## Quantum markovian master equations: Resonance theory overcomes the weak coupling regime

Marco Merkli \*
Department of Mathematics and Statistics
Memorial University of Newfoundland
St. John's, Canada A1C 5S7

August 7, 2019

#### Abstract

Quantum systems coupled to environments exhibit intricate dynamics. The master equation gives a Markov approximation of the dynamics, allowing for analytic and numerical treatments. It is ubiquitous in theoretical and applied quantum sciences. The accuracy of the master equation approximation was so far proven in the regime where time must not exceed an upper bound depending on the systemenvironment interaction strength (weak coupling regime). Here, we show that the Markov approximation is valid for fixed coupling strength and for all times. We also construct a new approximate markovian dynamics – a completely positive, trace preserving semigroup – which is asymptotically in time exact, to all orders in the coupling.

## 1 Explanation of the main results

We consider open quantum system Hamiltonians

$$H = H_{\rm S} + H_{\rm R} + \lambda G \otimes \varphi(g) \tag{1.1}$$

where  $H_{\rm S}$  is an  $N \times N$  hermitian matrix with eigenvalues  $E_i$  and eigenvectors  $\phi_i$ ,

$$H_{\rm S} = \sum_{j=1}^{N} E_j |\phi_j\rangle\langle\phi_j| \tag{1.2}$$

<sup>\*</sup>merkli@mun.ca, https://www.math.mun.ca/~merkli/

and  $H_{\rm R}$  is the reservoir Hamiltonian

$$H_{\rm R} = \sum_{k} \omega_k a_k^* a_k, \tag{1.3}$$

describing modes of a collection of harmonic oscillators, labelled by k. Their frequencies are  $\omega_k > 0$  (we 'set  $\hbar = 1$ ') and the creation and annihilation operators  $a_k^*$ ,  $a_k$ , satisfy the canonical commutation relations  $[a_k, a_\ell^*] = \delta_{k,\ell}$  (Kronecker symbol). The interaction term contains a coupling constant  $\lambda \in \mathbb{R}$ , an interaction operator G (hermitian  $N \times N$  matrix), and it is linear in the field operator

$$\varphi(g) = \frac{1}{\sqrt{2}} \sum_{k} g_k a_k^* + \text{h.c.}, \qquad (1.4)$$

where h.c. denotes the hermitian conjugate. The collection of the numbers  $g_k \in \mathbb{C}$  constitutes the 'form factor' g. The size of  $g_k$  determines how strongly the mode k is coupled to the system.

To describe irreversible effects it is necessary to pass to a limit where the oscillator frequencies  $\omega_k$  take on *continuous* values (and hence so must k). In principle, the parameter k belongs to an arbitrary 'continuous set'. For instance, having in mind a reservoir modeling a (scalar) quantized field in physical space  $\mathbb{R}^3$  (infinite volume limit), the oscillatory frequencies are indexed by  $k \in \mathbb{R}^3$ , and  $\omega_k$ ,  $g_k$ ,  $a_k^*$  and  $a_k$  become functions  $\omega(k)$ , g(k),  $a^*(k)$ , a(k) with  $[a(k), a^*(\ell)] = \delta(k - \ell)$  (Dirac function). In the continuous mode limit, the reservoir Hamiltonian (1.3) and field operator (1.4) are

$$H_{R} = \int_{\mathbb{R}^{3}} \omega(k) a^{*}(k) a(k) d^{3}k,$$

$$\varphi(g) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}^{3}} \left( g(k) a^{*}(k) + \text{h.c.} \right) d^{3}k.$$
(1.5)

The Hilbert space on which the operators (1.5) act is the Bosonic Fock space over the single particle wave function space  $L^2(\mathbb{R}^3, d^3k)$  (momentum representation),

$$\mathcal{F} = \mathbb{C} \oplus_{n \ge 1} S_{+}L^{2}(\mathbb{R}^{3}, d^{3}k)^{\otimes n}, \tag{1.6}$$

where  $S_{+}$  is the symmetrization operator (Bosons).

