^\dagger(k)a(l)) = \frac{\delta(k-l)}{e^{\beta\omega(k)} - 1}. \quad (8)$$

This encodes Planck's law of black body radiation, where $n(k) = (e^{\beta\omega(k)} - 1)^{-1}$ is the momentum density distribution in the reservoir. (That is, the number of modes per unit volume in a given region $\Lambda \in \mathbb{R}^3$ in momentum space is $\int_\Lambda n(k)d^3k$.)

The state (6) is Gaussian and centered. Its covariance operator $\mathcal{C}$ acting on $L^2(\mathbb{R}^3, d^3k)$ is the operator of multiplication with the function $\coth(\beta\omega/2)$. We may consider more general Gaussian states of the form

$$\omega(W(f)) = e^{-\frac{1}{4}\langle f, \mathcal{C}f \rangle}, \quad (9)$$

where $\mathcal{C}$ is a general covariance operator on $L^2(\mathbb{R}^3, d^3k)$, satisfying

$$\mathcal{C} \geq \mathbb{1}. \quad (10)$$

The condition (10) is known to be necessary and sufficient for the right hand side of (9) to be the expectation functional of a quantum state; the case $\mathcal{C} = \mathbb{1}$ is the field vacuum (zero temperature case). Instead of the thermal distribution (8) we may consider reservoir states with an arbitrary energy distribution $\mu(k) \geq 0$, $\omega_{\text{R}}(a^\dagger(k)a(l)) = \mu(k)\delta(k-l)$, which corresponds to the covariance (compare with (6)) $\mathcal{C} = C(k) = 1 + 2\mu(k)$. The corresponding state ω_{R} (9) is stationary, $\omega_{\text{R}}(e^{itH_{\text{R}}}W(f)e^{-itH_{\text{R}}}) = \omega_{\text{R}}(W(e^{it\omega}f)) = \omega_{\text{R}}(W(f))$. Covariance operators $\mathcal{C}$ which are not multiplication operators by a function of k result in non-stationary Gaussian reservoir states, and they are included in the discussion and results.

We take initial system-reservoir states are of the form

$$\omega_{\text{SR}} = \omega_{\text{S}} \otimes \omega_{\text{R}}, \quad (11)$$

where ω_{R} is the Gaussian state (9) for a general covariance operator $\mathcal{C} \geq \mathbb{1}$, and where

$$\omega_{\text{S}}(\cdot) = \text{tr}_{\text{S}}(\rho_{\text{S}} \cdot) \quad (12)$$

is a system state determined by a density matrix ρ_{S} of the d -level system with Hilbert space $\mathbb{C}^d$. Let $A \in \mathcal{B}(\mathbb{C}^d)$ be a system observable. The reduced system density matrix $\rho_{\text{S}}(t)$ at time $t \geq 0$ in the Zeno limit is defined by the relation

$$\text{tr}_{\text{S}}(\rho_{\text{S}}(t)A) = \lim_{\lambda \rightarrow \infty} \omega_{\text{S}} \otimes \omega_{\text{R}}(e^{itH}(A \otimes \mathbb{1}_{\text{R}})e^{-itH}), \quad (13)$$

holding for all system observables $A \in \mathcal{B}(\mathbb{C}^d)$.

We make the following assumptions on the form factor $g(k)$ and the dispersion $\omega(k)$ in the Hamiltonian (2),

(A1) We have the regularity property

$$\mathcal{C}^{1/2} \frac{e^{i\omega(k)t} - 1}{\omega(k)} g(k) \in L^2(\mathbb{R}^3, d^3k), \quad \forall t > 0 \quad \text{and} \quad \frac{g(k)}{\omega(k)} \in L^2(\mathbb{R}^3, d^3k). \quad (14)$$

(A2) We have the effective coupling property

$$g(k) \neq 0 \quad \text{for } k \in \mathbb{R}^3 \text{ satisfying } a < |k| < b \text{ for some } 0 \leq a < b. \quad (15)$$

The condition (14) is used in the so-called *polaron transformation* (see [14]). However, if one assumes some regularity on the state (9) then the condition (14) is not needed. In particular, it is not needed if the reservoir state is the thermal state $\omega_{R,\beta}$, for any $0 < \beta \leq \infty$. We explain this further in [14]. The non-vanishing condition (15) on g is satisfied for instance if g is continuous (and not the zero function) — it guarantees that the system is coupled in an effective way to the reservoir.

Theorem 1 (Zeno coupling, [14]). *Assume conditions (A1) and (A2). Then for all $t > 0$,*

$$\rho_S(t) = e^{-itH_Z} \left(\sum_{l=1}^{\nu} P_l \rho_S P_l \right) e^{itH_Z}, \quad (16)$$

where H_Z is the Zeno Hamiltonian (see (4))

$$H_Z = \sum_{l=1}^{\nu} P_l H_S P_l. \quad (17)$$

The result shows that in the Zeno coupling limit ($t > 0$ fixed, $\lambda \rightarrow \infty$), the system dynamics is that of a non-selective measurement with respect to the measurement observable G (defining the interaction, see (2))

$$\rho_S \mapsto \sum_{l=1}^{\nu} P_l \rho_S P_l$$

plus a Schrödinger dynamics generated by the Hamiltonian H_Z . The dynamics is happening independently on spectral subspaces $\text{Ran} P_l$ of G — the Hamiltonian H_Z is block diagonal with respect to the decomposition

$$\mathcal{H}_S = \bigoplus_{l=1}^{\nu} \text{Ran} P_l.$$

In the case when G has simple spectrum, $\dim P_l = 1$ for all l , the blocks of H_Z are 1×1 and then (16) reduces to the time-independent state (Zeno effect)

$$\rho_S(t) = \sum_{l=1}^{\nu} P_l \rho_S P_l, \quad t > 0.$$

The right side is the state after a non-selective von Neumann projective measurement, associated to the measurement observable G , has been performed on ρ_S . The Zeno coupling implements an *instantaneous* measurement on the system S . Unless the initial state ρ_S is already block diagonal, the measurement causes a discontinuity in the dynamics at $t = 0$,

$$\lim_{t \rightarrow 0_+} \rho_S(t) \neq \rho_S. \quad (18)$$

Let us try to understand heuristically why the Zeno limit implements instantaneous decoherence. For this we consider a Hamiltonian of the SR-type (2), given by

$$H(\varepsilon, \lambda) = \varepsilon H_S + H_R + \lambda G \otimes X, \quad (19)$$

where ε is another parameter and X is a reservoir operator. Let $\rho_S(t)$ be the reduced system density matrix at time t . It depends on ε and λ . Let $\{\psi_k\}$ be an eigenbasis of G . The populations of the density matrix $\rho_S(t)$ in this basis are (by definition) the diagonal density matrix elements, $\langle \psi_k, \rho_S(t) \psi_k \rangle$. The change of the populations for small times are given by

$$\partial_t|_0 \text{tr}_S(\rho_S(t) |\psi_k\rangle \langle \psi_k|) = -i\omega_{SR} \left([H(\varepsilon, \lambda), |\psi_k\rangle \langle \psi_k| \otimes \mathbb{1}_R] \right) = -i\varepsilon\omega_S \left([H_S, |\psi_k\rangle \langle \psi_k|] \right) \propto \varepsilon, \quad (20)$$

