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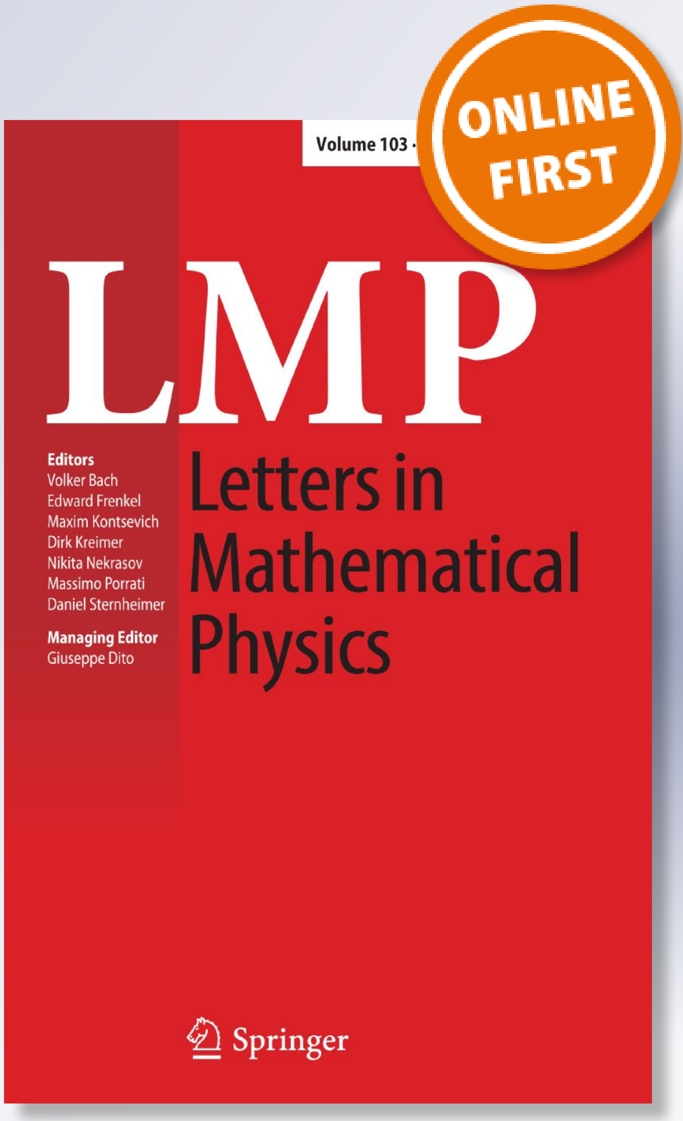

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Completely positive dynamical semigroups and quantum resonance theory

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Abstract Starting from a microscopic system–environment model, we construct a quantum dynamical semigroup for the reduced evolution of the open system. The difference between the true system dynamics and its approximation by the semigroup has the following two properties: It is (linearly) small in the system–environment coupling constant for all times, and it vanishes exponentially quickly in the large time limit. Our approach is based on the quantum dynamical resonance theory.

Keywords Open quantum system · Quantum resonances · Dynamical semigroup · Complete positivity

Mathematics Subject Classification 82C10 · 81S22

1 The issue

Due to the entanglement of an open system with its surroundings, its dynamics $V(t) : \rho_0 \mapsto \rho_t$, mapping an initial system density matrix ρ_0 to its value at time t, is not a semigroup in time. For each fixed t, the mapping $V(t)$, called a *dynamical*

[1] We recall that a map on bounded operators on a Hilbert space, $V : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, is called completely positive if $V \otimes \mathbf{1} : \mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n) \to \mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n)$ is positive (maps positive operators into positive ones) for all $n \in \mathbb{N}$.

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map, is a linear, completely positive, trace preserving transformation.[1] Under certain assumptions, one can approximate the dynamics of an open system by a continuous one-parameter semigroup of dynamical maps, called a *quantum dynamical semigroup* [5,12]. The dynamics given by such a semigroup has two important features: (i) It is Markovian due to the semigroup property and (ii) it maps density matrices into density matrices due to its trace and positivity preserving quality. *Complete* positivity of the dynamical semigroup implies its positivity preservation, but not vice versa. It is a crucial physical property which ensures that the dynamics of initially entangled systems interacting with an environment is well defined [1,3]. The semigroup property is particularly convenient since the spectral analysis of the generator $\mathcal{L}$ of the semigroup yields dynamical properties of the system, such as the final state(s) and convergence speeds. Controlling the remainder in the approximation $V(t)\rho_0 \approx \mathrm{e}^{t\mathcal{L}}\rho_0$ rigorously is difficult. Microscopic derivations, passing from a full (Hamiltonian) model of system plus environment and tracing out the environment degrees of freedom, involve approximations (Born, Markov, rotating wave) that are hard to deal with mathematically. In some situations where the system–environment interaction is weak, measured by a small coupling constant λ, one can implement a (time-dependent) perturbation theory, $\lambda = 0$ giving the unperturbed (uncoupled) case. For certain systems, it has been shown [7,8] that for all $a > 0$,

$$\lim_{\lambda\to 0} \sup_{0\leqslant\lambda^2 t<a} \|V(t) - \mathrm{e}^{t(\mathcal{L}_0+\lambda^2 K)}\| = 0,$$

where $\mathcal{L}_0$ is the generator of the uncoupled (Hamiltonian) dynamics and K is a (lowest order) correction responsible for dissipative effects. We discuss here finite-dimensional open systems and so the nature of the norm is immaterial. This weak coupling result allows a description of the dynamics by a semigroup up to times $t = O(\lambda^{-2})$. However, the asymptotics $t \to \infty$ is not resolved correctly by the dynamical semigroup $\mathrm{e}^{t(\mathcal{L}_0+\lambda^2 K)}$. For instance, the invariant state of the latter is typically the *uncoupled* system Gibbs equilibrium state, while the true asymptotic state is the restriction of the *coupled* system–environment equilibrium to the system alone. A more recent dynamical resonance theory [13,20–22] improves the weak coupling result to

$$\|V(t) - \mathrm{e}^{tM(\lambda)}\| \leqslant C\lambda^2 \mathrm{e}^{-\gamma' t}, \qquad t \geqslant 0,$$

where $M(\lambda) = \mathcal{L}_0 + \lambda^2 K + \cdots$ is analytic in λ and $\gamma' > 0$. This approach grew out of works proving "return to equilibrium" of open systems using elements of algebraic quantum field theory and spectral theory [4,14] and is useful in different physical settings [16–19]. While it is known that the "Davies generator" $\mathcal{L}_0 + \lambda^2 K$, describing the weak coupling limit, generates a dynamical semigroup [7,10], this is not known for the generator $M(\lambda)$ emerging from the dynamical resonance theory. In the present paper, we construct a dynamical semigroup $\mathcal{T}_t$ satisfying

$$\mathcal{T}_0 = \mathbf{1}, \qquad \mathcal{T}_{t+s} = \mathcal{T}_t\,\mathcal{T}_s, \quad \forall s, t \geqslant 0$$

and

$$\|V(t)-\mathcal{T}_t\| \leqslant C|\lambda|\left(1+\lambda^2 t\right)\mathrm{e}^{-\lambda^2(1+O(\lambda))\gamma t}, \qquad t \geqslant 0,$$

where $\gamma > 0$. Giving the Schrödinger dynamics $\mathcal{T}_t$ is equivalent to giving the completely positive, identity preserving semigroup τ^t acting on the algebra of observables of the system (Heisenberg dynamics), defined by the relation $\mathrm{Tr}(\{\mathcal{T}_t\rho_0\}X) = Tr(\rho_0\,\tau^t(X))$ for all system density matrices ρ_0 and all system observables X. Our main result, Theorem 2.1, shows the existence of the Heisenberg dynamics τ^t. We construct it by modifying the dynamical resonance theory approach right at its starting point. Namely, instead of taking the uncoupled system equilibrium state as a reference state, we take for it the effective, coupled system equilibrium state, which contains all orders of interactions with the reservoir. We show that this leads to a dynamics that is a quantum dynamical semigroup and that has the correct final state.

Our paper is organized as follows. In Sect. 2, we give the setup of the problem, state our assumptions and present the main result, Theorem 2.1. At the beginning of Sect. 3, we explain the mathematical description of the reservoir, and in Sect. 3.2 we construct the renormalized quantities (i.e., the system reference state). We provide the proof of Theorem 2.1 in Sect. 3.3 (representation of the dynamics by τ^t) and Sect. 3.4 (complete positivity).

2 Main result

The Hilbert space of a finite-dimensional quantum system S in contact with a bosonic quantum field (reservoir) R is

$$\mathcal{H} = \mathcal{H}_\mathrm{S} \otimes \mathcal{H}_\mathrm{R}, \tag{2.1}$$

where $\mathcal{H}_\mathrm{S} = \mathbb{C}^d$ and $\mathcal{H}_\mathrm{R} = \oplus_{n\geqslant 0} L^2_{\mathrm{sym}}(\mathbb{R}^{3n}, d^{3n}k)$ is the Fock space over the single particle space $L^2(\mathbb{R}^3, d^3k)$. We consider Hamiltonians

$$H = H_\mathrm{S} + H_\mathrm{R} + \lambda\, V_\mathrm{S} \otimes \varphi(g), \tag{2.2}$$

where H_S and V_S are self-adjoint matrices on $\mathcal{H}_\mathrm{S}$,

$$H_\mathrm{S} = \sum_{j=1}^d E_j |\phi_j\rangle\langle\phi_j|, \quad \text{and} \quad H_\mathrm{R} = \int_{\mathbb{R}^3} |k|\, a^*(k)a(k)d^3k \tag{2.3}$$

is the second quantization of multiplication with the function $|k|$, the energy of the mode k. The creation operators $a^*(k)$ and annihilation operator $a(k)$ satisfy the Bose canonical commutation relations $[a(k), a^*(l)] = \delta(k-l)$ (Dirac delta). We assume for convenience of exposition that all eigenvalues E_j of H_S are simple and that $\min_{1\leqslant j\leqslant d} E_j = 0$. Our arguments are readily generalized to degenerate (and shifted) spectrum. The interaction strength is gauged by the coupling constant $\lambda \in \mathbb{R}$ and

$$\varphi(g) = \frac{1}{\sqrt{2}}\big(a^*(g) + a(g)\big), \qquad a^*(g) = \int_{\mathbb{R}^3} g(k) a^*(k) d^3k,$$

is the field and the creation operator [whose adjoint is $a(f)$, the annihilation operator], respectively, smoothed out with a form factor $g \in L^2(\mathbb{R}^3, d^3k)$.