It is customary in the physics literature to carry out calculations for discrete modes ((1.3), (1.4)) and take the continuous limit in quantities of interest 'at the end'. However, it might be advantageous to start off directly with the continuous model, because then one can attack the dynamical problem by spectral analysis of the Hamiltonian, using that continuous spectrum is associated with scattering effects and irreversibility. This is the approach we take here. A (minor) trade off is that in the continuous mode models, defining the equilibrium state is slightly more complicated: while the operator  $e^{-\beta H_R}$  has a finite trace for (1.3) this is not the case when  $H_R$  has continuous spectrum, (1.5). The notion of

reservoir equilibrium density matrix  $\rho_{R,\beta} \propto e^{-\beta H_R}$  has therefore to be replaced by that of a state (normalized linear functional)  $\omega_{R,\beta}$  on reservoir observables. The latter is obtained by taking the thermodynamic limit of the discrete mode model and is determined entirely by its two point function  $(k, l \in \mathbb{R}^3)$ 

$$\omega_{R,\beta}(a^*(k)a(l)) = \frac{\delta(k-l)}{e^{\beta\omega(k)} - 1}.$$
(1.7)

Averages of general reservoir observables are found using Wick's theorem ('quasi free', or 'Gaussian' state). We explain this in Section 2. The analysis presented here can be carried out for more general states, where the right side of (1.7) is replaced by  $\mu(k)\delta(k-l)$  for general functions  $\mu(k) > 0$ , see e.g. Section 4.3 of [21]. Having in mind spectral methods, as mentioned above, it will be useful to take a purification of reservoir state, i.e., to describe  $\omega_{R,\beta}$  by a vector state in a (new) Hilbert space.

In this paper, it is understood that the continuous mode limit is performed and all statements are given for continuous models. In other words, we consider Hamiltonians (1.1) with  $H_{\rm R}$  and  $\varphi(g)$  given in (1.5). Our method works for initial system-reservoir states belonging to the 'folium' of the equilibrium state, namely, for which the reservoir is spatially asymptotically close to equilibrium at temperature  $T=1/\beta>0$ . Within this folium, the initial system-reservoir states are allowed to be entangled. We explain this point below in Section 2, and (2.40) is our fundamental result for the dynamics, equally valid for entangled and product initial states. The dynamics for non-factorized initial states in the weak coupling regime was analyzed in [31, 34] (see also the references therein) and we will address the detailed analysis of our results on the dynamics of entangled states elsewhere.

The main goal of Sections 1.1-1.3 is to make a link with the 'usual' setup and results, where the system dynamics is given by a 'propagator'  $V_t$ . The latter is well defined for disentangled initial states of the form  $\rho_S \otimes \rho_{R,\beta}$ , where  $\rho_{R,\beta}$  is the equilibrium state (in the thermodynamic limit) and  $\rho_S$  is an arbitrary system state. (Strictly speaking,  $\rho_{R,\beta}$  here is the density matrix representing  $\omega_{R,\beta}$  in the purification Hilbert space – this point is explained in detail in Section 2.) The system dynamics is described by the reduced system density matrix

$$\rho_{S}(t) = \operatorname{tr}_{R} e^{-itH} (\rho_{S} \otimes \rho_{R,\beta}) e^{itH}, \qquad (1.8)$$

where  $tr_R$  is the partial trace over the reservoir degrees of freedom. The relation (1.8) defines a linear map on system density matrices, called the *dynamical map*  $V_t$ , by

$$\rho_{\rm S} \mapsto V_t \rho_{\rm S} \equiv \rho_{\rm S}(t).$$
(1.9)

Equivalently, one can introduce the Heisenberg dynamics  $t \mapsto \alpha_t A$  of system observables A (hermitian matrices acting on the system), by setting

$$\operatorname{tr}_{S}(V_{t}\rho_{S})A = \operatorname{tr}_{S}\rho_{S}(\alpha_{t}A). \tag{1.10}$$

It is well known (and a source of great difficulty in theory and applications) that the map  $t \mapsto V_t$  is not a group in t, namely  $V_{t+s} \neq V_t \circ V_s$ . Of course, for  $\lambda = 0$ ,  $V_t \rho_S = e^{-itH_S} \rho_S e^{itH_S}$ 

does have the group property, but when the system interacts with the reservoir ( $\lambda \neq 0$ ), correlations between the two are built up and the group property is destroyed. Still, being the reduction of a unitary dynamics of a bigger physical system (namely, the system plus the reservoir), the reduced dynamics  $V_t$  has a special structure. Indeed, for each t fixed,  $V_t$  is a completely positive, trace preserving map, for short,  $V_t$  is CPT <sup>1</sup>. Using (1.10) it is not difficult to understand that, for any t fixed,  $V_t$  is CPT if and only if  $\alpha_t$  is completely positive and identity preserving ( $\alpha_t \mathbf{1} = \mathbf{1}$ ).