(we assume $\omega_{SR} = \omega_S \otimes \omega_R$) while change of the coherences, which (by definition) are the off-diagonal density matrix elements in the G -eigenbasis, are given for small times by

$$\begin{aligned} \partial_t|_0 \text{tr}_S(\rho_S(t) |\psi_k\rangle \langle \psi_l|) &= -i\omega_{SR} \left([H(\varepsilon, \lambda), |\psi_k\rangle \langle \psi_l| \otimes \mathbb{1}_R] \right) \\ &= -i\varepsilon\omega_S \left([H_S, |\psi_k\rangle \langle \psi_l|] \right) - i\lambda(\gamma_k - \gamma_l)\omega_S(|\psi_k\rangle \langle \psi_l|)\omega_R(X) \\ &= \varepsilon C_{k,l} + \lambda C''_{k,l}. \end{aligned} \quad (21)$$

It follows from (20), (21) that for $\lambda \gg \varepsilon$ the time scale $\propto 1/\varepsilon$ at which the populations change is much longer than the time scale $\propto 1/\lambda$ at which the coherences change. (If $C''_{k,l} = 0$, say for $\omega_R(X) = 0$ then one looks at the second derivative at zero which is $\propto \lambda^2 \omega_R(X^2)$.) This is the heuristic reason why, in the setting of the Zeno coupling of Section 2, where $\varepsilon = 1$, $t > 0$ fixed and $\lambda \rightarrow \infty$, the coherences of $\rho_S(t)$ in the G eigenbasis evolve very fast leading to the instantaneous projective measurement and successive Zeno dynamics while the populations are constant (see (16)).

In order to resolve the dynamics of the measurement process induced by the Zeno limit, we must look at finite but large coupling constants λ and short times t . This leads us to consider the *ultrastrong coupling regime* (1).

3 Fine graining of time

Consider a SR bipartite open system with Hilbert space

$$\mathcal{H}_{SR} = \mathcal{H}_S \otimes \mathcal{H}_R \quad (22)$$

with

$$\dim \mathcal{H}_S = d < \infty$$

and Hamiltonian

$$H(\lambda) = H_S + H_R + \lambda G \otimes X \quad (23)$$

where $\lambda \in \mathbb{R}$, H_S and H_R are the Hamiltonians of the system and the reservoir, and where G and X are self-adjoint operators on the Hilbert spaces $\mathcal{H}_S$ and $\mathcal{H}_R$ of the system and the reservoir, respectively. Let

$$\omega_{SR} = \omega_S \otimes \omega_R \equiv \text{tr}_S(\rho_S \cdot) \otimes \text{tr}_R(\rho_R \cdot) \quad (24)$$

be the initial SR state, where the ρ_S and ρ_R are density matrices of S and R.² We are interested in the dynamics of the system, described by the density matrix

$$\rho_S(t) = \text{tr}_R(e^{-itH(\lambda)}(\rho_S \otimes \rho_R)e^{itH(\lambda)}) \quad (25)$$

on $\mathcal{H}_S$. In (25) the trace is a partial one, taken over $\mathcal{H}_R$. In terms of the fine grained time $\tau = \lambda t$, (1), the propagator of the dynamics (25) is

$$e^{-itH(\lambda)} = e^{-i\tau\left(\frac{H_S+H_R}{\lambda}+G\otimes X\right)}. \quad (26)$$

We obtain formally,

$$\lim_{\substack{t \rightarrow 0+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} e^{-itH(\lambda)} = e^{-i\tau G \otimes X}. \quad (27)$$

For bounded operators H_R, X (H_S, G are automatically bounded as we assume $\dim \mathcal{H}_S < \infty$) the equality (27) in the sense of operator norm convergence follows directly from ($H_0 = H_S + H_R$)

$$e^{-i\tau\left(\frac{H_0}{\lambda}+G\otimes X\right)} - e^{-i\tau G \otimes X} = \frac{-i}{\lambda} \int_0^\tau e^{-is\left(\frac{H_0}{\lambda}+G\otimes X\right)} H_0 e^{i(s-\tau)G \otimes X} ds.$$

However, we are usually interested in unbounded reservoir operators H_R and X , and the precise meaning of the limit (27) needs to be elucidated. We do this later in Section 5 for spin-Boson type models. For now we examine some implications of (27). From (25) and (27) we obtain for $\tau > 0$,

$$\varrho_S(\tau) \equiv \lim_{\substack{t \rightarrow 0+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \rho_S(t) = \text{tr}_R(e^{-i\tau G \otimes X}(\rho_S \otimes \rho_R)e^{i\tau G \otimes X}). \quad (28)$$

Using the diagonal form (4) of G gives

$$\varrho_S(\tau) = \sum_{l,r=1}^{\nu} D_{l,r}(\tau) P_l \rho_S P_r, \quad \text{with} \quad D_{l,r}(\tau) \equiv \text{tr}_R(\rho_R e^{-i\tau(\gamma_l - \gamma_r)X}). \quad (29)$$

As $D_{l,r}(0) = 1$ the continuity at time zero is restored,

$$\lim_{\tau \rightarrow 0+} \varrho_S(\tau) = \rho_S. \quad (30)$$

Assume that $\lim_{|s| \rightarrow \infty} \text{tr}_R(\rho_R e^{isX}) = 0$. Then (29) shows that

$$\lim_{\tau \rightarrow \infty} \varrho_S(\tau) = \sum_l P_l \rho_S P_l. \quad (31)$$

In the $\tau \rightarrow \infty$ limit we thus recover the Zeno result (albeit with $H_S = 0$, as the effect of H_S is eliminated by taking $t \rightarrow 0$ in the current scaling, (28)). The function

$$D(s) = \omega_R(e^{-isX}), \quad s \in \mathbb{R}, \quad (32)$$

²For the reservoir typically the state is obtained by a thermodynamic limit and so ω_R should generally be viewed as a state in the algebraic sense, that is, a positive normalized functional on an algebra of observables. Then, by the Gelfand-Naimark-Segal construction, ω_R can always be represented by a density matrix (of rank one even) on a suitable Hilbert space.

is of positive type, meaning that the matrix D with elements $D_{ij} = D(s_i - s_j)$ is a positive semidefinite matrix for any $s_1, \dots, s_N$ and any $N \geq 1$.³ Moreover, $D(0) = 1$. Suppose that D is continuous. Then it follows from Bochner's theorem that there exists a unique Borel probability measure μ on $\mathbb{R}$ such that

$$D(s) = \int_{\mathbb{R}} d\mu(\alpha) e^{-i\alpha s}. \quad (33)$$

If $D(s)$ is a square integrable function, that is,

$$\int_{\mathbb{R}} |D(s)|^2 ds < \infty,$$

then we have

$$d\mu(\alpha) = \mu(\alpha) d\alpha, \quad \mu(\alpha) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\alpha s} D(s) ds. \quad (34)$$

This follows from (33) and the Fourier inversion theorem on $L^2(\mathbb{R}, ds)$ and the uniqueness of $d\mu(\alpha)$ for a given $D(s)$. We summarize these findings in the following result.