In this work, we are concerned with the time evolution of observables $X \in \mathcal{B}(\mathcal{H}_S)$ under the coupled system–reservoir Heisenberg dynamics α_λ^t generated by the Hamiltonian H,

$$t \mapsto \omega\big(\alpha_\lambda^t(X \otimes \mathbf{1}_R)\big). \tag{2.4}$$

The initial state ω is a "normal state," characterized by the fact that asymptotically in space, the reservoir is in its thermal equilibrium state. We do not demand that the system and reservoir are initially disentangled. There is a slight mathematical complication in the precise definition of (2.4) because thermal reservoirs are spatially infinitely extended systems. We explain this point in Sect. 3.1.

The non-interacting dynamics is the product $\alpha_0^t = \alpha_S^t \otimes \alpha_R^t$, where the individual dynamics of each factor is generated by its own Hamiltonian H_S or H_R. For small coupling constants λ, one can use a perturbation theory for the reduced system dynamics. Effectively, the energy levels of H_S acquire *complex valued* corrections [of $O(\lambda^2)$] which describe irreversibility of the open system dynamics. It is convenient to express this scheme in terms of the system *Liouville operator*

$$L_S = H_S \otimes \mathbf{1}_S - \mathbf{1}_S \otimes H_S \tag{2.5}$$

acting on the doubled space $\mathcal{H}_S \otimes \mathcal{H}_S$. The Liouville representation is quite standard [23]. The eigenvalues of L_S are the differences of those of H_S. They describe the temporal oscillations of the system density matrix elements in the energy basis under the uncoupled dynamics. Namely, the density matrix elements oscillate in time with frequencies that are the eigenvalues of L_S. The coupling with the reservoir produces corrections. To lowest order in λ, the corrected eigenvalues are those of $L_S + \lambda^2\Lambda$, where Λ is the so-called *level shift operator*, a non-self-adjoint matrix on $\mathcal{H}_S \otimes \mathcal{H}_S$, which can be calculated explicitly [c.f. (3.17)]. The operators L_S and Λ commute and satisfy

$$(L_S + \lambda^2\Lambda)\Omega_{S,\beta} = 0 \tag{2.6}$$

for all $\lambda \in \mathbb{R}$, where [c.f. (2.3)]

$$\Omega_{S,\beta} = Z_S^{-1/2} \sum_j e^{-\beta E_j/2} \phi_j \otimes \phi_j, \qquad Z_S = Tr\, e^{-\beta H_S} \tag{2.7}$$

is the system Gibbs (equilibrium) vector, defining the equilibrium state

$$\omega_{S,\beta}(X) = Z_S^{-1} Tr_S(e^{-\beta H_S} X) = \big\langle \Omega_{S,\beta}, (X \otimes \mathbf{1}_S)\Omega_{S,\beta}\big\rangle, \qquad X \in \mathcal{B}(\mathcal{H}_S). \tag{2.8}$$

Relation (2.6) reflects the fact that the system Gibbs state is invariant under the coupled dynamics, to lowest order in the perturbation. (In fact, generically, it is the final system state, as $t \to \infty$, to lowest order in λ.) For simplicity of the exposition, we assume that

(A1) (i) All eigenvalues of Λ are simple.
(ii) All eigenvalues of Λ but zero have strictly positive imaginary part,

$$\gamma = \min\left\{\mathrm{Im}\, a \ :\ a \in \mathrm{spec}(\Lambda)\backslash\{0\}\right\} > 0. \tag{2.9}$$

Since L_{S} and Λ commute, the eigenvalues of $L_{\mathrm{S}} + \lambda^2\Lambda$ are of the form $e + \lambda^2 a$, with $e \in \mathrm{spec}(L_{\mathrm{S}})$, $a \in \mathrm{spec}(\Lambda)$. In particular, for small enough, but non-vanishing λ, the operator $L_{\mathrm{S}} + \lambda^2\Lambda$ has only simple eigenvalues and, apart from zero, all its spectrum has imaginary part $\geqslant \gamma$. Both assumptions are readily and generically verified in concrete examples. Assumption (i) simplifies the analysis somewhat and guarantees in particular that $L_{\mathrm{S}} + \lambda^2\Lambda$ is diagonalizable. Assumption (ii) is commonly referred to as the *Fermi Golden Rule Condition* and ensures that irreversible effects are visible already in the lowest order correction to the dynamics.

In the dynamical theory of quantum resonances, the resonances (complex energy eigenvalues) associated with the Liouville operator are determined using spectral deformation or Mourre theory [4,13,14,16–22]. In order not to muddle the core ideas of the current work, we follow here the technically least complicated situation, where the Hamiltonian is "translation deformation analytic" [4,14]. This requires a regularity assumption on the form factor $g \in L^2(\mathbb{R}^3, d^3k)$. To state it, define the complex valued function g_β on $\mathbb{R} \times S^2$ by

$$g_\beta(u, \Sigma) = \sqrt{\frac{u}{1 - \mathrm{e}^{-\beta u}}}\ |u|^{1/2} \begin{cases} g(u, \Sigma), & u \geq 0 \\ -\overline{g}(-u, \Sigma), & u < 0 \end{cases} \tag{2.10}$$

where $g(u, \Sigma)$ is $g(k)$ in spherical coordinates $(u, \Sigma) \in \mathbb{R}_+ \times S^2$. The regularity condition is the following.

(A2) For $\theta \in \mathbb{R}$, define $(T_\theta g_\beta)(u, \Sigma) = g_\beta(u - \theta, \Sigma)$. There is a $\theta_0 > 0$ such that, viewed as a map from $\mathbb{R}$ to $L^2(\mathbb{R} \times S^2, du \times d\Sigma)$, the function $\theta \mapsto T_\theta g_\beta$ has an analytic extension to $0 < \mathrm{Im}\theta < 2\theta_0$ which is continuous as $\mathrm{Im}\theta \to 0_+$.

This condition is satisfied for instance for the following family of form factors, given in spherical coordinates $(r, \Sigma) \in \mathbb{R}_+ \times S^2 = \mathbb{R}^3$,

$$g(k) = g(r, \Sigma) = r^p \mathrm{e}^{-r^m} g_1(\Sigma),$$

where $p = -1/2 + n$, $n = 0, 1, 2, \ldots$, $m = 1, 2$ and $g_1(\sigma) = \mathrm{e}^{i\phi}\bar{g}_1(\sigma)$ for an arbitrary phase ϕ (see also [11]).

Let α_λ^t be the coupled system–reservoir dynamics. The resonance approach, developed in [20–22], gives the expansion (2.11) below. We give an outline of the derivation at the end of this section. If $0 < |\lambda| < \lambda_0$ for a sufficiently small λ_0, then we have for all system–reservoir initial states ω_0 belonging to a dense set $\mathcal{S}_0$, all system observables $X \in \mathcal{B}(\mathcal{H}_{\mathrm{S}})$ and all times $t \geqslant 0$,

$$\omega_0\big(\alpha_\lambda^t(X \otimes \mathbf{1}_{\mathrm{R}})\big) = \omega_{\mathrm{SR},\beta,\lambda}(X \otimes \mathbf{1}_{\mathrm{R}}) + \omega_0\big(\delta_\lambda^t(X) \otimes \mathbf{1}_{\mathrm{R}}\big) + R_{\lambda,t}(X), \tag{2.11}$$

where $\omega_{\mathrm{SR},\beta,\lambda}$ is the coupled system–reservoir equilibrium state, where $\delta_\lambda^t : \mathcal{B}(\mathcal{H}_\mathrm{S}) \to \mathcal{B}(\mathcal{H}_\mathrm{S})$ and the remainder $R_{\lambda,t}(X)$ satisfy

$$|\delta_\lambda^t(X)| \leqslant C\mathrm{e}^{-\lambda^2\gamma t}\,\|X\| \tag{2.12}$$

$$|R_{\lambda,t}(X)| \leqslant C\,|\lambda|\,\left(\mathrm{e}^{-\theta_0 t} + \lambda^2 t\,\mathrm{e}^{-\lambda^2\gamma t}\right)\|X\|. \tag{2.13}$$

Here, γ is the gap (2.9) and θ_0 is given in Assumption (A2).[2] The resonance approach requires that $\lambda^2\gamma \ll \theta_0$. The map δ_λ^t is defined by the relation

$$\left(\delta_\lambda^t(X)\otimes \mathbf{1}_\mathrm{S}\right)\Omega_{\mathrm{S},\beta} = \mathrm{e}^{it(L_\mathrm{S}+\lambda^2\Lambda)}\,P_{\mathrm{S},\beta}^{\perp}\left(X\otimes\mathbf{1}_\mathrm{S}\right)\Omega_{\mathrm{S},\beta}, \tag{2.14}$$

where $\Omega_{\mathrm{S},\beta} \in \mathcal{H}_\mathrm{S}\otimes\mathcal{H}_\mathrm{S}$ is the system Gibbs vector (2.7), $P_{\mathrm{S},\beta} = |\Omega_{\mathrm{S},\beta}\rangle\langle\Omega_{\mathrm{S},\beta}|$ and $P_{\mathrm{S},\beta}^{\perp} = \mathbf{1}_\mathrm{S} - P_{\mathrm{S},\beta}$.[3] The operators L_S and Λ are the system Liouville and the level shift operators, respectively, acting on $\mathcal{H}_\mathrm{S}\otimes\mathcal{H}_\mathrm{S}$ and commuting with each other. Under typical well-coupledness conditions (e.g., “the Fermi Golden Rule condition”), one has

$$\mathrm{Ker}(L_\mathrm{S}+\lambda^2\Lambda) = \mathbb{C}\Omega_{\mathrm{S},\beta}, \tag{2.15}$$

which sharpens (2.6). The property of return to equilibrium follows from (2.11), namely,

$$\lim_{t\to\infty}\omega_0(\alpha_\lambda^t(X\otimes\mathbf{1}_\mathrm{R})) = \omega_{\mathrm{SR},\beta,\lambda}(X\otimes\mathbf{1}_\mathrm{R}). \tag{2.16}$$

By modifying δ_λ^t, (2.14), on the “stationary subspace” Ran $P_{\mathrm{S},\beta}$, we define the map $\sigma_\lambda^t : \mathcal{B}(\mathcal{H}_\mathrm{S}) \to \mathcal{B}(\mathcal{H}_\mathrm{S})$ by

$$\left(\sigma_\lambda^t(X)\otimes\mathbf{1}_\mathrm{S}\right)\Omega_{\mathrm{S},\beta} = \mathrm{e}^{it(L_\mathrm{S}+\lambda^2\Lambda)}\left(X\otimes\mathbf{1}_\mathrm{S}\right)\Omega_{\mathrm{S},\beta}. \tag{2.17}$$

It follows from (2.14) and (2.6) that

$$\sigma_t^\lambda(X) = \delta_t^\lambda(X) + \omega_{\mathrm{S},\beta}(X)\mathbf{1}_\mathrm{S}, \qquad X\in\mathcal{B}(\mathcal{H}_\mathrm{S}). \tag{2.18}$$

Expanding the joint equilibrium state for small λ,

$$\omega_{\mathrm{SR},\beta,\lambda}(X\otimes\mathbf{1}_\mathrm{R}) = \omega_{\mathrm{S},\beta}(X) + R_\lambda'(X), \tag{2.19}$$

where

$$|R_\lambda'(X)| \leqslant C\lambda^2\|X\|, \tag{2.20}$$

[2] If the initial state is of product form $\omega_\mathrm{S}\otimes\omega_{\mathrm{R},\beta}$, then the term $C|\lambda|\mathrm{e}^{-\theta_0 t}$ in (2.13) can be replaced by $C\lambda^2\mathrm{e}^{-\theta_0 t}$, see Theorem 3.1 of [20], *Resonance theory of decoherence and thermalization*.