Importance of the group property. If the group property  $V_{t+s} = V_t \circ V_s$  is satisfied, then there is a generator  $\mathcal{L}$ , a linear operator acting on density matrices, such that  $V_t = e^{t\mathcal{L}}$ . The open system dynamics is entirely determined by the spectral data (eigenvalues and eigenvectors) of  $\mathcal{L}$ . Assume for the moment that one can show a spectral representation

$$e^{t\mathcal{L}} = \sum_{j} e^{t\epsilon_j} P_j, \tag{1.11}$$

where  $\epsilon_j$  are the eigenvalues of  $\mathcal{L}$  and  $P_j$  the corresponding eigenprojections. All dynamical information is then contained in the  $\epsilon_j$  and  $P_j$ . Namely, the  $\epsilon_j$  with  $\operatorname{Re} \epsilon_j < 0$  drive irreversible decay (t > 0), with decay rates  $|\operatorname{Re} \epsilon_j|$  and the associated  $P_j$  determine the decay directions in state space. Stationary states are in the range of the projections  $P_j$  with j such that  $\epsilon_j = 0$ .

Importance of complete positivity. Suppose you have a bipartite system AB in an entangled initial state  $\rho_{AB}$ . Suppose that the subsystem B evolves independently, according to its own unitary dynamics  $U_t$  (generated by a Hamiltonian  $H_B$ ) and that the dynamics of subsystem A is given by  $V_t$  (emerging for instance by interaction with a reservoir). The state of AB at time t is then  $\rho_{AB}(t) = (V_t \otimes U_t)\rho_{AB}(0)$ . This state is guaranteed to be a density matrix only because  $V_t$  is completely positive. (If  $V_t$  was not completely positive, then one could find an initial density matrix  $\rho_{AB}(0)$  for which  $\rho_{AB}(t)$  would have some negative eigenvalues!) On the mathematical side, complete positivity of a map V is equivalent with V having a Kraus representation, which is again equivalent with V being the reduction of a unitary map acting on a bigger system (adding an 'ancilla' reservoir system). We refer to [5, 1, 7, 8] for more detail about this.

Markovian approximation in the van Hove weak coupling regime. Intuitively, if the reservoir dynamics is very fast, maybe if local disturbances of the reservoir state are quickly propagated far away (short lived reservoir memory), and if the system-reservoir

<sup>&</sup>lt;sup>1</sup>A map V acting on  $\mathcal{B}(\mathcal{H})$ , the bounded operators on a Hilbert space  $\mathcal{H}$ , is called CPT if (i) for all  $\rho \in \mathcal{B}(\mathcal{H})$  having finite trace,  $\operatorname{tr}V\rho = \operatorname{tr}\rho$  (trace preserving) and (ii)  $V \otimes \mathbf{1}$  is positivity preserving on the space of operators  $\mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^K)$ , for all  $K \geq 1$  (complete positivity). Positivity preserving in turn means that if X is a bounded non-negative operator acting on  $\mathcal{H} \otimes \mathbb{C}^K$  (having non-negative spectrum only), then  $(V \otimes \mathbf{1})X$  is a bounded non-negative operator acting on  $\mathcal{H} \otimes \mathbb{C}^K$ . If V is completely positive then it is positivity preserving, but the converse is not true. For instance, consider two qubits and take V to the partial transpose operator. This is a positivity preserving map but it is not CP. Indeed the positive partial transpose (PPT) criterion to check for entanglement in quantum information theory is based on the fact that the partial transpose is not CP.

interaction is not too large, then the back reaction from the reservoir onto the system might be minor. In this situation, one expects the group property to hold for  $t \mapsto V_t$ . Quantifying this idea is an important problem, leading to the *Markovian approximation*. The challenge is to show the validity of a Markovian approximation

$$V_t = e^{t\mathcal{L}} + R(t, \lambda) \tag{1.12}$$

and to find a parameter regime in which the remainder term  $R(t,\lambda)$  is small. When the remainder is squarely neglected,  $V_t = e^{t\mathcal{L}}$  is the integrated version of the differential equation  $\frac{d}{dt}V_t = \mathcal{L}V_t$ , or as per (1.9),  $\frac{d}{dt}\rho_{\rm S}(t) = \mathcal{L}\rho_{\rm S}(t)$ , which is called the *Markovian master equation* for the system density matrix  $\rho_{\rm S}(t)$ . It is a difficult problem to find quantitative and controlled (not heuristic) bounds on the remainder  $R(t,\lambda)$  in (1.12). There is one rigorous approach, called the *van Hove*-, or *weak coupling limit*. It states that for all a > 0,

$$\lim_{\lambda \to 0} \sup_{0 \le \lambda^2 t \le a} \left\| V_t - e^{t(\mathcal{L}_S + \lambda^2 K)} \right\| = 0. \tag{1.13}$$