Theorem 2. *For all $\tau > 0$, the state $\varrho_S(\tau)$, (28) has the expression*

$$\varrho_S(\tau) = \sum_{l,r=1}^{\nu} D_{l,r}(\tau) P_l \rho_S P_r \quad (35)$$

$$= \int_{\mathbb{R}} e^{i\tau\alpha G} \rho_S e^{-i\tau\alpha G} d\mu(\alpha) \quad (\text{if } D(s) \text{ is continuous}) \quad (36)$$

$$= \int_{\mathbb{R}} \mu(\alpha) e^{i\tau\alpha G} \rho_S e^{-i\tau\alpha G} d\alpha \quad (\text{if } D(s) \text{ is continuous and square integrable}) \quad (37)$$

where $D_{l,r}(\tau) = D(\tau(\gamma_l - \gamma_r))$, μ the measure given by (33), which satisfies (34) for square integrable D .

According to (35) the populations (in the eigenbasis of G) are time-independent; this can be understood as a consequence of the fact that in the considered limit $t \rightarrow 0$, the system Hamiltonian H_S does not play any role (see also (80)). The second and third equality in (35) show that $\varrho_S(\tau)$ is a convex combination of density matrices $e^{i\tau\alpha G} \rho_S e^{-i\tau\alpha G}$, each following a Markovian dynamics at a different speed given by the scaling of time, $\tau\alpha$ for varying α . It is known that a convex combination of Markovian dynamics is generally non-Markovian [29]. We now investigate the Markovianity properties of $\Lambda(\tau) : \rho_S \rightarrow \varrho_S(\tau)$ more closely.

4 Markovianity in the fine grained time regime

4.1 General Results

Motivated by (35) we consider the dynamics of density matrices ρ of dimension $d \times d$ given by a dynamical map $\Lambda(\tau)$ of the form

$$\Lambda(\tau)\rho = \sum_{l,r=1}^{\nu} D_{l,r}(\tau) P_l \rho P_r, \quad (38)$$

³Let $N \geq 1$, denote the inner product of $\mathbb{C}^N$ by $\langle \cdot, \cdot \rangle$ and let $z = (z_1, \dots, z_N)^T \in \mathbb{C}^N$. Then $\langle z, Dz \rangle = \omega_R(Y^\dagger Y) \geq 0$, where $Y = \sum_{l=1}^N z_l e^{is_l X}$. So D is positive semidefinite.

where $\tau \geq 0$ and the P_l are a complete family of orthogonal projections (possibly of rank higher than one, in which case $\nu < d$),

$$P_l^\dagger = P_l, \quad P_l P_r = \delta_{l,r} P_l, \quad \sum_{l=1}^{\nu} P_l = \mathbb{1}. \quad (39)$$

We assume that for each $\tau \geq 0$, $D_{l,r}(\tau)$ defines a positive definite matrix, that $D_{l,r}(0) = 1$ and that $D_{l,l}(\tau) = 1$. As we show below, these assumptions imply that $\Lambda(\tau)$ is completely positive, that $\Lambda(0) = \mathbb{1}$ and that $\Lambda(\tau)$ is trace preserving, respectively. In order to study the Markovianity of $\Lambda(\tau)$, we further assume that $D_{l,r}(\tau) \neq 0$ for all l, r and $\tau \geq 0$, so that the inverse map $\Lambda(\tau)^{-1}$ exists⁴ for all $\tau \geq 0$ and reads explicitly

$$\Lambda(\tau)^{-1} \rho = \sum_{l,r=1}^{\nu} (D_{l,r}(\tau))^{-1} P_l \rho P_r. \quad (40)$$

An invertible map $\Lambda(\tau)$ is called CP-divisible if the intermediate propagator

$$V(\tau, \sigma) := \Lambda(\tau) \Lambda(\sigma)^{-1} \quad (41)$$

is completely positive for all $\tau \geq \sigma \geq 0$. CP-divisibility is one of the definitions of quantum Markovianity [3]. If $V(\tau, \sigma)$ is positivity preserving then $\Lambda(\tau)$ is called P-divisible. Maps that are P-divisible but not CP-divisible are called weakly non-Markovian. If there is a $\tau \geq \sigma \geq 0$ such that $V(\tau, \sigma)$ is not positive, then the dynamics is called essentially non-Markovian.

Based on (38) and (40) we have

$$V(\tau, \sigma) \rho = \sum_{l,r=1}^{\nu} Q_{l,r}(\tau, \sigma) P_l \rho P_r, \quad \text{where} \quad Q_{l,r}(\tau, \sigma) := \frac{D_{l,r}(\tau)}{D_{l,r}(\sigma)}, \quad (42)$$

so that the map $V(\tau, \sigma)$ has the same structure as $\Lambda(\tau)$ with a different coefficient matrix. For this class of dynamics and rank-one projections P_l , the Markovianity properties have been studied in [13] (Proposition 4.1). Our next result is a slight generalization to arbitrary rank.

Proposition 1 (Slight generalization of Lonigro-Chruściński [13]). *Let P_l , $l = 1, \dots, \nu$ be a family of projections on $\mathbb{C}^d$ satisfying (39) and let $A = (A_{l,r})$ be a $\nu \times \nu$ complex matrix. Consider the map $\Pi_A \rho = \sum_{l,r=1}^{\nu} A_{l,r} P_l \rho P_r$, where ρ is an operator on $\mathbb{C}^d$. The following are equivalent:*

- (a) Π_A is CP
- (b) Π_A is P
- (c) A is positive semi-definite

Proof of Proposition 1. The proof follows closely [13]. To see that (c) $\Rightarrow$ (a) we note that for a positive definite A , the formula $\sum_{l,r=1}^{\nu} A_{l,r} P_l(\cdot) P_r$ is a (non-diagonal) Kraus representation for Π_A and therefore Π_A is CP. By definition, (a) $\Rightarrow$ (b). Finally, the implication (b) $\Rightarrow$ (c) is proved

⁴The characterization of Markovianity for non-invertible maps is more involved, see for instance [5].

by showing the contrapositive. This is the only part where the rank of the projections plays a role. We will show that if A is not positive semi-definite, then there are vectors $x = (x_1, \dots, x_d)$, $y = (y_1, \dots, y_d) \in \mathbb{C}^d$ such that $\langle x, (\Pi_A|y\rangle\langle y|)x \rangle < 0$. We consider the canonical basis as the one in which the P_l are diagonal. We have

$$\langle x, (\Pi_A|y\rangle\langle y|)x \rangle = \sum_{l,r=1}^{\nu} A_{l,r} \langle x, P_l y \rangle \langle y, P_r x \rangle = \langle v, Av \rangle,$$

where $v = (v_1, \dots, v_{\nu}) \in \mathbb{C}^{\nu}$ is the vector with components $v_k = \langle y, P_k x \rangle$. (Note that the last inner product above is that of $\mathbb{C}^{\nu}$ while other ones are that of $\mathbb{C}^d$.) Suppose that A is not positive definite. Then there is a (normalized) $v \in \mathbb{C}^{\nu}$ such that $\langle v, Av \rangle < 0$. Choosing $x = (1, \dots, 1)$ we have $\langle y, P_k x \rangle = \sum_{j \in J_k} y_j$, where J_k is the set of indices associated with the coordinates of the subspace $\text{Ran} P_k$. Now we take $y_j = \frac{v_k}{|J_k|}$ for $j \in J_k$, and we do this for all k . Then $\langle y, P_k x \rangle = v_k$ for all k . It follows that $\langle x, (\Pi_A|y\rangle\langle y|)x \rangle < 0$, which shows that $\Pi_A|y\rangle\langle y|$ is not positive definite, hence Π_A is not positivity preserving. This completes the proof of Proposition 1. $\square$

Applying the Proposition 1 to $A = (Q_{l,r}(\tau, \sigma))$ given in (42) we obtain the next result.