[3] $\Omega_{\mathrm{S},\beta}$ is *cyclic*, meaning that $(\mathcal{B}(\mathcal{H}_\mathrm{S})\otimes\mathbf{1}_\mathrm{S})\Omega_{\mathrm{S},\beta} = \mathcal{H}_\mathrm{S}\otimes\mathcal{H}_\mathrm{S}$ and $\Omega_{\mathrm{S},\beta}$ is *separating*, meaning that if $(X\otimes\mathbf{1}_\mathrm{S})\Omega_{\mathrm{S},\beta} = 0$ then $X = 0$. Due to the cyclic and separating property, (2.14) defines the map δ_λ^t uniquely, and it shows that $t\mapsto\delta_\lambda^t$ is a group.

and combining (2.11) and (2.18) we obtain

$$\omega_0\big(\alpha_\lambda^t(X\otimes\mathbf{1}_{\rm R})\big)=\omega_0\big(\sigma_\lambda^t(X)\otimes\mathbf{1}_{\rm R}\big)+R'_\lambda(X)+R_{\lambda,t}(X), \tag{2.21}$$

where $R_{\lambda,t}(X)$ and $R'_\lambda(X)$ satisfy (2.13) and (2.20), respectively.

The expansion (2.21) has an advantage and a disadvantage over the expansion (2.11).

- The advantage: The main term in (2.21) is given by σ_λ^t, which is a *quantum dynamical semigroup* (in the Heisenberg picture). This means that σ_λ^t is a semigroup of completely positive maps and satisfies $\sigma_\lambda^t(\mathbf{1}_{\rm S})=\mathbf{1}_{\rm S}$. The latter property (which is equivalent to the dual map acting on density matrices being trace preserving) follows directly from definition (2.17) and (2.15). We give a derivation of its complete positivity in Sect. 3.4.
- The disadvantage: The main term of expansion (2.21) describes the time asymptotics only up to an accuracy of $O(\lambda^2)$. Indeed, the final state of σ_λ^t is the uncoupled equilibrium $\omega_{{\rm S},\beta}$ while the true final state is the reduction to S of the coupled state $\omega_{{\rm SR},\beta,\lambda}$, as correctly described by (2.11). In other words, the remainder in expansion (2.21) does not vanish as $t\to\infty$, but stays of $O(\lambda^2)$.

The main result of this paper is Theorem 2.1 below, which gives an effective system dynamics τ_λ^t that *combines the advantages* of the above expansions (2.11) and (2.21), namely

(i) τ_λ^t is a quantum dynamical semigroup of the system, and
(ii) τ_λ^t describes the correct long time asymptotics (vanishing remainder as $t\to\infty$).

Theorem 2.1 *There is a constant $\lambda_0>0$ such that the following holds for $|\lambda|<\lambda_0$. There is a completely positive, identity preserving semigroup τ_λ^t acting on $\mathcal{B}(\mathcal{H}_{\rm S})$, the observables of the system, such that $\forall\omega_0\in\mathcal{S}_0$, $\forall t\geqslant 0$, $\forall X\in\mathcal{B}(\mathcal{H}_{\rm S})$,*

$$\omega_0\big(\alpha_\lambda^t(X\otimes\mathbf{1}_{\rm R})\big)=\omega_0\big(\tau_\lambda^t(X)\otimes\mathbf{1}_{\rm R}\big)+R_{\lambda,t}(X), \tag{2.22}$$

where $R_{\lambda,t}(X)$ satisfies

$$|R_{\lambda,t}(X)|\leqslant C|\lambda|\left(1+\lambda^2 t\right){\rm e}^{-\lambda^2(1+O(\lambda))\gamma t}\,\|X\|. \tag{2.23}$$

The dynamical semigroup τ_λ^t can be constructed perturbatively in λ, by using the resonance data (energies and vectors) of a renormalized, λ-dependent system Hamiltonian.

In analogy with (2.14) and (2.17), we will construct τ_λ^t by the definition

$$\big(\tau_\lambda^t(X)\otimes\mathbf{1}_{\rm S}\big)\widetilde{\Omega}_{{\rm S},\beta,\lambda}={\rm e}^{it(\widetilde{L}_{\rm S}+\lambda^2\widetilde{\Lambda})}(X\otimes\mathbf{1}_{\rm S})\widetilde{\Omega}_{{\rm S},\beta,\lambda}, \tag{2.24}$$

where $\widetilde{L}_{\rm S}=\widetilde{L}_{\rm S}(\lambda)$ and $\widetilde{\Lambda}=\widetilde{\Lambda}(\lambda)$ are suitably renormalized Liouville and level shift operators, respectively, which commute with each other. Here, $\widetilde{\Omega}_{{\rm S},\beta,\lambda}$ is a cyclic and separating vector spanning the kernel of $\widetilde{L}_{\rm S}+\lambda^2\widetilde{\Lambda}$.

2.1 Outline of the derivation of (2.11)–(2.13)

The detailed derivation is found in [20–22]. We sum it up as follows. A purification (GNS representation) of the state ω_0 gives the expression

$$\omega_0(\alpha_\lambda^t(X\otimes \mathbf{1}_{\mathrm{R}})) = \left\langle \Psi_0, \mathrm{e}^{itL_\lambda}\pi(X\otimes \mathbf{1}_{\mathrm{R}})\mathrm{e}^{-itL_\lambda}\Psi_0\right\rangle, \tag{2.25}$$

where Ψ_0 is a normalized vector in a suitable representation Hilbert space with inner product $\langle\cdot,\cdot\rangle$, L_λ is the self-adjoint *Liouville operator* and π is a $*$-representation, mapping system–reservoir observables to bounded operators on the representation Hilbert space. The algebraic structure (Tomita–Takesaki theory) implies that it suffices to consider vectors of the form $\Psi_0 = B\Omega_{\mathrm{SR},\beta,\lambda}$, where B is a bounded operator in the commutant of Ran π, and where $\Omega_{\mathrm{SR},\beta,\lambda}$ is the purification of the coupled system–reservoir equilibrium state $\omega_{\mathrm{SR},\beta,\lambda}$ [the (α_λ^t,β)-KMS state], satisfying $L_\lambda\Omega_{\mathrm{SR},\beta,\lambda}=0$ (stationary state). Then, (2.25) takes the form

$$\omega_0\left(\alpha_\lambda^t(X\otimes \mathbf{1}_{\mathrm{R}})\right) = \left\langle \Psi_0, B\mathrm{e}^{itL_\lambda}\pi(X\otimes \mathbf{1}_{\mathrm{R}})\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle. \tag{2.26}$$

The right side is now most easily analyzed using spectral deformation (complex scaling) techniques as in [20–22], similarly to what we do in the present paper in Sect. 3, see in particular (3.38).[4] The complex deformation effectively replaces the propagator e^{itL_λ} by $\mathrm{e}^{itL_{\lambda,\theta}}$, where $L_{\lambda,\theta}$ is the deformed, non-self-adjoint Liouville operator. For a fixed deformation parameter θ, the spectrum of $L_{\lambda,\theta}=L_{0,\theta}+\lambda I_\theta$ [in accordance with (3.6)] can be analyzed using standard analytic perturbation theory in λ, since the eigenvalues of $L_{0,\theta}$, which are real, are *isolated*, separated from the continuous spectrum, which is shifted by $\mathrm{Im}\theta>0$ into the upper complex plane (this is the action of the deformation). The eigenvalues of $L_{\lambda,\theta}$ (θ fixed, such that $\mathrm{Im}\theta \gg \lambda^2$) close to an unperturbed eigenvalue e of L_0 are $e+\lambda^2\lambda_{e,j}+O(\lambda^3)$, $j=1,\ldots,m_e$ (multiplicity of e, $m_0=d$) and the corresponding eigenprojections are $\Pi_{e,j}=Q_{e,j}+O(\lambda)$. Here $\lambda_{e,j}$ and $Q_{e,j}$ are the eigenvalues and eigenprojections of the level shift operator Λ_e [see (3.17), (3.18)]. The deformed propagator is then "diagonalized" as

$$\mathrm{e}^{itL_{\lambda,\theta}} = |\Omega_{\mathrm{SR},\beta,\lambda}\rangle\langle\Omega_{\mathrm{SR},\beta,\lambda}| + \textstyle\sum_{j=1}^{d-1}\mathrm{e}^{it\lambda^2(\lambda_{0,j}+O(\lambda))}\,\Pi_{0,j} \tag{2.27}$$

$$+\textstyle\sum_{e\in\mathrm{spec}(L_{\mathrm{S}})\setminus\{0\}}\sum_{j=1}^{m_e}\mathrm{e}^{it(e+\lambda^2(\lambda_{e,j}+O(\lambda)))}\,\Pi_{e,j} \tag{2.28}$$

$$+O(\lambda\mathrm{e}^{-\theta_0 t}). \tag{2.29}$$

This last equality sign has to be taken *cum grano salis*, in the weak sense on suitable vectors, and it is proven rigorously by means of a resolvent representation of the propagator (complex path integral over the resolvent). The term $|\Omega_{\mathrm{SR},\beta,\lambda}\rangle\langle\Omega_{\mathrm{SR},\beta,\lambda}|$ is the projection onto the invariant state (associated with the simple eigenvalue zero of $L_{\lambda,\theta}$). The sums on lines (2.27) and (2.28) describe the bifurcation of complex

[4] One may also follow an extended Mourre theory approach, recently developed in [15]. This method is more powerful in that it requires less restrictive assumptions, but it is technically somewhat more demanding.