Here,  $\mathcal{L}_{\mathrm{S}}$  and K are commuting operators acting on system density matrices and for each t fixed,  $e^{t(\mathcal{L}_{\mathrm{S}}+\lambda^2K)}$  is CPT  $^2$ . The operator  $\mathcal{L}_{\mathrm{S}}=-\mathrm{i}[H_{\mathrm{S}},\cdot]$  generates the free system dynamics (no interaction) and K is a (lowest order) correction term, encoding coupling effects. The  $\lambda^2 t$  scaling was used in [32] and later analyzed with mathematical rigour in [9, 10]. The literature on the weak coupling regime and markovian master equations is huge and growing. It has important applications not only to physics and mathematics, but also to chemistry, biology and the quantum information sciences [28, 15, 23, 6]. It is worthwhile to note that many different (heuristic) approximations and candidates for generators have been proposed over time, often violating the CPT requirement, with the 'Davies generator'  $\mathcal{L}_{\mathrm{S}} + \lambda^2 K$  above emerging as the 'correct' one [11, 30].

The relation (1.13) is the same as (1.12) with  $\mathcal{L} = \mathcal{L}_S + \lambda^2 K$  and (1.13) says

$$\lim_{\lambda \to 0} \sup_{0 \le \lambda^2 t < a} ||R(t, \lambda)|| = 0. \tag{1.14}$$

The shortcoming of (1.13), (1.14) is that only times up to  $t \approx a/\lambda^2$  are resolved by the Markovian approximation. Beyond that time scale,  $e^{t(\mathcal{L}_S + \lambda^2 K)}$  is not guaranteed to be accurate (the remainder may not be small). Of course, a is arbitrary, so in principle one can consider large times – but the bigger one takes a, the smaller  $\lambda$  has to be in order to make the remainder smaller than a given accuracy. (In other words, the speed of convergence in (1.14) depends on a). Another way of saying this is that, when considering  $t \to \infty$  one has to take at the same time  $\lambda \to 0$  in such a way that  $\lambda^2 t$  stays bounded (< a), in order to be sure that the Markovian approximation is valid. This is called the weak coupling regime.

One of our main results is to remove the condition that  $\lambda^2 t$  needs to be bounded. We show the accuracy of the Markovian approximation for all times  $t \geq 0$ .

<sup>&</sup>lt;sup>2</sup>Which norm  $\|\cdot\|$  we take in (1.13) is not too important here, as we assume that the system Hilbert space has finite dimension and so all norms are equivalent.

Decay of reservoir correlations. The symmetrized correlation function is defined as  $C_{\beta}(t) = \text{Re }\omega_{R,\beta}\left(\varphi(g)\varphi\left(e^{i\omega t}g\right)\right)$ , where g is the form factor in the interaction (1.1) and  $\omega_{R,\beta}$  is the reservoir thermal equilibrium state at temperature  $T=1/\beta$ . The resonance theory we develop requires some regularity of the function g, which translates into time decay of the correlation function  $C_{\beta}(t)$ . Instead of stating the precise regularity assumption on g, let us give the following admissible family (polar coordinates):  $g(k) = g(|k|, \Sigma) = |k|^p e^{-r^m} g_1(\Sigma)$ , with p = -1/2 + n,  $n = 0, 1, 2, \ldots$  and m = 1, 2 and  $g_1(\Sigma) = e^{i\alpha} \bar{g}_1(\Sigma)$  for an arbitrary phase  $\alpha$  and angular function  $g_1$ . The precise regularity condition involves analyticity of g and is given in (2.22) below (see also [18]). It is readily seen that analyticity of the form factor (in the sense of (2.22)) leads to exponential time decay of the correlation function  $C_{\beta}(t)$ . One can significantly weaken the regularity requirements on g (replacing analyticity by just real differentiability), which implies that  $C_{\beta}(t)$  will decay polynomially in time only. This demands a technically more involved technique developed in [19] (Mourre theory).

#### 1.1 Result 1: Resonance expansion of the dynamics.

The resonance theory is a mathematically rigorous approach for the analysis of the evolution of the system-reservoir complex. It does not only describe the dynamics of the system state or observables, but also that of the reservoir. Here we explain the results on the system Schrödinger dynamics. To state our results in terms of the dynamical map  $V_t$ , we assume that the initial system-reservoir state is disentangled, of the form (1.8) for t = 0. (The result for general initial states is given in (2.40).)