Corollary 1. *The following statements about the dynamics $\Lambda(\tau)$, (38) are equivalent:*

- (a) $\Lambda(\tau)$ is CP-divisible
- (b) $\Lambda(\tau)$ is P-divisible
- (c) The $\nu \times \nu$ matrix $Q = (Q_{l,r}(\tau, \sigma))_{l,r}$ defined in (42) is positive semi-definite for every $\tau \geq \sigma \geq 0$

A necessary condition for CP-divisibility is $|D_{l,r}(\tau)| \leq |D_{l,r}(\sigma)|$ for $\tau \geq \sigma \geq 0$. This is also sufficient for $d = 2$.

Proof of Corollary 1. The equivalences follow directly from Proposition 1 applied to the map $\Pi_{Q(\tau, \sigma)} = V(\tau, \sigma)$. Moreover, the positive semi-definiteness of Q implies that all principal minors are nonnegative (see e.g. the equivalent characterizations of positive semi-definite matrices in [22] p. 566). In particular, all 2×2 principal minors are nonnegative, i.e. for any pair of indices i_1, i_2 we have

$$Q_{i_1, i_1}(\tau, \sigma)Q_{i_2, i_2}(\tau, \sigma) - Q_{i_1, i_2}(\tau, \sigma)Q_{i_2, i_1}(\tau, \sigma) \geq 0. \quad (43)$$

Using (42), the hermiticity $D_{l,r}(\tau) = \overline{D_{r,l}(\tau)}$ and $D_{r,r}(\tau) = 1$, we obtain from (43) that $|Q_{l,r}(\tau, \sigma)|^2 \leq 1$, which implies $|D_{l,r}(\tau)| \leq |D_{l,r}(\sigma)|$ for $\tau \geq \sigma \geq 0$. Finally, for $d = 2$, Q is a 2×2 matrix with trace equal to 2. Therefore, it is positive semi-definite whenever the determinant is nonnegative, which in turn is guaranteed by the monotonicity of $|D_{l,r}(\tau)|$, as we just discussed. Corollary 1 is proven. $\square$

Counterexample: Monotonicity without CP-divisibility. We now show that already for $d = 3$ the monotonicity condition in Corollary 1 is not sufficient for CP-divisibility. The matrix

$$D = \begin{pmatrix} 1 & a & b \\ a & 1 & a \\ b & a & 1 \end{pmatrix}, \quad a, b \geq 0, \quad (44)$$

has determinant $\det D = (1 - b)(1 + b - 2a^2)$. Let $D(\tau)$ be the matrix D with $a(\tau) = e^{-\tau/4}$ and $b(\tau) = (1 + \tau^3/2)^{-1}$. One easily sees that $D(\tau) \geq 0$ for all $\tau \geq 0$ (check for instance that all the principal minors are non-negative) and furthermore, the matrix elements $D_{l,r}(\tau)$ satisfy $|D_{l,r}(\tau)| \leq |D_{l,r}(\sigma)|$ for $\tau \geq \sigma \geq 0$. However, there are $\tau \geq \sigma \geq 0$ such that the matrix $Q(\tau, \sigma)$ with the elements $Q_{l,r}(\tau, \sigma) = D_{l,r}(\tau)/D_{l,r}(\sigma)$ is not positive semi-definite. Indeed, $Q(\tau, \sigma)$ is again of the form (44) above, with matrix elements $a(\tau, \sigma) = e^{-(\tau-\sigma)/4}$ and $b(\tau, \sigma) = (2 + \sigma^3)/(2 + \tau^3)$. The 2×2 principal minors of $Q(\tau, \sigma)$ are always non-negative, therefore $Q(\tau, \sigma)$ is positive semi-definite if and only if $\det Q(\tau, \sigma) \geq 0$. Now

$$\det Q(\tau, \sigma) = \left(1 - \frac{2 + \sigma^3}{2 + \tau^3}\right) \left(1 + \frac{2 + \sigma^3}{2 + \tau^3} - 2e^{-(\tau-\sigma)/2}\right)$$

and the first factor is strictly positive for all $\tau > \sigma$. For $\tau = 2$ and $\sigma = 3/2$ the second factor is $< -1/50$. It follows that $Q(2, 3/2)$ is not positive semi-definite.

Remark. The counterexample we provided has a different qualitative time-dependence for the different matrix elements of $D(\tau)$. However, dynamical maps that are obtained in the fine-grained-time regime from the interaction with a reservoir correspond to $D_{l,r}(\tau) = \omega_R(e^{-i\tau(\gamma_l - \gamma_r)X})$, so that the different matrix elements share the same functional form of the time-dependence. Finding a counterexample within this class seems more difficult. In particular, for a natural ansatz like $D_{l,r}(\tau) = e^{-a_{lr}\tau^\alpha}$, with non-negative coefficients a_{lr} and some exponent $\alpha > 0$, one has that $D(\tau) \geq 0 \Rightarrow Q(\tau, \sigma) \geq 0$ for $\tau \geq \sigma \geq 0$. Indeed, $Q(\tau, \sigma) = D(\sqrt[\alpha]{\tau^\alpha - \sigma^\alpha})$.

4.2 Markovianity properties via the generator

An alternative way of studying Markovianity is to investigate the master equation, that is the dynamical equation for the time-dependent density matrix $\Lambda(\tau)\rho$,

$$\partial_\tau \Lambda(\tau)\rho = \mathcal{L}_\tau \Lambda(\tau)\rho, \quad (45)$$

where the time-dependent generator is defined by

$$\mathcal{L}_\tau(\cdot) := (\partial_\tau \Lambda(\tau))\Lambda(\tau)^{-1}(\cdot), \quad (46)$$

and we of course assume that $\Lambda(\tau)$ is differentiable in τ and invertible as before. By construction, as $\Lambda(\tau)$ is trace-preserving and hermiticity-preserving (that is, $\text{tr}(\Lambda(\tau)A) = \text{tr}(A)$ and $\Lambda(\tau)(A^\dagger) = (\Lambda(\tau)(A))^\dagger$), the generator $\mathcal{L}_\tau$ satisfies

$$(i) \text{tr}(\mathcal{L}_\tau(A)) = 0, \quad \text{and} \quad (ii) \mathcal{L}_\tau(A^\dagger) = (\mathcal{L}_\tau(A))^\dagger. \quad (47)$$

When talking about generators in the following, we always consider linear maps having the properties (i) and (ii) in (47). There are many equivalent ways of expressing a given generator. Some of those are called canonical [6].