resonance energies of $L_{\lambda,\theta}$ out of the zero and nonzero real (Bohr) system energies [the eigenvalues of L_{S}, (2.5), which are the same as the eigenvalues of $L_{0,\theta}$]. The remainder term (2.29) is brought about by the (continuous) spectrum of $L_{\lambda,\theta}$, all of whose spectral points have imaginary part exceeding $\theta_0 = \mathrm{Im}\theta$. We now use the expansion (2.27)–(2.29) in (2.26). The projection onto $\Omega_{\mathrm{SR},\beta,\lambda}$ contributes with

$$\left\langle \Psi_0, B\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle\left\langle \Omega_{\mathrm{SR},\beta,\lambda}, \pi\left(X\otimes \mathbf{1}_{\mathrm{R}}\right)\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle = \omega_{\mathrm{SR},\beta,\lambda}\left(X\otimes \mathbf{1}_{\mathrm{R}}\right). \tag{2.30}$$

A general term in the sums of (2.27), (2.28) contributes in (2.26) with

$$\begin{aligned}&\left\langle \Psi_0, B\mathrm{e}^{it(e+\lambda^2(\lambda_{e,j}+O(\lambda)))}\Pi_{e,j}\,\pi(X\otimes \mathbf{1}_{\mathrm{R}})\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle\\ &\quad=\left\langle \Psi_0, B\mathrm{e}^{it(e+\lambda^2\lambda_{e,j})}\,Q_{e,j}\,\pi(X\otimes \mathbf{1}_{\mathrm{R}})(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}})\right\rangle + O\Big(|\lambda|\,\|X\|(1+\lambda^2 t)\mathrm{e}^{-\lambda^2\gamma t}\Big).\end{aligned} \tag{2.31}$$

We have replaced $\mathrm{e}^{it(e+\lambda^2(\lambda_{e,j}+O(\lambda)))}$ by $\mathrm{e}^{it(e+\lambda^2\lambda_{e,j})}$, leading to an error term $O(|\lambda|^3\|X\|\,t\mathrm{e}^{-\lambda^2\gamma t})$, where γ is given in (2.9) (see also footnote 5). Then, we have replaced $\Pi_{e,j}$ by $Q_{e,j}$, making an error of $O(|\lambda|\,\|X\|\,\mathrm{e}^{-\lambda\gamma t})$ and the same error is incurred by replacing the coupled KMS vector $\Omega_{\mathrm{SR},\beta,\lambda}$ by the uncoupled KMS vector $\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}$, since $\|\Omega_{\mathrm{SR},\beta,\lambda}-\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}\| = O(\lambda)$. Next, summing (2.31) over all e and j, as dictated by the sums in (2.27) and (2.28), turns $\mathrm{e}^{it(e+\lambda^2(\lambda_{e,j}))}Q_{e,j}$ into $\mathrm{e}^{it(L_{\mathrm{S}}+\lambda\Lambda)}P^{\perp}_{\mathrm{S},\beta}$ [the eigenvalue zero of Λ is excluded as it is taken care of in the term coming from $|\Omega_{\mathrm{SR},\beta,\lambda}\rangle\langle\Omega_{\mathrm{SR},\beta,\lambda}|$ in (2.27)]. Consequently,

$$\begin{aligned}\omega_0\left(\alpha^t_\lambda\left(X\otimes \mathbf{1}_{\mathrm{R}}\right)\right) &= \omega_{\mathrm{SR},\beta,\lambda}\left(X\otimes \mathbf{1}_{\mathrm{R}}\right) + \left\langle \Psi_0, B\mathrm{e}^{it(L_{\mathrm{S}}+\lambda\Lambda)}P^{\perp}_{\mathrm{S},\beta}\,\pi\left(X\otimes \mathbf{1}_{\mathrm{R}}\right)\left(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}\right)\right\rangle\\ &\quad+O\Big(|\lambda|\,\|X\|(1+\lambda^2 t)\mathrm{e}^{-\lambda^2\gamma t}\Big).\end{aligned} \tag{2.32}$$

Next, we use definition (2.14) of δ^t_λ to see that

$$\begin{aligned}&\left\langle \Psi_0, B\mathrm{e}^{it(L_{\mathrm{S}}+\lambda\Lambda)}P^{\perp}_{\mathrm{S},\beta}\,\pi\left(X\otimes \mathbf{1}_{\mathrm{R}}\right)\left(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}\right)\right\rangle\\ &\quad=\left\langle \Psi_0, B\left(\delta^t_\lambda(X)\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}}\right)\left(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}\right)\right\rangle\\ &\quad=\left\langle \Psi_0, \left(\delta^t_\lambda(X)\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}}\right)B\left(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}\right)\right\rangle\\ &\quad=\left\langle \Psi_0, \pi\left(\delta^t_\lambda(X)\otimes \mathbf{1}_{\mathrm{R}}\right)\Psi_0\right\rangle + O\left(|\lambda|\,\|X\|\,\mathrm{e}^{-\lambda^2\gamma t}\right).\end{aligned} \tag{2.33}$$

In the last step, we have exploited that $B(\Omega_{\mathrm{S},\beta}\otimes\Omega_{\mathrm{R}}) = B\Omega_{\mathrm{SR},\beta,\lambda} + O(\lambda)$ and $B\Omega_{\mathrm{SR},\beta,\lambda} = \Psi_0$. Finally, combining (2.32) and (2.33), voilà, we obtain the expansion (2.11).

3 The renormalized dynamics and complete positivity

3.1 States and dynamics

The description (2.1)–(2.3) given above is common in the theoretical physics literature and serves, in particular, to introduce the system–reservoir interaction operators [taken here to be linear in the field, (2.2)]. It is, however, well known that the Fock space $\mathcal{H}_{\rm R}$ above is not the correct Hilbert space on which one can represent the state of a spatially infinitely extended Bose gas in thermal equilibrium. To find that Hilbert space, one has to first perform the thermodynamic limit of the reservoir equilibrium state and then reconstruct its Hilbert space representation using the Gelfand–Naimark–Segal construction. This is the Araki–Woods representation for thermal reservoirs [2].

It consists of a triple $(\mathcal{H}_{{\rm R},\beta}, \pi_\beta, \Omega_{\rm R})$, where $\mathcal{H}_{{\rm R},\beta}$ is the representation Hilbert space, $\pi_\beta : \mathfrak{W} \to \mathcal{B}(\mathcal{H}_{{\rm R},\beta})$ is a representation of the Weyl algebra and $\Omega_{\rm R} \in \mathcal{H}_{{\rm R},\beta}$ is a normalized vector representing the equilibrium state. Explicitly,

$$\mathcal{H}_{{\rm R},\beta} = \mathcal{F}\left(L^2\left(\mathbb{R}\times S^2, {\rm d}u \times {\rm d}\Sigma\right)\right) \equiv \bigoplus_{n\geqslant 0} L^2_{\rm sym}\left(\left(\mathbb{R}\times S^2\right)^n, ({\rm d}u\times{\rm d}\Sigma)^n\right) \tag{3.1}$$

is the bosonic Fock space over the single particle space $L^2(\mathbb{R}\times S^2, du \times d\Sigma)$, where $d\Sigma$ is the uniform measure on the sphere S^2. The vector $\Omega_{\rm R}$ is the vacuum vector of $\mathcal{F}$, and the representation map is given by

$$\pi_\beta\left(W(f)\right) = W\left(f_\beta\right), \tag{3.2}$$

where $f \mapsto f_\beta$ was defined by (2.10). The operator $W(f)$ on the left side of (3.2) is an (abstract) Weyl operator in $\mathfrak{W}$, while the represented $W(f_\beta)$ on the right side is given by $W(f_\beta) = {\rm e}^{i\varphi(f_\beta)}$, with $\varphi(f_\beta) = 2^{-1/2}[a(f_\beta) + a^*(f_\beta)]$. Here, $a^*(f_\beta)$ is the creation operator smoothed out with f_β, acting on $\mathcal{F}$ and $a(f_\beta)$ its adjoint. The reservoir equilibrium state at temperature $T = 1/\beta$ is represented as

$$\omega_{{\rm R},\beta}\left(W(f)\right) = \langle\, \Omega_{\rm R} \,|\, \pi_\beta\left(W(f)\right) \Omega_{\rm R}\,\rangle.$$

The free reservoir dynamics is implemented as $\pi_\beta(W({\rm e}^{i\omega t} f)) = {\rm e}^{itL_{\rm R}} \pi_\beta(W(f))$ ${\rm e}^{-itL_{\rm R}}$, where

$$L_{\rm R} = {\rm d}\Gamma(u) \tag{3.3}$$

is the reservoir Liouville operator, the second quantization of multiplication with the radial variable u.

Together with (2.5), the joint system–reservoir Hilbert space and non-interacting Liouville operator are given by

$$\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathcal{H}_{{\rm R},\beta} \quad \text{and} \quad L_0 = L_{\rm S} + L_{\rm R}. \tag{3.4}$$

The interaction associated with (2.2) is represented by the operator

$$I = V_{\rm S} \otimes \mathbf{1}_{\rm S} \otimes \varphi(g_\beta) - J\big(V_{\rm S} \otimes \mathbf{1}_{\rm S} \otimes \varphi(g_\beta)\big) J, \tag{3.5}$$

where $J = J_S \otimes J_R$ is the modular conjugation. It is given explicitly as follows. Let $\mathcal{C}$ be the antilinear operator acting on $\mathbb{C}^d$ by taking complex conjugates of vector coordinates in the energy basis $\{\varphi_n\}$, then J_S acts on $\mathbb{C}^d \otimes \mathbb{C}^d$ as $J_S \chi \otimes \psi = \mathcal{C}\psi \otimes \mathcal{C}\chi$. Similarly, J_R acts on $\mathcal{F}$ sector-wise and on the n-sector, its action is $J_R \psi_n(u_1, \Sigma_1, \ldots, u_n, \Sigma_n) = \overline{\psi_n(-u_1, \Sigma_1, \ldots, -u_n, \Sigma_n)}$. The full Liouville operator is then

$$L_\lambda = L_0 + \lambda I. \tag{3.6}$$

The non-interacting and interacting systems, whose dynamics is generated by L_0 and L_λ, have unique β-KMS states $\omega_{SR,\beta,0}$ and $\omega_{SR,\beta,\lambda}$, which are represented by the KMS vectors $\Omega_{SR,\beta,0}$ and $\Omega_{SR,\beta,\lambda}$ respectively, where [recall (2.7)]

$$\Omega_{SR,\beta,0} = \Omega_{S,\beta} \otimes \Omega_R \qquad \text{and} \qquad \Omega_{SR,\beta,\lambda} = \frac{e^{-\beta(L_0+\lambda V_S \otimes \mathbf{1}_S \otimes \varphi(g_\beta))/2}\Omega_{SR,\beta,0}}{\|e^{-\beta(L_0+\lambda V_S \otimes \mathbf{1}_S \otimes \varphi(g_\beta))/2}\Omega_{SR,\beta,0}\|}. \tag{3.7}$$

We refer to [4,6,9] for more detail on the construction of the interacting KMS state.