We show that if  $|\lambda| \leq \lambda_0$  (for some  $\lambda_0 > 0$ ), then for all times  $t \geq 0$ ,

$$\|V_t - W_t - \rho_{S,\beta,\lambda} \langle tr| \| \le C\lambda^2 e^{-\gamma(\lambda)t}.$$
 (1.15)

The constant  $C < \infty$  is independent of  $\lambda$ , t and  $\gamma(\lambda) \geq 0$  does not depend on t. In (1.15),  $\langle \text{tr} | \text{ is the linear functional } \rho \mapsto \text{tr}(\rho) = 1$ . Moreover,  $\rho_{S,\beta,\lambda}$  is the effective system equilibrium state, obtained by taking the full, coupled system-reservoir equilibrium state (relative to H, (1.1)) and tracing out the reservoir degrees of freedom.  $W_t$  is a linear map on system states (density matrices), describing how, and if, the system approaches the equilibrium  $\rho_{S,\beta,\lambda}$ . It has an expansion of the type (1.11),

$$W_t = \sum_j e^{it\epsilon_j(\lambda)} \mathcal{P}_j, \tag{1.16}$$

where the  $\mathcal{P}_j$  are  $\lambda$ -independent projection operators (acting on system density matrices). They satisfy

$$\mathcal{P}_{j}\mathcal{P}_{k} = \delta_{j,k}\mathcal{P}_{j} \quad \text{and} \quad \sum_{j} \mathcal{P}_{j} = W_{0} = \mathbb{1} - \rho_{S,\beta,0} \langle \text{tr} |,$$
 (1.17)

where  $\rho_{S,\beta,0} = e^{-\beta H_S}/\text{tr}(e^{-\beta H_S})$  is the (uncoupled) system equilibrium state. The  $\epsilon_j(\lambda) \in \mathbb{C}$  are analytic in  $\lambda$  at the origin,

$$\epsilon_j(\lambda) = \epsilon_j^{(0)} + \lambda^2 \epsilon_j^{(2)} + O(\lambda^4)$$
(1.18)

and  $\epsilon_j^{(0)}$  are differences of eigenvalues of  $H_S$  (Bohr energies). It is clear from (1.16) and the properties of the  $\mathcal{P}_j$  that

$$W_{t+s} = W_t \circ W_s. \tag{1.19}$$

Symmetries or degeneracies in the spectrum of  $H_{\rm S}$  can cause some of the  $\epsilon_j(\lambda)$  to vanish (or to be real). In this case, the associated  $\mathcal{P}_j$  project onto additional stationary states, other than  $\rho_{{\rm S},\beta,\lambda}$ . However, generically, in the absence of symmetries and degeneracies, one has  ${\rm Im}\epsilon_j(\lambda)>0$  for all j (for small, nonzero  $\lambda$ ). Then all terms in (1.16) decay in time, the jth one at the rate  ${\rm Im}\epsilon_j(\lambda)$ . Denoting by  $2\ell_j$  the order of the zero of  ${\rm Im}\epsilon_j(\lambda)$  at the origin, i.e.,  ${\rm Im}\epsilon_j\propto\lambda^{2\ell_j}$  to leading order in  $\lambda$ , we see that  $W_t$  is a sum of terms decaying at (possibly different) rates  $\lambda^{2\ell_j}$ . The slowest decay rate is

$$\gamma(\lambda) = \min_{j} \operatorname{Im} \epsilon_{j}(\lambda) \ge 0 \tag{1.20}$$

and coincides with that of the remainder in (1.15). Note, however, the additional factor  $\lambda^2$  on the right side of (1.15). The result (1.15) can be expressed as

$$V_t \rho = \rho_{S,\beta,\lambda} + W_t \rho + O\left(\lambda^2 e^{-\gamma(\lambda)t}\right)$$
(1.21)

for any density matrix  $\rho$ , with an error term which is (quadratically) small in  $\lambda$  for all times, and which also decays to zero exponentially quickly in time.

## 1.2 Result 2: Approximation of the dynamics by a CPT semigroup for all times.

In applications it is often observed that the imaginary parts of all the  $\epsilon_j(\lambda)$  are strictly positive already to second order in  $\lambda$  (see (1.18)), *i.e.*, that

$$\gamma_{\text{FGR}} \equiv \min_{j} \operatorname{Im} \epsilon_{j}^{(2)} > 0. \tag{1.22}$$

If (1.22) is satisfied we say that the Fermi Golden Rule Condition holds [2, 4, 16, 25, 26]. In this situation,  $W_t$  contains the single characteristic time scale  $\lambda^{-2}$ . We assume (1.22) now. Retaining only the leading terms of  $W_t$  and  $\rho_{S,\beta,\lambda}$  on the left side of (1.15), namely

$$\epsilon_j(\lambda) \approx \epsilon_j^{(0)} + \lambda^2 \epsilon_j^{(2)}, \quad \rho_{S,\beta,\lambda} \approx \rho_{S,\beta,0} = \frac{e^{-\beta H_S}}{\text{tr } e^{-\beta H_S}},$$
(1.23)