Definition. A canonical form of a (possibly time-dependent) generator $\mathcal{L}_\tau : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ is

$$\mathcal{L}_\tau(\cdot) = -i[H(\tau), \cdot] + \sum_{l,r=1}^{d^2-1} \hat{C}_{lr}(\tau) \left(F_l(\tau)(\cdot) F_r^\dagger(\tau) - \frac{1}{2} \{ F_r^\dagger(\tau) F_l(\tau), \cdot \} \right), \quad (48)$$

where for each $\tau \geq 0$, $H(\tau)$ is a hermitian $d \times d$ matrix, $\hat{C}(\tau) := (\hat{C}_{lr}(\tau))_{lr}$ is a hermitian $(d^2 - 1) \times (d^2 - 1)$ matrix, and the set $\{F_i(\tau)\}_{i=1}^{d^2-1} \cup \{\mathbb{1}/\sqrt{d}\}$ is a orthonormal basis of $M_d(\mathbb{C})$. Equivalently, the operators $F_i(\tau)$ are orthonormal and traceless.

The orthonormality is with respect to the Hilbert-Schmidt inner product, that is, here and in the following we consider the bounded operators $M_d(\mathbb{C})$ on $\mathbb{C}^d$ with inner product $\langle X, Y \rangle = \text{tr}(X^\dagger Y)$ and induced norm $\|X\|^2 = \text{Tr}(X^\dagger X)$. It is readily checked that the form (47) implies (i) and (ii) of (47) — in particular, the hermiticity of $\hat{C}(\tau)$ implies the hermiticity-preservation (ii). The canonical form of a given generator is not unique. All canonical forms are related by a change of basis that keeps one element fixed, the multiple of the identity $\mathbb{1}/\sqrt{d}$. Therefore, the coefficient matrix $\hat{C}(\tau)$ — called Kossakowski matrix — depends on the specific canonical form considered. However, some properties, such as hermiticity or semi-definiteness of the Kossakowski matrix, are representation independent.

Definition ([6]). A (possibly time-dependent) generator $\mathcal{L}_\tau : M_d(\mathbb{C}) \rightarrow M_d(\mathbb{C})$ is in diagonal canonical form if it is written as (48) with a diagonal matrix $\hat{C}(\tau)$. Equivalently, $\forall \tau \geq 0$

$$\mathcal{L}_\tau(\cdot) = -i[H(\tau), \cdot] + \sum_{i=1}^{d^2-1} \Gamma_i(\tau) \left(\hat{F}_i(\tau)(\cdot) \hat{F}_i^\dagger(\tau) - \frac{1}{2} \{ \hat{F}_i^\dagger(\tau) \hat{F}_i(\tau), \cdot \} \right) \quad (49)$$

for real numbers $\{\Gamma_i(\tau)\}_{i=1}^{d^2-1}$ and orthonormal traceless operators $\{\hat{F}_i(\tau)\}_{i=1}^{d^2-1}$.

A generator given in canonical form can always be put in diagonal canonical form: As $\hat{C}(\tau)$ is hermitian we have for any fixed τ , $\hat{C}(\tau) = U^\dagger(\tau) \Gamma(\tau) U(\tau)$ for some unitary matrix $U(\tau)$ and diagonal matrix $\Gamma(\tau)$ with real entries $\Gamma_{ij}(\tau) = \Gamma_i(\tau) \delta_{ij}$. Defining $\hat{F}_i(\tau) := \sum_l U_{li} F_l(\tau)$ one passes from (48) to (49). Coming back to our original motivation of studying Markovianity, a well-known result connecting the structure of the generator with Markovianity is the following.

Theorem 3 (Corollary 7 in [6]). A time-dependent generator $\mathcal{L}_\tau$ written in diagonal canonical form (49) defines a CP-divisible dynamics if and only if all the coefficients $\Gamma_i(\tau)$ are non-negative for all times τ .

According to Theorem 3, a strategy to characterize Markovianity is to write the generator in a canonical form (48), diagonalize the matrix $\hat{C}(\tau)$ in order to arrive at a diagonal canonical form and check the sign of the eigenvalues $\Gamma_i(\tau)$. In particular, the positive-definiteness of the matrix $\hat{C}(\tau)$ will not depend on the specific canonical form considered.

Let us now focus the discussion on dynamics of the form (38), like those emerging under strong coupling in the fine grained time regime. Explicitly, from the definition (46) one can compute

$$\mathcal{L}_\tau(\cdot) = \sum_{l,r=1}^{\nu} C_{lr}(\tau) P_l(\cdot) P_r, \quad \text{where} \quad C_{lr}(\tau) = \frac{\partial_\tau D_{l,r}(\tau)}{D_{l,r}(\tau)}. \quad (50)$$

Since $\partial_\tau D_{l,l}(\tau) = 0$ for all l, τ , the sum in (46) is effectively only over $l \neq r$. Also, for $l \neq r$ one has $P_l P_r = 0$ because these are orthogonal projections. Therefore, (50) can be written equivalently

$$\mathcal{L}_\tau(\cdot) = \sum_{l,r=1}^{\nu} C_{lr}(\tau) \left(P_l(\cdot) P_r - \frac{1}{2} \{ P_r P_l, \cdot \} \right), \quad (51)$$

that at a first look resembles a canonical form. However, the operators P_r , despite being orthogonal, are not normalized, $\langle P_r, P_r \rangle := \text{tr} P_r^\dagger P_r \neq 1$ (unless the P_r are rank-one) and moreover they are not traceless. Therefore, this is not a canonical form.

To write the generator in a canonical form, we use a Gram-Schmidt orthogonalization procedure. The set of ν operators $\{\mathbb{1}, P_1, \dots, P_{\nu-1}\}$ is linearly independent because the P_j are spectral projections (4) satisfying $\sum_{j=1}^{\nu} P_j = \mathbb{1}$. By Gram-Schmidt we construct the orthonormal set $\{F_i\}_{i=0}^{\nu-1}$ as

$$F_0 = \frac{\mathbb{1}}{\sqrt{d}}, \quad F_i = \frac{\tilde{F}_i}{\|\tilde{F}_i\|} \quad \text{with} \quad \tilde{F}_i = P_i - \sum_{j=0}^{i-1} \frac{\text{tr}(P_i \tilde{F}_j)}{\|\tilde{F}_j\|^2} \tilde{F}_j, \quad 1 \leq i \leq \nu-1. \quad (52)$$

This gives

$$P_i = \|\tilde{F}_i\| F_i + \sum_{j=0}^{i-1} F_j \text{tr}(P_i F_j), \quad i = 1, \dots, \nu-1, \quad P_\nu = \mathbb{1} - \sum_{j=1}^{\nu-1} P_j = \sqrt{d} F_0 - \sum_{j=1}^{\nu-1} P_j. \quad (53)$$