3.2 Construction of the renormalized quantities

The reduction in the joint equilibrium state to the system is given by the density matrix $\rho_{S,\beta,\lambda}$, defined by

$$Tr_S\big(\rho_{S,\beta,\lambda} X\big) = \omega_{SR,\beta,\lambda}\,(X \otimes \mathbf{1}_R) \qquad \text{for all } X \in \mathcal{B}(\mathcal{H}_S). \tag{3.8}$$

Since $\omega_{SR,\beta,\lambda}$ is faithful, it is readily seen that $\rho_{S,\beta,\lambda}$ is *strictly* positive. Set

$$\widetilde{Z} := \|\rho_{S,\beta,\lambda}\|^{-1} \tag{3.9}$$

(operator norm) and define the renormalized system Hamiltonian by

$$\widetilde{H}_S = -\tfrac{1}{\beta} \ln\big(\widetilde{Z}\rho_{S,\beta,\lambda}\big), \tag{3.10}$$

so that

$$\rho_{S,\beta,\lambda} = \widetilde{Z}^{-1}\, e^{-\beta \widetilde{H}_S}. \tag{3.11}$$

Note that $\widetilde{Z} = Tr_S\, e^{-\beta\widetilde{H}_S}$. The operator $\widetilde{H}_S$ depends on λ, and we have $\widetilde{H}_S|_{\lambda=0} = H_S$ and $\widetilde{Z}|_{\lambda=0} = Tr_S\, e^{-\beta H_S} \equiv Z_S$ [c.f. (2.7)].

Remark Given $\rho_{S,\beta,\lambda}$, the relation $\rho_{S,\beta,\lambda} = (\widetilde{Z}(\lambda))^{-1} e^{-\beta\widetilde{H}_S(\lambda)}$ [c.f. (3.11)] implies that $\widetilde{Z}(\lambda) = Tr_S\, e^{-\beta\widetilde{H}_S(\lambda)}$ but defines the operator $\widetilde{H}_S(\lambda)$ only up to an additive term $\propto \mathbf{1}_S$. Let $\widetilde{E}_0(\lambda) = \min \operatorname{spec}(\widetilde{H}_S(\lambda))$, then taking the operator norm gives $\|\rho_{S,\beta,\lambda}\| = e^{-\beta\widetilde{E}_0(\lambda)}/\widetilde{Z}(\lambda)$. The ground-state energy normalization $\widetilde{E}_0(\lambda) = 0$, in accordance with $\min \operatorname{spec}(H_S) = 0$ [see after (2.3)], gives the choice (3.9).

Lemma 3.1 *Let $\{\phi_n\}_{n=1,\dots,d}$ be an orthonormal basis of eigenvectors of H_S, such that $H_S\phi_n = E_n\phi_n$. The eigenvalues of $\widetilde{H}_S$ are $\widetilde{E}_n$, satisfying $E_n - \widetilde{E}_n = O(\lambda)$. The normalized eigenvectors, $\widetilde{H}_S\widetilde{\phi}_n = \widetilde{E}_n\widetilde{\phi}_n$, satisfy $\phi_n - \widetilde{\phi}_n = O(\lambda)$.*

Proof of Lemma 3.1 Araki's perturbation theory of KMS states [4,6,9] yields $\|\rho_{S,\beta,\lambda} - \rho_{S,\beta,0}\| = O(\lambda)$. It follows from (3.9) that $|\widetilde{Z} - Z_S| = O(\lambda)$, where Z_S is the unperturbed system partition function, (2.7). Then, (3.10) gives $\|\widetilde{H}_S - H_S\| = O(\lambda)$. The lemma then follows from usual analytic perturbation theory for matrices. □

We define

$$\widetilde{L}_S = \widetilde{H}_S \otimes \mathbf{1}_S - \mathbf{1}_S \otimes \mathcal{C}\widetilde{H}_S\mathcal{C} \tag{3.12}$$

$$\widetilde{\Omega}_{S,\beta,\lambda} = \widetilde{Z}^{-1/2}\sum_{n=1}^{d} e^{-\beta\widetilde{E}_n/2}\widetilde{\phi}_n \otimes \mathcal{C}\widetilde{\phi}_n, \tag{3.13}$$

where $\mathcal{C}$ is the antilinear map satisfying $\mathcal{C}\phi_n = \phi_n$ (i.e., $\mathcal{C}$ implements complex conjugation of coordinates in the basis $\{\phi_n\}$). The vector $\widetilde{\Omega}_{S,\beta,\lambda}$ represents the state $\rho_{S,\beta,\lambda}$, meaning

$$\left\langle \widetilde{\Omega}_{S,\beta,\lambda}, (X \otimes \mathbf{1}_S)\widetilde{\Omega}_{S,\beta,\lambda}\right\rangle = \mathrm{Tr}_S\,(\rho_{S,\beta,\lambda}X), \qquad X \in \mathcal{B}(\mathcal{H}_S). \tag{3.14}$$

$\widetilde{\Omega}_{S,\beta,\lambda}$ and is a β-KMS vector with respect to the dynamics $e^{it\widetilde{L}_S} \cdot e^{-it\widetilde{L}_S}$ of the system observable algebra $\mathcal{B}(\mathcal{H}_S) \otimes \mathbf{1}_S$. We let

$$\widetilde{L}_0 = \widetilde{L}_S + L_R \tag{3.15}$$

$$\widetilde{\Omega}_0 = \widetilde{\Omega}_{S,\beta,\lambda} \otimes \Omega_R \tag{3.16}$$

and denote by $\widetilde{P}_{\widetilde{e}}$ the eigenprojection onto the eigenvalue $\widetilde{e}$ of $\widetilde{L}_0$.

The level shift operators of the original (not renormalized) system are given as follows. For each $e \in \mathrm{spec}(L_S)$,

$$\Lambda_e = -P_e I P_e^{\perp}(L_0 - e + i0_+)^{-1} I P_e, \qquad \text{and} \qquad \Lambda = \sum_{e\in\mathrm{spec}(L_S)} \Lambda_e, \tag{3.17}$$

where P_e is the spectral projection of L_0 onto the eigenvalue e (having multiplicity m_e). Λ_e is diagonalizable and has the spectral representation

$$\Lambda_e = \sum_{j=1}^{m_e} \lambda_{e,j} Q_{e,j}, \tag{3.18}$$

where $Q_{e,j} = P_e Q_{e,j} = Q_{e,j} P_e$ and $\lambda_{e,j}$ are the spectral projections and eigenvalues, which are all simple [Assumption (A1)(i)]. According to Assumption (A1)(ii), we have $\ker\Lambda = \mathbb{C}\Omega_{S,\beta}$ and $\mathrm{Im}\lambda_{e,j} > 0$ for all $e \neq 0$ and j, $\mathrm{Im}\lambda_{0,j} > 0$ for $j = 1,\dots,d-1$ and $\lambda_{0,d} = 0$ (one-dimensional kernel of Λ).

We now define the level shift operator $\widetilde{\Lambda}$ of the renormalized system. For each $\widetilde{e}\in\mathrm{spec}(\widetilde{L}_{\mathrm{S}})$, set

$$\widetilde{\Lambda}_{\widetilde{e}}=-\widetilde{P}_{\widetilde{e}}I\widetilde{P}_{\widetilde{e}}^{\perp}(\widetilde{L}_0-\widetilde{e}+i0_+)^{-1}I\widetilde{P}_{\widetilde{e}},\qquad\text{and}\qquad\widetilde{\Lambda}=\sum_{\widetilde{e}\in\mathrm{spec}(\widetilde{L}_{\mathrm{S}})}\widetilde{\Lambda}_{\widetilde{e}}\widetilde{P}_{\widetilde{e}}.\tag{3.19}$$

Proposition 3.2 *The operator $\widetilde{\Lambda}_{\widetilde{e}}$ exists for each $\widetilde{e}\in\mathrm{spec}(\widetilde{L}_{\mathrm{S}})$ and satisfies $\Lambda_e-\widetilde{\Lambda}_{\widetilde{e}}=O(\lambda)$. Its spectrum consists of simple eigenvalues $\widetilde{\lambda}_{\widetilde{e},j}$, $j=1,\ldots,m_e$, satisfying $\lambda_{e,j}-\widetilde{\lambda}_{\widetilde{e},j}=O(\lambda)$. The associated Riesz spectral projections $\widetilde{Q}_{\widetilde{e},j}$ satisfy $Q_{e,j}-\widetilde{Q}_{\widetilde{e},j}=O(\lambda)$. Moreover,* $\ker\widetilde{\Lambda}=\mathbb{C}\widetilde{\Omega}_0$.

The proposition implies that $\widetilde{\Lambda}$ has the spectral representation

$$\widetilde{\Lambda}=\sum_{j=1}^{d-1}\widetilde{\lambda}_{0,j}\,\widetilde{Q}_{0,j}+\sum_{\widetilde{e}\neq 0}\sum_{j=1}^{m_e}\widetilde{\lambda}_{\widetilde{e},j}\,\widetilde{Q}_{\widetilde{e},j}.\tag{3.20}$$

Proof of Proposition 3.2 Let $U_\theta=\mathrm{e}^{i\theta\mathrm{d}\Gamma(-i\partial_u)}$, so that $U_\theta L_0U_\theta^*=L_0+\theta N$, where $N=\mathrm{d}\Gamma(\mathbf{1}_{\mathrm{R}})$ is the number operator. Setting $I_\theta=U_\theta IU_\theta^*$ and using that $U_\theta P_e=P_eU_\theta=P_e$, we have for all $\theta\in\mathbb{R}$ and $\epsilon>0$

$$P_eI\,(L_0-e+i\epsilon)^{-1}\,IP_e=P_eI_\theta\,(L_0+\theta N-e+i\epsilon)^{-1}\,I_\theta P_e.$$

By Assumption (A2), the right side has an analytic extension into values of θ in a strip with $\mathrm{Im}\,\theta<2\theta_0$, for some $\theta_0>0$ and so

$$\begin{aligned}P_eI\,(L_0-e+i\epsilon)^{-1}\,IP_e&=P_eI_{i\theta_0}\,(L_0+i\theta_0N-e+i\epsilon)^{-1}\,I_{i\theta_0}P_e\\&=\widetilde{P}_{\widetilde{e}}I_{i\theta_0}\left(\widetilde{L}_0+i\theta_0N-\widetilde{e}+i\epsilon\right)^{-1}I_{i\theta_0}\widetilde{P}_{\widetilde{e}}+O(\lambda),\end{aligned}$$

where the error term bounded uniformly in $\epsilon>0$. As $U_\theta\widetilde{P}_{\widetilde{e}}=\widetilde{P}_{\widetilde{e}}U_\theta=\widetilde{P}_{\widetilde{e}}$, we can undo the spectral deformation in the main term on the right side and take $\epsilon\to 0_+$ to obtain

$$\Lambda_e=\widetilde{\Lambda}_{\widetilde{e}}+O(\lambda).\tag{3.21}$$

The statements about the eigenvalues and Riesz eigenprojections follow from basic perturbation theory. [Recall that Λ_e has simple, λ-independent eigenvalues by Assumption (A1).] To show that $\ker\widetilde{\Lambda}=\mathbb{C}\widetilde{\Omega}_0$ it suffices to show that $\widetilde{\Lambda}_0\widetilde{\Omega}_0=0$, as all the eigenvalues $\widetilde{\lambda}_{\widetilde{e},j}$ associated with $e\neq 0$ and for $e=0$ and $j=1,\ldots,d-1$, have strictly positive imaginary part, a property which is inherited from the eigenvalues of Λ (for λ small).