we can show the following result. There is a  $\lambda_0 > 0$  such that if  $|\lambda| \leq \lambda_0$ , then for all  $t \geq 0$ ,

$$||V_t - e^{t(\mathcal{L}_S + \lambda^2 K)}|| \le C\lambda^2. \tag{1.24}$$

Here,  $\mathcal{L}_{S} = -i[H_{S}, \cdot]$  (commutator) and K are commuting operators acting on system density matrices, and K is constructed entirely in terms of  $\epsilon_{j}^{(2)}$  and  $\mathcal{P}_{j}$ . Moreover,  $e^{t(\mathcal{L}_{S}+\lambda^{2}K)}$  is a CPT semigroup satisfying

$$e^{t(\mathcal{L}_S + \lambda^2 K)} \rho_{S,\beta,0} = \rho_{S,\beta,0}. \tag{1.25}$$

It is the same semigroup as the one in the weak coupling result (1.13). In passing from (1.16) to (1.24) we have gained the CPT and semigroup properties of the approximation, but we have traded it for a worse error estimate. Namely, the approximation (1.24) is still  $O(\lambda^2)$  for all  $t \geq 0$ , but it does not decay to zero for large times, as it did in (1.15). The inequality (1.24) proves that the Markovian approximation, implemented by a CPT semigroup, is valid for all times  $t \geq 0$ . It can be phrased as

$$\sup_{t>0} \|V_t - e^{t(\mathcal{L}_S + \lambda^2 K)}\| \le C\lambda^2. \tag{1.26}$$

This is a significant improvement of the weak coupling result (1.13).

The generator K can be obtained by perturbation theory or by the relation

$$\lim_{\lambda \to 0} V_{\frac{\tau}{\lambda^2}} \circ e^{-\frac{\tau}{\lambda^2} \mathcal{L}_S} = e^{\tau K}, \qquad \tau \ge 0, \tag{1.27}$$

which identifies it as the 'Davies generator' (the same K as in (1.13)), [9, 10, 1, 7, 8, 12]. It can be calculated explicitly, see the Appendix A.

# 1.3 Result 3: Approximation of the dynamics by an asymptotically exact CPT semigroup.

The origin of the loss of time decay in the remainder, when passing from (1.15) to (1.24) as described in the previous section, comes from replacing  $\rho_{S,\beta,\lambda}$  by  $\rho_{S,\beta,0}$  (see (1.23)). We recall that  $\rho_{S,\beta,\lambda}$  is the restriction to the system of the full, coupled system-reservoir equilibrium state. This replacement unavoidably introduces an error of  $O(\lambda^2)$  for large times, as the true final  $(t \to \infty)$  system state is  $\rho_{S,\beta,\lambda}$ , while the one predicted by the approximation is  $\rho_{S,\beta,0}$ , differing from the true one by  $O(\lambda^2)$ . Above, this replacement was necessary in order to incorporate the 'final state' into the approximate dynamical group, as an element in the kernel of the generator  $\mathcal{L}_S + \lambda^2 K$ , see (1.25). To avoid the approximation of  $\rho_{S,\beta,\lambda}$ , we might try to modify the generator into a new one,  $M(\lambda)$ , by adding supplementary terms of all orders in  $\lambda$ , as to make the full  $\rho_{S,\beta,\lambda}$  an invariant state. This is the result we explain now, and in this result we restore the time decay of the remainder (obtaining thus an asymptotically exact approximation).

We introduce a 'renormalization',  $\widetilde{H}_{S}(\lambda)$ , of the system Hamiltonian, satisfying

$$\frac{e^{-\beta \widetilde{H}_{S}(\lambda)}}{\operatorname{tr} e^{-\beta \widetilde{H}_{S}(\lambda)}} = \rho_{S,\beta,\lambda}.$$
(1.28)

By carrying out the resonance theory leading to the results of Subsection 1.1, but now with this renormalized 'reference state' (1.28), the CPT semigroup approximating the true dynamics  $V_t$  turns out to be  $e^{t(\tilde{\mathcal{L}}_S + \lambda^2 \tilde{K})}$ , with  $\lambda$  dependent operators  $\tilde{\mathcal{L}}_S$  and  $\tilde{K}$ . The crucial point is that  $e^{t(\tilde{\mathcal{L}}_S + \lambda^2 \tilde{K})} \rho_{S,\beta,\lambda} = \rho_{S,\beta,\lambda}$ , which replaces the property (1.25) in the previous argument and allows us to obtain a remainder which decays to zero for large times. We show the following.