Substituting these expressions for P_l, P_r into (51) we obtain

$$\begin{aligned} \mathcal{L}_\tau(\cdot) &= \sum_{l,r=0}^{\nu-1} \hat{C}_{lr}^0(\tau) \left(F_l(\cdot) F_r - \frac{1}{2} \{F_r F_l, \cdot\} \right) \\ &= \sum_{l,r=1}^{\nu-1} \hat{C}_{lr}^0(\tau) \left(F_l(\cdot) F_r - \frac{1}{2} \{F_r F_l, \cdot\} \right) + i \sum_{r=1}^{\nu-1} \frac{\text{Im} \hat{C}_{r0}^0(\tau)}{\sqrt{d}} [F_r, \cdot] \end{aligned} \quad (54)$$

where the explicit expression for $\hat{C}_{lr}^0(\tau)$ can be obtained in principle from $C_{lr}(\tau)$ by exploiting the recursive definition of the F_i . The last equality follows from isolating the terms with $l = 0$, $r = 0$: the term with $l = r = 0$ vanishes; for $l = 0$ and $r \neq 0$ one has for any matrix A

$$\sum_{r=1}^{\nu-1} \frac{\hat{C}_{0r}^0(\tau)}{\sqrt{d}} \left(A F_r - \frac{F_r A}{2} - \frac{A F_r}{2} \right) = - \sum_{r=1}^{\nu-1} \frac{\hat{C}_{0r}^0(\tau)}{\sqrt{d}} \frac{[F_r, A]}{2}.$$

The terms with $l \neq 0$ and $r = 0$ give the same expression as on the right side, with $\hat{C}_{0r}^0(\tau)$ replaced by $-\hat{C}_{r0}^0(\tau)$. Exploiting the hermiticity⁵ of $\hat{C}^0(\tau)$ one arrives at (54).

Note that the $(\nu-1) \times (\nu-1)$ matrix $\hat{C}(\tau)$, that is obtained from $\hat{C}^0(\tau)$ eliminating the elements with $l = 0$ or $r = 0$, is also hermitian. The generator (54) is in canonical form⁶ and therefore, according to Theorem 3, the positivity of $\hat{C}(\tau)$ for any τ gives a further explicit criterion to determine the Markovianity of the dynamics (38).

⁵The hermiticity of $\hat{C}^0(\tau)$ is guaranteed by the property (47)-(ii), see e.g. [6].

⁶The orthonormal set $\{F_i\}_{i=0}^{\nu-1}$ is not a basis because the dimension of $M_d(\mathbb{C})$ is $d^2 > \nu$. However, it becomes a basis once completed with arbitrary orthonormal elements $\{F_i\}_{i=\nu}^{d^2-1}$ that do not play a role in the considered dynamics. Therefore, the $(d^2-1) \times (d^2-1)$ Kossakowski matrix has a block-diagonal structure $\begin{pmatrix} [\hat{C}]_{(\nu-1) \times (\nu-1)} & [0]_{(\nu-1) \times (d^2-\nu)} \\ [0]_{(d^2-\nu) \times (\nu-1)} & [0]_{(d^2-\nu) \times (d^2-\nu)} \end{pmatrix}$ and it is positive semi-definite if and only if $\hat{C}$ is.

Remark. We can normalize the projections in (50), (51) and introduce the orthonormal family $\tilde{P}_l := P_l / \sqrt{\text{tr}(P_l)}$ to arrive at

$$\mathcal{L}_\tau(\cdot) = \sum_{l,r=1}^{\nu} \tilde{C}_{lr}(\tau) \left(\tilde{P}_l(\cdot) \tilde{P}_r - \frac{1}{2} \{ \tilde{P}_r \tilde{P}_l, \cdot \} \right), \quad (55)$$

with $\tilde{C}_{lr}(\tau) := \sqrt{\text{tr}(P_l) \text{tr}(P_r)} C_{lr}(\tau)$. Still, this is not a canonical form of the generator, because the $\tilde{P}_j$ are not traceless. The matrix $\tilde{C}(\tau)$ is hermitian and traceless (all diagonal elements are vanishing) and so unless $\tilde{C}(\tau)$ is the zero matrix, it cannot be positive semi-definite. A naive (and wrong!) application of Theorem 3 would lead us to conclude that the dynamics is not CP-divisible. This is not true however, as we show in the following example.

Example. Consider the case of a free Bosonic reservoir as in Section 2 in a centered Gaussian state ω_R , with interaction operator (see (23)) $X = \varphi(g)$. The decoherence function is

$$D_{l,r}(\tau) := \omega_R \left(W(\tau(\gamma_r - \gamma_l)g) \right) = e^{-\frac{\tau^2}{4}(\gamma_l - \gamma_r)^2 \langle g, Cg \rangle}$$

and the elements of the matrix $Q(\tau, \sigma)$ are

$$Q_{l,r}(\tau, \sigma) = e^{-\frac{\tau^2 - \sigma^2}{4}(\gamma_l - \gamma_r)^2 \langle g, Cg \rangle} = D_{l,r}(\sqrt{\tau^2 - \sigma^2}). \quad (56)$$

$Q(\tau, \sigma)$ positive semi-definite for any $\tau \geq \sigma \geq 0$ because $D(s)$ is positive semi-definite for all $s \geq 0$. Corollary 1 implies that the dynamics $\Lambda(\tau)$ is Markovian. However, it is not of semigroup type, because $\Lambda(\tau - \sigma)\Lambda(\sigma) \neq \Lambda(\tau)$, as can be easily checked from the definition (38). *We have shown that the fine-grained time scaling can lead to a dynamics that does not satisfy the semigroup composition law but is still Markovian in the sense of CP-divisibility.* This has to be compared with other scaling regimes studied in the literature, such as the weak coupling, singular coupling, or low density scaling, which all lead to a semigroup dynamics.

We further develop the above example to illustrate the connection between Markovianity and the form of the generator. We already know that the dynamics is Markovian, so the Kossakowski matrix in any canonical form of the generator will be positive-semidefinite. Let us see how to get to a canonical form without using the Gram-Schmidt procedure in this specific case. Since all the elements $D_{l,r}(\tau)$ are strictly positive, we can rewrite the generator (46) as

$$\mathcal{L}_\tau(\cdot) = \sum_{\substack{1 \leq l, r \leq \nu \\ l \neq r}} \partial_\tau [\ln(D_{l,r}(\tau))] P_l(\cdot) P_r = -\frac{\tau}{2} \|\sqrt{C}g\|^2 \sum_{\substack{1 \leq l, r \leq \nu \\ l \neq r}} (\gamma_r - \gamma_l)^2 P_l(\cdot) P_r. \quad (57)$$