To show $\widetilde{\Lambda}_0\widetilde{\Omega}_0=0$, we introduce the auxiliary Liouville operator

$$\widetilde{L}_\mu=\widetilde{L}_0+\lambda\mu I,\tag{3.22}$$

where I is given in (3.5). By Araki's perturbation theory of KMS states, we know that

$$\widetilde{L}_\mu\widetilde{\Omega}_\mu=0,\tag{3.23}$$

where

$$\widetilde{\Omega}_\mu = \frac{\mathrm{e}^{-\beta\{\widetilde{L}_0+\lambda\mu V_S\otimes\mathbf{1}_S\otimes\varphi(g_\beta)\}/2}\widetilde{\Omega}_0}{\|\mathrm{e}^{-\beta\{\widetilde{L}_0+\lambda\mu V_S\otimes\mathbf{1}_S\otimes\varphi(g_\beta)\}/2}\widetilde{\Omega}_0\|}. \tag{3.24}$$

Lemma 3.3 *Let $g_0 > 0$ be the spectral gap of $\widetilde{L}_S$ at zero. The operator $\widetilde{L}_\mu^\perp := \widetilde{P}_0^\perp \widetilde{L}_\mu \widetilde{P}_0^\perp|_{\mathrm{Ran}\,\widetilde{P}_0^\perp}$ has purely absolutely continuous spectrum in the open interval $(-g_0/2, g_0/2)$. In particular, zero is not an eigenvalue of $\widetilde{L}_\mu^\perp$.*

Proof of Lemma 3.3 Let φ be a U_θ-analytic vector. For $\mathrm{Im}z < 0$

$$\begin{aligned}\left\langle \varphi, (\widetilde{L}_\mu^\perp - z)^{-1}\varphi\right\rangle &= \left\langle \varphi_{\bar\theta}, (\widetilde{L}_0^\perp + \theta N^\perp + \lambda\mu I_\theta^\perp - z)^{-1}\varphi_\theta\right\rangle \\ &= \left\langle \varphi_{\bar\theta}, (\widetilde{L}_0^\perp + \theta N^\perp - z)^{-1}\sum_{n\geq 0}(-\lambda\mu)^n\left[I_\theta^\perp(\widetilde{L}_0^\perp + \theta N^\perp - z)^{-1}\right]^n \varphi_\theta\right\rangle,\end{aligned} \tag{3.25}$$

where $X^\perp = \widetilde{P}_0^\perp X \widetilde{P}_0^\perp|_{\mathrm{Ran}\,\widetilde{P}_0^\perp}$. Using the decomposition $\widetilde{P}_0^\perp = \widetilde{P}_S^\perp \otimes P_R + \mathbf{1}_S \otimes P_R^\perp$, where $\widetilde{P}_S$ is the orthogonal projection onto the kernel of $\widetilde{L}_S$ and $P_R = |\Omega_R\rangle\langle\Omega_R|$, we easily obtain the bounds

$$\left\|\left(\widetilde{L}_0^\perp + i\theta_0 N^\perp - z\right)^{-1}\right\| \leqslant \max\left\{\max_{\widetilde{e}\neq 0}|\widetilde{e} - z|^{-1}, |\theta_0 - \mathrm{Im}z|^{-1}\right\} \tag{3.26}$$

$$\left\|I_{i\theta_0}^\perp\left(\widetilde{L}_0^\perp + i\theta_0 N^\perp - z\right)^{-1}\right\| \leqslant C_{\theta_0}\max\left\{\max_{\widetilde{e}\neq 0}|\widetilde{e} - z|^{-1}, |\theta_0 - \mathrm{Im}z|^{-1}\right\}. \tag{3.27}$$

Thus, for $\mathrm{Im}z \leqslant 0$ and $|Rez| \leqslant g_0/2$, where $g_0 > 0$ is the spectral gap of $\widetilde{L}_S$ at zero, the combination of (3.25), (3.26) and (3.27) gives the limiting absorption principle

$$\sup_{z:|Rez|\leqslant g_0/2, \mathrm{Im}z\leqslant 0}\left|\left\langle\varphi, (\widetilde{L}_\mu^\perp - z)^{-1}\varphi\right\rangle\right| \leqslant C(\varphi).$$

This implies that $\widetilde{L}_\mu^\perp$ has purely absolutely continuous spectrum in the interval $(-g_0/2, g_0/2)$. Lemma 3.3 is proven.

Combining (3.23) with Lemma 3.3, and invoking the isospectrality of the Feshbach map (see for instance Proposition B.2 in [15]), we obtain

$$\mathfrak{F}\left(\widetilde{L}_\mu; \widetilde{P}_0\right)\widetilde{P}_0\widetilde{\Omega}_\mu = 0, \tag{3.28}$$

where

$$\mathfrak{F}\left(\widetilde{L}_\mu; \widetilde{P}_0\right) = -\lambda^2\mu^2\widetilde{P}_0 I \widetilde{P}_0^\perp\left(\widetilde{L}_\mu^\perp + i0_+\right)^{-1} I\widetilde{P}_0. \tag{3.29}$$

We now use the translation analyticity to obtain

$$\widetilde{P}_0 I\left(\widetilde{L}_\mu^\perp + i0_+\right)^{-1} I\widetilde{P}_0 = \widetilde{P}_0 I_{i\theta_0}\left(\widetilde{L}_0^\perp + i\theta_0 N^\perp + \lambda\mu I_{i\theta_0}^\perp\right)^{-1} I_{i\theta_0}\widetilde{P}_0. \tag{3.30}$$

Combining (3.28), (3.29) and (3.30), and taking $\mu \to 0$, gives

$$\widetilde{P}_0 I_{i\theta_0} \left(\widetilde{L}_0^\perp + i\theta_0 N^\perp\right)^{-1} I_{i\theta_0} \widetilde{P}_0 \widetilde{\Omega}_0 = 0. \tag{3.31}$$

Reversing the spectral deformation (i.e., taking $\theta_0 \to 0_+$) on the left hand side of (3.31) gives precisely $\widetilde{\Lambda}_0 \widetilde{\Omega}_0 = 0$. This completes the proof of Proposition 3.2. □

3.3 Representation of the dynamics: proof of (2.22)

We first introduce the dense set of initial states for which the dynamical resonance theory based on spectral deformation can be applied. The three vectors $\widetilde{\Omega}_0$, $\Omega_{\mathrm{SR},\beta,0}$ and $\Omega_{\mathrm{SR},\beta,\lambda}$ play a role in what follows. We recall their definitions, (3.16) and (3.7).

Let $\mathfrak{M}_0 \subset \mathfrak{M}$ be the set of all finite linear combinations of operators of the form $\pi(A_{\mathrm{S}} \otimes W(f))$, where $A_{\mathrm{S}} \in \mathcal{B}(\mathcal{H}_{\mathrm{S}})$ and $W(f)$ is a Weyl operator smoothed out with a test function f that satisfies Assumption (A2). The following properties of the set of vectors $J\mathfrak{M}_0\widetilde{\Omega}_0 = J\mathfrak{M}_0 J\widetilde{\Omega}_0$ are not difficult to verify:

$$J\mathfrak{M}_0\widetilde{\Omega}_0 \text{ is dense in} \mathcal{H} \quad \text{and} \quad J\mathfrak{M}_0\widetilde{\Omega}_0 \subset \mathcal{A}_{\theta_0} \cap \mathrm{Dom}\left(\mathrm{e}^{\alpha N}\right) \text{ for all } \alpha \in \mathbb{R}. \tag{3.32}$$

Here, $\mathcal{A}_{\theta_0}$ is the set of vectors $\psi \in \mathcal{H}$ such that $\theta \mapsto \mathrm{e}^{i\theta A}\psi$, $A = \mathrm{d}\Gamma(-i\partial_u)$, is analytic in θ in a strip $\mathrm{Im}\theta < \theta_0$ and $N = \mathrm{d}\Gamma(\mathbf{1}_{\mathrm{R}})$ is the number operator. We consider the set of states

$$\mathcal{S}_0 = \left\{\omega(\cdot) = \langle JC\widetilde{\Omega}_0, \pi(\cdot)JC\widetilde{\Omega}_0\rangle \ : \ C \in \mathfrak{M}_0\right\}. \tag{3.33}$$

Lemma 3.4 *We have* $\widetilde{\Omega}_0 = JD\Omega_{\mathrm{SR},\beta,\lambda}$ *for an operator* D *affiliated with* $\mathfrak{M}$. *Moreover, given any* $\alpha > 0$, *we have for small enough* λ, $\mathrm{Dom}(D^\#) \supset \mathrm{Dom}(\mathrm{e}^{\alpha N})$ *and* $D^\#\mathrm{e}^{-\alpha N}\mathcal{A}_{\theta_0} \subset \mathcal{A}_{\theta_0}$. *Here,* $D^\#$ *stands for* D *or its adjoint* D^*. *Moreover,* $\Omega_{\mathrm{SR},\beta,\lambda} \in \mathcal{A}_{\theta_0}$.

Remark The vectors $\Omega_{\mathrm{SR},\beta,0}$, $\Omega_{\mathrm{SR},\beta,\lambda}$ and $\widetilde{\Omega}_0$ are all invariant under the action of the modular conjugation J. This implies that $\widetilde{\Omega}_0 = D\Omega_{\mathrm{SR},\beta,\lambda} = JDJ\Omega_{\mathrm{SR},\beta,\lambda}$.