Suppose that the Fermi Golden Rule Condition  $\gamma_{\text{FGR}} > 0$  is satisfied (c.f. (1.22)). Then there is a  $\lambda_0 > 0$  such that for  $|\lambda| < \lambda_0$ , and all times  $t \ge 0$ ,

$$||V_t - e^{tM(\lambda)}|| \le C(|\lambda| + \lambda^2 t) e^{-\lambda^2 \gamma_{FGR} t (1 + O(\lambda^2))}.$$

$$(1.29)$$

Here,  $e^{tM(\lambda)}$  is a CPT semigroup with a generator  $M(\lambda)$  analytic in  $\lambda$ , containing all orders of  $\lambda$ . Its Taylor series can be calculated by perturbation theory. The result (1.29) shows that we can construct a CPT semigroup which approximates the true dynamics and which is asymptotically exact, meaning that  $\lim_{t\to\infty}(V_t-e^{tM(\lambda)})=0$ . Note, however, that for  $t\sim 1/\lambda^2$ , the right hand side of (1.29) is not small. Still, for times  $t>1/(\lambda^2\gamma_{\rm FGR})$  the remainder becomes negligible.

We get a better result for the evolution of the populations ("Pauli equations", see also [2]) of the state  $V_t \rho$ , *i.e.*, the diagonal of the density matrix  $V_t \rho$  in the energy basis of  $H_S$ . For an operator A, set

$$[A]_{k,\ell} = \langle \phi_k, A\phi_\ell \rangle, \tag{1.30}$$

where  $\phi_k$  is the eigenvector of  $H_S$  associated to the eigenvalue  $E_k$ , see (1.2). The population of the energy  $E_k$  at time t is then

$$[V_t \rho]_{k,k} = \langle \phi_k, (V_t \rho) \phi_k \rangle. \tag{1.31}$$

We show that there is a  $\lambda_0 > 0$  such that for  $|\lambda| < \lambda_0$  and all k, and for all  $t \ge 0$ ,

$$[V_t \rho]_{k,k} = \left[ e^{t\lambda^2 M_d(\lambda)} \rho \right]_{k,k} + O\left( \left( |\lambda| + \lambda^4 t \right) e^{-\lambda^2 t (\gamma_{\text{FGR}} + O(\lambda^2))} \right), \tag{1.32}$$

where  $e^{t\lambda^2 M_d(\lambda)}$  is a CPT semigroup with a generator  $M_d(\lambda)$  ("d" for diagonal) analytic in  $\lambda$ , which is explicitly constructable by perturbation theory and satisfies  $M_d(0) = K$ , the Davies generator (see (1.27)). The relation (1.32) shows that there is a CPT semigroup which approximates the populations to accuracy  $O(\lambda)$  for all times, and on top of this, is asymptotically exact. The generators  $M(\lambda)$  and  $M_d(\lambda)$  are related by

$$M(\lambda) = -i[\widetilde{H}_{S}(\lambda), \cdot] + \lambda^{2} M_{d}(\lambda)$$
(1.33)

and the two operators on the right side commute.

## 2 Mechanism of the resonance theory

## 2.1 History.

The method we develop has its origins in works using a  $C^*$ -dynamical system approach, pioneered in [16, 4]. In those works, it was shown that an initial system-reservoir state, which does not deviate much from the equilibrium state, will converge to the equilibrium

in the limit of large times. In this setup, the approach to equilibrium is driven by a spectral gap of the (complex deformed) Liouville operator for the resonance located at the origin. In [25, 26] it was realized that the other resonances govern the evolution of the system coherences and consequently a rigorous analysis of the dynamics of decoherence and entanglement in various physical settings became possible, see e.q. [22, 24]. The CPT properties and asymptotic exactness of the approximating markovian dynamics have not been addressed until very recently. In [18] we give a short (two page) outline of a proof of the Results 1 and 2 presented in the current work. The paper [18] focuses on the construction of an asymptotically exact markovian approximation, which is part of Result 3 of the present publication. However, there is a gap in the proof of the main result in [18]. This is explained in an erratum to [18], where it is also announced that we can still show the result in its full strength for the dynamics of the populations of the system (but not the coherences). We give the corresponding precise statement and proof of it here in (1.32). An approximate system dynamics valid for all times was constructed [17], using a semigroup with a generator depending on all powers of  $\lambda$ , but which is not asymptotically exact, and which is not shown to be CPT. In contrast, we show here that the approximation by the CPT semigroup given by the free dynamics plus the Davies generator, which is merely quadratic in  $\lambda$ , works for all times. By adding higher orders in  $\lambda$  to the generator, we achieve an asymptotically exact CPT semigroup. Of course, non markovian effects play an important role in quantum physics and are heavily studied (see for instance the review [29]). A refined weak coupling limit which captures non-markovian effects has been developed in [27]. It will be interesting to examine how our resonance theory will contribute to this line of study.