Let us assume that the projections $P_l = |l\rangle\langle l|$ are rank 1, so that $1 \leq l \leq \nu = d = \dim(\mathcal{H}_S)$, and make the ansatz

$$\mathcal{L}_\tau(\cdot) = \sum_{l=1}^d \eta_{ll}(\tau) \left(P_l(\cdot) P_l - \frac{1}{2} \{ P_l, \cdot \} \right) + \sum_{\substack{1 \leq l, r \leq d \\ l \neq r}} \eta_{lr}(\tau) P_l(\cdot) P_r, \quad (58)$$

with real coefficients η_{lr} that satisfy $\eta_{lr} = \eta_{rl}$. We obtain on the one hand from (58),

$$\mathcal{L}_\tau(|j\rangle\langle k|) = \left(-\frac{1}{2}(\eta_{jj} + \eta_{kk}) + \eta_{jk} \right) |j\rangle\langle k| = -\frac{1}{2}(\eta_{jj} + \eta_{kk} - 2\eta_{jk}) |j\rangle\langle k| \quad (59)$$

and on the other hand from (57),

$$\mathcal{L}_\tau(|j\rangle\langle k|) = -\frac{\tau}{2}\|\sqrt{\mathcal{C}}g\|^2(\gamma_k - \gamma_j)^2|j\rangle\langle k|. \quad (60)$$

Comparing (59) and (60) gives

$$\tau\|\sqrt{\mathcal{C}}g\|^2(\gamma_k - \gamma_j)^2 = \eta_{jj} + \eta_{kk} - 2\eta_{jk}, \quad k, l = 1, \dots, d. \quad (61)$$

For $j = k$ the expression (61) is satisfied without giving constraints on η_{jk} , and the symmetry of the left side implies that $\eta_{kj} = \eta_{jk}$. We have thus $(d^2 + d)/2$ unknowns η_{jk} with $1 \leq j \leq k \leq d$ for the $(d^2 - d)/2$ independent equations (61) with $1 \leq j < k \leq d$. This means that we have an underdetermined system and so there is some freedom in choosing the η_{jk} . With the choice $\eta_{jk}(\tau) = \tau\|\sqrt{\mathcal{C}}g\|^2\gamma_j\gamma_k$, $j, k = 1, \dots, d$ the expression (58) becomes

$$\mathcal{L}_\tau(\cdot) = \tau\|\sqrt{\mathcal{C}}g\|^2 \sum_{l,r=1}^d \gamma_l \gamma_r \left(P_l(\cdot)P_r - \frac{1}{2}\{P_l P_r, \cdot\} \right) = \tau\|\sqrt{\mathcal{C}}g\|^2 \left(L'(\cdot)L' - \frac{1}{2}\{(L')^2, \cdot\} \right),$$

with a single global jump operator $L' = \sum_{l=1}^d \gamma_l P_l$. We shift it to the traceless $L'' = L' - \sum_{l=1}^d \gamma_l$ and then normalize it $L = L''/\sqrt{\sum_l \gamma_l^2 + (d-2)(\sum_l \gamma_l)^2}$, so that we arrive at the generator

$$\mathcal{L}_\tau(\cdot) = \Gamma(\tau) \left(L(\cdot)L - \frac{1}{2}\{L^2, \cdot\} \right), \quad \Gamma(\tau) = \tau\|\sqrt{\mathcal{C}}g\|^2 \left(\sum_{l=1}^d \gamma_l^2 + (d-2) \left(\sum_{l=1}^d \gamma_l \right)^2 \right). \quad (62)$$

This is a canonical diagonal form of $\mathcal{L}_\tau$. Theorem 3 implies that the dynamics is CP-divisible.

5 Ultrastrongly coupled spin-boson models

The main result of Section 3, Theorem 2, describes the evolution of the system density matrix

$$\varrho_S(\tau) = \lim_{\substack{t \rightarrow 0_+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \text{tr}_R \left(e^{-it(H_0 + \lambda G \otimes X)} \rho_S \otimes \rho_R e^{it(H_0 + \lambda G \otimes X)} \right) \quad (63)$$

where $H_0 = H_S + H_R$, under the condition (27),

$$\lim_{\substack{t \rightarrow 0_+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} e^{-it(H_0 + \lambda G \otimes X)} = e^{-i\tau G \otimes X}. \quad (64)$$

As we have mentioned, (64) is easily shown to be correct if H_R and X are bounded operators. We now consider the SR model introduced in Section 2, with the Hamiltonian (2) and $X = \varphi(g)$, (5). Both these two operators are unbounded. Our main result here is Theorem 4, which demonstrates that the expression for $\varrho_S(\tau)$ given in Theorem 2 is correct for this model.

In order to state a regularity condition on the state ω_R and the form factor g used to derive our result (which guarantees (64) to hold in a weak sense, see the proof of Theorem 4), we start by noticing that $\forall \tau \geq 0$,

$$\frac{e^{i\tau\omega(k)/\lambda} - 1}{i\omega(k)/\lambda} g(k) \rightarrow \tau g(k)$$

in the $L^2(\mathbb{R}^3, d^3k)$ sense as $\lambda \rightarrow \infty$. We then make the following mild regularity assumption:

(R) For all $\tau \geq 0$,

$$\lim_{\lambda \rightarrow \infty} \omega_R \left(W \left(\frac{e^{i\tau\omega/\lambda} - 1}{i\omega/\lambda} g \right) \right) = \omega_R(W(\tau g)). \quad (65)$$

Example. For a Gaussian ω_R , (9) the condition (65) holds if

$$\sqrt{\mathcal{C}} \frac{e^{i\tau\omega/\lambda} - 1}{i\omega/\lambda} g \rightarrow \sqrt{\mathcal{C}} \tau g \quad (66)$$

in the $L^2(\mathbb{R}^3, d^3k)$ sense, as $\lambda \rightarrow \infty$. If the covariance operator is a multiplication operator by a function $C(k)$ then (66) holds if $\sqrt{C(k)}g(k) \in L^2(\mathbb{R}^3, d^3k)$. For a thermal reservoir state at inverse temperature $\beta > 0$, we have $C(k) = \coth(\beta\omega(k)/2)$.

Theorem 4. *Let H be the spin-Boson Hamiltonian (2) and consider the system density matrix (63). Assume the condition (R) and let $D_{l,r}(\tau) = \omega_R(W(\tau(\gamma_r - \gamma_l)g))$. Then for all $\tau \geq 0$,*

$$\varrho_S(\tau) = \sum_{l,r=1}^{\nu} D_{l,r}(\tau) P_l \rho_S P_r. \quad (67)$$

We present the proof of Theorem 4 in Section 5.1. As in Theorem 2, the dynamics (67) can be written in the form (36), (37) under the appropriate continuity and integrability condition on

$$D(s) = \omega_R(e^{-isX}) = \omega_R(W(-sg)) = \int_{\mathbb{R}} d\mu(\alpha) e^{-i\alpha s},$$

where W is the Weyl operator, see (7) and μ is the associated Borel probability measure, see (33).

Examples.