Proof of Lemma 3.4 We first construct an operator G satisfying $\Omega_0 = JG\Omega_{\mathrm{SR},\beta,\lambda}$ having the desired regularity properties. The perturbation theory of KMS states gives

$$\Omega_{\mathrm{SR},\beta,\lambda} = c^{-1}\mathrm{e}^{-\beta(L_0+\lambda K)/2}\mathrm{e}^{\beta L_0/2}\Omega_{\mathrm{SR},\beta,0} \quad \text{and} \quad \Omega_{\mathrm{SR},\beta,0} = c\mathrm{e}^{-\beta L_0/2}\mathrm{e}^{\beta(L_0+\lambda K)/2}\Omega_{\mathrm{SR},\beta,\lambda}, \tag{3.34}$$

where c is a normalization constant and, for short, $K = V_{\mathrm{S}} \otimes \mathbf{1}_{\mathrm{S}} \otimes \varphi(g_\beta)$. A Dyson series expansion yields

$$\mathrm{e}^{-\beta L_0/2}\mathrm{e}^{\beta(L_0+\lambda K)/2} = \sum_{n\geqslant 0}\lambda^n \int_{0\leqslant s_1\leqslant\cdots\leqslant s_n\leqslant\beta/2} \mathrm{d}s_1\cdots\mathrm{d}s_n\, K(s_n)\cdots K(s_1) =: c^{-1}G, \tag{3.35}$$

where $K(s) = \mathrm{e}^{-sL_0} K \mathrm{e}^{sL_0}$. Using that

$$\sup_{0 \leqslant s \leqslant \beta/2} \left\| \mathrm{e}^{\alpha N} K(s) \mathrm{e}^{-\alpha N} (N+1)^{-1/2} \right\| < \infty,$$

one readily sees that, for any $\alpha > 0$ fixed and λ small enough, the series in (3.35) converges strongly on $\mathrm{Dom}(\mathrm{e}^{\alpha N})$ and defines an element affiliated with $\mathfrak{M}$, and that furthermore, $\mathrm{Ran}(G\mathrm{e}^{-\alpha N}) \subset \mathrm{Dom}(\mathrm{e}^{\alpha N})$. The analogous expansion and result can be obtained starting with $\mathrm{e}^{-\beta(L_0+\lambda K)/2} \mathrm{e}^{\beta L_0/2}$, which shows that $\Omega_{\mathrm{SR},\beta,\lambda} \in \mathrm{Dom}(\mathrm{e}^{\alpha N})$. Combining this with (3.34) gives

$$\Omega_{\mathrm{SR},\beta,0} = G \Omega_{\mathrm{SR},\beta,\lambda} = J G \Omega_{\mathrm{SR},\beta,\lambda}. \tag{3.36}$$

The last equality follows from $J\Omega_{\mathrm{SR},\beta,0} = \Omega_{\mathrm{SR}\,\beta,0}$. The cyclicity of $\Omega_{\mathrm{S},\beta}$ implies that there is a $D_\mathrm{S} \in \mathcal{B}(\mathcal{H}_\mathrm{S})$ satisfying $\widetilde{\Omega}_0 = J(D_\mathrm{S} \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\Omega_{\mathrm{SR},\beta,0}$. Thus, from (3.36),

$$\widetilde{\Omega}_0 = J\,(D_\mathrm{S} \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\, G \Omega_{\mathrm{SR},\beta,\lambda} =: J D \Omega_{\mathrm{SR},\beta,\lambda}. \tag{3.37}$$

It remains to prove the analyticity statement, which is the same as $G\mathrm{e}^{-\alpha N} \mathcal{A}_{\theta_0} \subset \mathcal{A}_{\theta_0}$. This follows again from the series expansion of G, (3.35), and the fact that $\mathrm{e}^{i\theta A} K(s_n) \cdots K(s_1) \mathrm{e}^{-i\theta A} = K_\theta(s_n) \cdots K_\theta(s_1)$, where $K_\theta(s) = \mathrm{e}^{i\theta A} \mathrm{e}^{-sL_0} K \mathrm{e}^{sL_0}$ $\mathrm{e}^{-i\theta A}$, is analytic.

Finally, to show that $\Omega_{\mathrm{SR},\beta,\lambda} \in \mathcal{A}_{\theta_0}$, we note that the adjoint of the Dyson series expansion (3.35) gives that $G^* \mathrm{e}^{-\alpha N} \mathcal{A}_{\theta_0} \subset \mathcal{A}_{\theta_0}$ and the desired result follows from (3.34). □

For $\omega_0 \in \mathcal{S}_0$ and $X \in \mathcal{B}(\mathcal{H}_\mathrm{S})$, we have

$$\begin{aligned}
\omega_0\left(\alpha_\lambda^t\,(X \otimes \mathbf{1}_\mathrm{R})\right) &= \left\langle JC\widetilde{\Omega}_0, \mathrm{e}^{itL}\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\,\mathrm{e}^{-itL} JC\widetilde{\Omega}_0 \right\rangle \\
&= \left\langle JC^*C\widetilde{\Omega}_0, \mathrm{e}^{itL}\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\,\mathrm{e}^{-itL} \widetilde{\Omega}_0 \right\rangle \\
&= \left\langle JC^*C\widetilde{\Omega}_0, \mathrm{e}^{itL}\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\,\mathrm{e}^{-itL} JDJ\Omega_{\mathrm{SR},\beta,\lambda} \right\rangle \\
&= \left\langle JC^*C\widetilde{\Omega}_0, JDJ\mathrm{e}^{itL}\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\,\Omega_{\mathrm{SR},\beta,\lambda} \right\rangle \\
&= \left\langle JD^*C^*C\widetilde{\Omega}_0, \mathrm{e}^{itL}\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\,\Omega_{\mathrm{SR},\beta,\lambda} \right\rangle.
\end{aligned} \tag{3.38}$$

Lemma 3.4 gives $\Omega_{\mathrm{SR},\beta,\lambda} \in \mathcal{A}_{\theta_0}$ and since $C^*C\widetilde{\Omega}_0 \in \mathrm{Dom}(\mathrm{e}^{\alpha N}) \cap \mathcal{A}_{\theta_0}$, it also gives $JD^*C^*C\widetilde{\Omega}_0 \in \mathcal{A}_{\theta_0}$. Thus, one can apply the spectral deformation method to (3.38) to obtain

$$\begin{aligned}
\omega_0\left(\alpha_\lambda^t\,(X \otimes \mathbf{1}_\mathrm{R})\right) &= \left\langle \left[JD^*C^*C\widetilde{\Omega}_0\right]_{\bar\theta}, \left(\left|\left[\Omega_{\mathrm{SR},\beta,\lambda}\right]_\theta\right\rangle\left\langle\left[\Omega_{\mathrm{SR},\beta,\lambda}\right]_{\bar\theta}\right|\right)\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\left[\Omega_{\mathrm{SR},\beta,\lambda}\right]_\theta \right\rangle \\
&\quad + \sum_{j=1}^{d-1} \mathrm{e}^{it\lambda^2 a_{0,j}} \left\langle \left[JC^*C\widetilde{\Omega}_0\right]_{\bar\theta}, \Pi_{0,j}(\theta)\,(X \otimes \mathbf{1}_\mathrm{S} \otimes \mathbf{1}_\mathrm{R})\left[\Omega_{\mathrm{SR},\beta,\lambda}\right]_\theta \right\rangle
\end{aligned}$$

$$+\sum_{e\neq 0}\sum_{j=1}^{m_e} \mathrm{e}^{it(e+\lambda^2 a_{e,j})}\left\langle \left[JC^*C\widetilde{\Omega}_0\right]_{\bar\theta}, \Pi_{e,j}(\theta)\,(X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\left[\Omega_{\mathrm{SR},\beta,\lambda}\right]_{\theta}\right\rangle$$
$$+ R(X,t), \tag{3.39}$$

where $[\psi]_\theta = \mathrm{e}^{i\theta A}\psi$ and [recall (3.18)]

$$\Pi_{e,j}(\theta) = Q_{e,j} + O(\lambda) \tag{3.40}$$
$$a_{e,j} = \lambda_{e,j} + O(\lambda). \tag{3.41}$$

The remainder $R(X,t)$ in (3.39) satisfies

$$|R(X,t)| \leqslant \mathrm{const.}|\lambda|\big(\mathrm{e}^{-\theta_0 t} + \mathrm{e}^{-\lambda^2(1+O(\lambda))\gamma t}\big)\|X\| \leqslant \mathrm{const.}|\lambda|\mathrm{e}^{-\lambda^2(1+O(\lambda))\gamma t}\,\|X\|. \tag{3.42}$$

The contribution $\propto \mathrm{e}^{-\theta_0 t}$ is the usual contour integral term (c.f. [20–22]), the other term is due to the fact that in the summands decaying in time t, we can replace D^* by $\mathbf{1}$ plus a remainder of $O(\lambda)$ and we have $|\mathrm{e}^{it\lambda^2 a_{e,j}}| = \mathrm{e}^{-\lambda^2(1+O(\lambda))\gamma t}$. The first term on the right side of (3.39) equals

$$\begin{aligned}
&\left\langle JD^*C^*C\widetilde{\Omega}_0, \Omega_{\mathrm{SR},\beta,\lambda}\right\rangle\left\langle \Omega_{\mathrm{SR},\beta,\lambda}, (X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\,\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle\\
&\quad= \left\langle \Omega_{\mathrm{SR},\beta,\lambda}, (X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\,\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle\\
&\quad= \left\langle \widetilde{\Omega}_0, (X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\,\widetilde{\Omega}_0\right\rangle\\
&\quad= \left\langle JC^*C\widetilde{\Omega}_0, \big(|\widetilde{\Omega}_0\rangle\langle\widetilde{\Omega}_0|\big)\,(X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\,\widetilde{\Omega}_0\right\rangle.
\end{aligned} \tag{3.43}$$

In the first step, we have made use of

$$\langle JD^*C^*C\widetilde{\Omega}_0, \Omega_{\mathrm{SR},\beta,\lambda}\rangle = \langle JC^*C\widetilde{\Omega}_0, JD\Omega_{\mathrm{SR},\beta,\lambda}\rangle = \langle JC^*C\widetilde{\Omega}_0, \widetilde{\Omega}_0\rangle = \|C\widetilde{\Omega}_0\|^2 = 1$$

and in the last step, again, $\langle JC^*C\widetilde{\Omega}_0, \widetilde{\Omega}_0\rangle = 1$. The second equality in (3.43) follows from (3.8), (3.14) and (3.16).