(i) For ω_R a (centered) Gaussian with covariance $\mathcal{C}$ we have

$$\omega_R(W(g)) = e^{-\frac{1}{4}\langle g, \mathcal{C}g \rangle}. \quad (68)$$

Then $D(s) = e^{-\frac{1}{4}s^2\|\sqrt{\mathcal{C}}g\|^2}$ is a Gaussian function and $d\mu(\alpha) = \mu(\alpha)d\alpha$ with

$$\mu(\alpha) = \frac{1}{\|\sqrt{\mathcal{C}}g\|\sqrt{\pi}} e^{-\frac{\alpha^2}{\|\sqrt{\mathcal{C}}g\|^2}}.$$

(ii) A particular case of (i) is when ω_R the equilibrium state at inverse temperature β . The covariance operator is the multiplication by the function $C(\omega) = \coth(\beta\omega/2)$, so

$$\|\sqrt{\mathcal{C}}g\|^2 = \int_{\mathbb{R}^3} |g(k)|^2 \coth(\beta\omega/2) d^3k.$$

The zero temperature case (vacuum) corresponds to $\mathcal{C} = \mathbb{1}$. If instead of the thermal distribution the reservoir has an arbitrary energy distribution $\varrho(k) \geq 0$, that is,

$$\omega_R(a^\dagger(k)a(l)) = \varrho(k)\delta(k-l),$$

then the covariance operator is the multiplication with the function $C(k) = 1 + 2\varrho(k)$. (The thermal distribution is $\varrho(k) = (e^{\beta\omega} - 1)^{-1}$.)

- (iii) A coherent state is given by $W(f)|\Omega\rangle$, where $f \in L^2(\mathbb{R}^3, d^3k)$ is fixed and $|\Omega\rangle$ is the vacuum vector. Then

$$D(s) = \omega_R(W(-sg)) = \langle \Omega | W(-f) W(-sg) W(f) | \Omega \rangle = e^{-is \operatorname{Im} \langle f, g \rangle} e^{-\frac{1}{4} s^2 \|g\|^2}.$$

The corresponding density μ , (34), becomes

$$\mu(\alpha) = \frac{1}{\sqrt{\pi} \|g\|} \exp \left(-\frac{(\alpha - \operatorname{Im} \langle f, g \rangle)^2}{\|g\|^2} \right). \quad (69)$$

5.1 Proof of Theorem 4

Define the operator

$$K = H_R + \lambda G \otimes \varphi(g). \quad (70)$$

We have for any system observable A ,

$$\omega_S \otimes \omega_R(e^{itK} A e^{-itK}) = \sum_{l,r} \omega_S(P_l A P_r) \omega_R(e^{it(H_R + \lambda \gamma_l \varphi(g))} e^{-it(H_R + \lambda \gamma_r \varphi(g))}). \quad (71)$$

The reservoir observable appearing in the state ω_R can be simplified by using the following formula, valid for all $x, y \in \mathbb{R}$,

$$e^{it(H_R + x\varphi(g))} e^{-it(H_R + y\varphi(g))} = e^{-\frac{i}{2}(x^2 - y^2) \operatorname{Im} \langle \frac{e^{i\omega t} - 1 - i\omega t}{\omega^2} g, g \rangle} W\left((x - y) \frac{e^{i\omega t} - 1}{i\omega} g\right). \quad (72)$$

This equality can be derived using the polaron transformation, see for instance [14], Lemma 1. Using (72) in (71) gives

$$\omega_S \otimes \omega_R(e^{itK} A e^{-itK}) = \sum_{l,r=1}^{\nu} \omega_S(P_l A P_r) e^{-\frac{i}{2} \lambda^2 (\gamma_l^2 - \gamma_r^2) \operatorname{Im} \langle (\frac{e^{i\omega t} - 1 - i\omega t}{\omega^2} g, g \rangle} \omega_R(W(\lambda(\gamma_l - \gamma_r) \frac{e^{i\omega t} - 1}{i\omega} g)). \quad (73)$$

Next with $\lambda t = \tau$, we get

$$\lambda^2 \operatorname{Im} \langle \frac{e^{i\omega t} - 1 - i\omega t}{\omega^2} g, g \rangle = \tau^2 \operatorname{Im} \langle \frac{e^{i\omega t} - 1 - i\omega t}{(\omega t)^2} g, g \rangle. \quad (74)$$

For every $\omega > 0$ we have $\lim_{t \rightarrow 0} \operatorname{Im} \frac{e^{i\omega t} - 1 - i\omega t}{(\omega t)^2} = 0$ and we have $\sup_{x>0} |\frac{e^{ix} - 1 - ix}{x^2}| < \infty$. Therefore, by the Lebesgue Dominated Convergence Theorem,

$$\lim_{\substack{t \rightarrow 0_+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \lambda^2 \operatorname{Im} \langle \frac{e^{i\omega t} - 1 - i\omega t}{\omega^2} g, g \rangle = 0. \quad (75)$$

The regularity assumption (65) together with the equations (73), (75) show that

$$\lim_{\substack{t \rightarrow 0_+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \omega_S \otimes \omega_R(e^{itK} A e^{-itK}) = \sum_{l,r=1}^{\nu} \omega_S(P_l A P_r) \omega_R(W(\tau(\gamma_l - \gamma_r)g)). \quad (76)$$

Note that the right hand side of (76) equals

$$\begin{aligned}
& \sum_{l,r=1}^{\nu} \omega_S \otimes \omega_R (W(\tau\gamma_l g) P_l A P_r W(-\tau\gamma_r g)) \\
&= \sum_{l,r=1}^{\nu} \omega_S \otimes \omega_R (e^{i\tau\gamma_l \varphi(g)} P_l A P_r e^{-i\tau\gamma_r \varphi(g)}) \\
&= \sum_{l,r=1}^{\nu} \omega_S \otimes \omega_R (e^{i\tau G \otimes \varphi(g)} P_l A P_r e^{-i\tau G \otimes \varphi(g)}) \\
&= \omega_S \otimes \omega_R (e^{i\tau G \otimes \varphi(g)} A e^{-i\tau G \otimes \varphi(g)}).
\end{aligned} \tag{77}$$

So (76) shows that

$$\lim_{\substack{t \rightarrow 0+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \omega_S \otimes \omega_R (e^{itK} (A \otimes \mathbb{1}_R) e^{-itK}) = \omega_S \otimes \omega_R (e^{i\tau G \otimes \varphi(g)} (A \otimes \mathbb{1}_R) e^{-i\tau G \otimes \varphi(g)}). \tag{78}$$

This means that in the considered limit, H_R does not play any role in the dynamics of system observables generated by K , as only the interaction term in (70) survives.

Next we deal with the dynamics when H_S does not vanish. The total Hamiltonian is given by $H = H_S + H_R + \lambda G \otimes \varphi(g)$. We have

$$e^{-itH} - e^{-itK} = \int_0^t e^{-isH} (-iH_S) e^{-i(t-s)K} ds, \tag{79}$$

which implies

$$\|e^{-itH} - e^{-itK}\| \leq t \|H_S\|. \tag{80}$$

Therefore, in the limit $t \rightarrow 0$, $\lambda \rightarrow \infty$, $\lambda t = \tau$ fixed, the system Hamiltonian does not play a role,

$$\lim_{\substack{t \rightarrow 0+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \omega_S \otimes \omega_R (e^{itH} A e^{-itH}) = \lim_{\substack{t \rightarrow 0+, \lambda \rightarrow \infty \\ \lambda t = \tau \text{ fixed}}} \omega_S \otimes \omega_R (e^{itK} A e^{-itK}). \tag{81}$$

The right side of (81) is given by (76), which is equivalently expressed as $\text{tr}(\varrho_S(\tau)A)$ with $\varrho_S(\tau)$ given in (67). This concludes the proof of Theorem 4. $\square$

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