Since all "directions" but the stationary one in (3.39) are decaying, i.e., $\mathrm{Im}\, a_{e,j} > 0$ for all e, j, we can replace in these terms in the exponents e and $a_{e,j}$ by $\widetilde{e}$ and $\widetilde{\lambda}_{\widetilde{e},j}$, $\Pi_{e,j}$ by $\widetilde{Q}_{\widetilde{e},j}$ and $\Omega_{\mathrm{SR},\beta,\lambda}$ by $\widetilde{\Omega}_0$ (see Proposition 3.2). This changes the remainder into a new one which, instead of (3.42), has the bound (2.23).[5] Making this replacement and using the spectral representation (3.20),

$$\mathrm{e}^{it(\widetilde{L}_{\mathrm{S}}+\lambda^2\widetilde{\Lambda})} = |\widetilde{\Omega}_0\rangle\langle\widetilde{\Omega}_0| + \sum_{j=1}^{d-1}\mathrm{e}^{it\lambda^2\widetilde{\lambda}_{0,j}}\,\widetilde{Q}_{0,j} + \sum_{\widetilde{e}\neq 0}\sum_{j=1}^{m_e}\mathrm{e}^{it(\widetilde{e}+\lambda^2\widetilde{\lambda}_{\widetilde{e},j})}\,\widetilde{Q}_{\widetilde{e},j},$$

we obtain

$$\omega_0\big(\alpha_\lambda^t(X\otimes \mathbf{1}_{\mathrm{R}})\big) = \left\langle JC^*C\widetilde{\Omega}_0, \mathrm{e}^{it(\widetilde{L}_{\mathrm{S}}+\lambda^2\widetilde{\Lambda})}(X\otimes \mathbf{1}_{\mathrm{S}}\otimes \mathbf{1}_{\mathrm{R}})\widetilde{\Omega}_0\right\rangle + R_{\lambda,t}(X), \tag{3.44}$$

---

5 Use the estimate $|\mathrm{e}^{-\lambda^2 t\mathrm{Im} a_{e,j}} - \mathrm{e}^{-\lambda^2 t\mathrm{Im}\widetilde{\lambda}_{e,j}}| = \mathrm{e}^{-\lambda^2 t\mathrm{Im} a_{e,j}}|1 - \mathrm{e}^{\lambda^2 t\mathrm{Im}(a_{e,j}-\widetilde{\lambda}_{\widetilde{e},j})}| \leqslant \mathrm{const.}|\lambda|^3 t\mathrm{e}^{-\lambda^2(1+O(\lambda))\gamma t}$.

where $R_{\lambda,t}(X)$ satisfies (2.23). According to definition (2.24) of τ_λ^t, the main term on the right side of (3.44) is

$$\langle JC^*C\widetilde{\Omega}_0, (\tau_\lambda^t(X)\otimes \mathbf{1}_S \otimes \mathbf{1}_R)\widetilde{\Omega}_0\rangle = \omega_0(\tau_\lambda^t(X)).$$

This shows the representation (2.22).

3.4 Proof of complete positivity of τ_λ^t

We first show complete positivity of the weak coupling dynamics σ_λ^t, (2.17). Then, we modify that argument just slightly to show complete positivity of τ_λ^t.

3.4.1 Complete positivity of the weak coupling dynamics σ_λ^t

Using (2.21) and a density argument, one sees that for any system–reservoir state ω,

$$\lim_{\lambda\to 0} \omega\big(\alpha_\lambda^{t/\lambda^2}\circ\alpha_0^{-t/\lambda^2}(X\otimes \mathbf{1}_R)\big) = \omega\big(\bar\sigma^t(X)\otimes \mathbf{1}_R\big), \tag{3.45}$$

where $\bar\sigma^t(X)$ is defined by $\big(\bar\sigma^t(X)\otimes \mathbf{1}_S\big)\Omega_{S,\beta} = e^{it\Lambda}\big(X\otimes \mathbf{1}_S\big)\Omega_{S,\beta}$ and satisfies [see (2.17)] $\sigma_\lambda^t = \bar\sigma^{\,\lambda^2 t}\circ\alpha_S^t = \alpha_S^t\circ\bar\sigma^{\,\lambda^2 t}$. Since α_S^t is completely positive, complete positivity of σ_λ^t follows from that of $\bar\sigma^t$. Let $\omega_{R,\beta}$ be the reservoir equilibrium state and let P_R be the partial trace over the reservoir, relative to $\omega_{R,\beta}$, defined by (linear extension of) $P_R(X\otimes B)P_R = X\,\omega_{R,\beta}(B)$. Taking $\omega=\omega_S\otimes\omega_{R,\beta}$ in (3.45), where ω_S is any system state, gives

$$\lim_{\lambda\to 0}\omega_S\big(P_R\alpha_\lambda^{t/\lambda^2}\circ\alpha_0^{-t/\lambda^2}(X\otimes\mathbf{1}_R)P_R\big) = \omega_S(\bar\sigma^t(X)).$$

As the system is finite-dimensional, this is equivalent to

$$\lim_{\lambda\to 0} P_R\alpha_\lambda^{t/\lambda^2}\circ\alpha_0^{-t/\lambda^2}(X\otimes\mathbf{1}_R)P_R = \bar\sigma^t(X).$$

The left side is the limit of a family of completely positive maps. Hence, $\bar\sigma^t$ is completely positive as well.

3.4.2 Complete positivity of τ_λ^t

We denote by $\gamma_{\lambda,\mu}^t(\cdot) = e^{it\widetilde{L}_\mu}\cdot e^{-it\widetilde{L}_\mu}$ the dynamics of $\mathfrak{M}$ generated by the Liouville operator $\widetilde{L}_\mu$ defined in (3.22). The level shift operator of $\widetilde{L}_\mu$ is $\lambda^2\mu^2\widetilde{\Lambda}$ [see also (3.19)]. Repeating the argument of the weak coupling limit, we have [c.f. (3.45)]

$$\lim_{\mu\to 0}\omega\big(\gamma_{\lambda,\mu}^{t/\mu^2}\circ\widetilde{\gamma}_{\lambda,0}^{-t/\mu^2}(X\otimes\mathbf{1}_R)\big) = \omega\big(\bar\tau_\lambda^t(X)\otimes\mathbf{1}_R\big), \tag{3.46}$$

where $\bar{\tau}_\lambda^t$ is defined by $(\bar{\tau}_\lambda^t(X)\otimes\mathbf{1}_\mathrm{S})\widetilde{\Omega}_{\mathrm{S},\beta,\lambda} = \mathrm{e}^{it\lambda^2\widetilde{\Lambda}}(X\otimes\mathbf{1}_\mathrm{S})\widetilde{\Omega}_{\mathrm{S},\beta,\lambda}$. Thus, by the same argument as in Sect. 3.4.1, $\bar{\tau}_\lambda^t$ is completely positive, and hence so is $\tau_\lambda^t = \bar{\tau}_\lambda^t \circ \widetilde{\alpha}_{\mathrm{S},\lambda}$, where $\widetilde{\alpha}_{\mathrm{S},\lambda}(\cdot) = \mathrm{e}^{it\widetilde{H}_\mathrm{S}} \cdot \mathrm{e}^{-it\widetilde{H}_\mathrm{S}}$.

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References

1. Alicki, R., Lendi, K.: Quantum dynamical semigroups and applications, Lecture notes on physics, vol. 717. Springer Verlag, New York (2007)
2. Araki, H., Woods, E.J.: Representation of the canonical commutation relations describing a nonrelativistic infinite free bose gas. J. Math. Phys. **4**, 637–662 (1963)
3. Benatti, F., Floreanini, R.: Open quantum dynamics: complete positivity and entanglement. Int. J. Mod. Phys. B **19**, 3063 (2005)
4. Bach, V., Fröhlich, J., Sigal, I.M.: Return to equilibrium. J. Math. Phys. **41**(6), 3985–4060 (2000)
5. Breuer, H.-P., Petruccione, F.: The theory of open quantum systems. Oxford University Press, Oxford (2006)
6. Bratteli, O., Robinson, D.W.: Operator algebras and quantum statistical mechanics, vol. 1 and 2. Springer Verlag, New York (1979)
7. Davies, E.B.: Markovian master equations. Commun. Math. Phys. **39**, 91–110 (1974)
8. Davies, E.B.: Markovian master equations, II. Math. Annalen **219**, 147–158 (1976)
9. Derezinski, J., Jaksic, V., Pillet, C.-A.: Perturbation theory of W^*-dynamics, Liouvilleans and KMS-states. Rev. Math. Phys. **15**(5), 447–489 (2003)
10. Dümke, R., Spohn, H.: The proper form of the generator in the weak coupling limit. Z. Phys. B **34**, 419–422 (1979)
11. Fröhlich, J., Merkli, M.: Another return of "return to equilibrium". Commun. Math. Phys. **251**(2), 235–262 (2004)
12. Gardiner, C.W., Zoller, P.: Quantum noise. Springer series in synergetics, 3rd edn. Springer, Berlin (2004)
13. Jaksic, V., Pillet, C.-A.: From resonances to master equations. Ann. Inst. H. Poincaré Phys. Théor. **67**(4), 425–445 (1997)
14. Jaksic, V., Pillet, C.-A.: On a model for quantum friction. II. Fermi's golden rule and dynamics at positive temperature. Commun. Math. Phys. **176**(3), 619–644 (1996)
15. Könenberg, M., Merkli, M.: On the irreversible dynamics emerging from quantum resonances. J. Math. Phys. **57**, 033302 (2016)
16. Merkli, M.: Entanglement evolution via quantum resonances. J. Math. Phys. **52**(9), 092201 (2011)
17. Merkli, M., Berman, G.P., Sayre, R.: Electron transfer reactions: generalized Spin–Boson approach. J. Math. Chem. **51**(3), 890–913 (2013)
18. Merkli, M., Berman, G.P., Song, H.: Multiscale dynamics of open three-level quantum systems with two quasi-degenerate levels. J. Phys. A Math. Theor. **48**, 275304 (2015)
19. Merkli, M., Berman, G.P., Sayre, R.T., Gnanakaran, S., Könenberg, M., Nesterov, A.I., Song, H.: Dynamics of a chlorophyll dimer in collective and local thermal environments. J. Math. Chem. **54**(4), 866–917 (2016)
20. Merkli, M., Sigal, I.M., Berman, G.P.: Resonance theory of decoherence and thermalization. Ann. Phys. **323**, 373–412 (2008)
21. Merkli, M., Sigal, I.M., Berman, G.P.: Decoherence and thermalization. Phys. Rev. Lett. **98**(13), 130401–130405 (2007)
22. Merkli, M., Sigal, I.M., Berman, G.P.: Dynamics of collective decoherence and thermalization. Ann. Phys. **323**(12), 3091–3112 (2008)
23. Mukamel, S.: Principles of nonlinear spectroscopy. Oxford series in optical and imaging sciences. Oxford University Press, Oxford (1995)