#### 2.2 Purification of the initial state.

Given any (initial) system density matrix  $\rho_{S}$  acting on  $\mathbb{C}^{N}$ , we take a purification, *i.e.*, a normalized vector  $\Psi_{S} \in \mathbb{C}^{N} \otimes \mathbb{C}^{N}$  satisfying

$$\operatorname{tr}_{S} \rho_{S} X = \langle \Psi_{S}, (X \otimes \mathbb{1}_{S}) \Psi_{S} \rangle \tag{2.1}$$

for all system operators  $X \in \mathcal{B}(\mathbb{C}^N)$  <sup>3</sup>. We also take a purification of the reservoir thermal equilibrium state (1.7), whose associated Hilbert space is again obtained by doubling the original one, namely the Fock space  $\mathcal{F}$ , (1.6). On  $\mathcal{F} \otimes \mathcal{F}$ , define the thermal annihilation operators

$$a_{\beta}(k) = \sqrt{1 + \mu(k)} \left( a(k) \otimes \mathbb{1} \right) + \sqrt{\mu(k)} \left( \mathbb{1} \otimes a^{*}(k) \right),$$

$$\mu(k) = \frac{1}{e^{\beta \omega(k)} - 1},$$
(2.2)

<sup>&</sup>lt;sup>3</sup>To do this explicitly, first diagonalize  $\rho_{\rm S} = \sum_j p_j |\chi_j\rangle \langle \chi_j|$ . Then the vector  $\Psi_{\rm S} = \sum_j \sqrt{p_j} \chi_j \otimes \chi_j$  does the job in (2.1).

and set  $(a_{\beta}(k))^* \equiv a_{\beta}^*(k)$ . This representation is due to [3]. One verifies that  $[a_{\beta}(k), a_{\beta}^*(l)] = \delta(k-l)$ , and that the purification of  $\omega_{R,\beta}$  is given by

$$\omega_{R,\beta}(\mathcal{P}) = \langle \Omega_R, \mathcal{P}_\beta \Omega_R \rangle, \qquad (2.3)$$

where

$$\Omega_{R} = \Omega \otimes \Omega \in \mathcal{F} \otimes \mathcal{F}, \tag{2.4}$$

 $\mathcal{P}$  is an arbitrary polynomial in creation and annihilation operators and  $\mathcal{P}_{\beta}$  is that same polynomial with each  $a^*(k)$ , a(l) replaced by  $a^*_{\beta}(k)$ ,  $a_{\beta}(l)$ . For the purposes of this paper, we shall call such  $\mathcal{P}_{\beta}$  reservoir observables <sup>4</sup>. We denote the smoothed out operators by  $(f \in L^2(\mathbb{R}^3, d^3k))$ 

$$a_{\beta}^{*}(f) = \int_{\mathbb{R}^{3}} f(k) a_{\beta}^{*}(k), \quad \varphi_{\beta}(f) = \frac{1}{\sqrt{2}} (a_{\beta}^{*}(f) + a_{\beta}(f))$$
 (2.5)

To show that (2.3) is a purification of the reservoir equilibrium state, one just has to check that

$$\omega_{R,\beta}(a^*(k)a(l)) = \langle \Omega_R, a_\beta^*(k)a_\beta(l)\Omega_R \rangle$$
(2.6)

equals the right side of (1.7), which is easy to do. The disentangled system reservoir state is thus represented in the purification Hilbert space by the 'reference vector'

$$\Psi_{\rm ref} = \Psi_{\rm S} \otimes \Omega_{\rm R} \in \mathcal{H}_{\rm ref} \equiv \mathbb{C}^N \otimes \mathbb{C}^N \otimes \mathcal{F} \otimes \mathcal{F}. \tag{2.7}$$

The initial states we consider are exactly those which are represented by a vector (or a density matrix) on the space  $\mathcal{H}_{ref}$ . This class contains entangled system-reservoir states. As an example, take an initial state obtained by entanglement via interaction, of the form (expressed before the continuous mode limit)  $\rho_{SR,0} = e^{-i\tau(G\otimes\mathcal{P})}(\rho_S\otimes\rho_{R,\beta})e^{i\tau(G\otimes\mathcal{P})}$ . Here,  $\tau$  is a 'preparation time' during which the disentangled  $\rho_S\otimes\rho_{R,\beta}$  builds up entanglement due the system reservoir interaction  $G\otimes\mathcal{P}$ , where G and  $\mathcal{P}$  are self-adjoint operators (e.g.  $\mathcal{P}$  a polynomial in field operators  $\varphi(g)$ , (1.5)). The purification vector of the entangled state  $\rho_{SR,0}$  is  $\Psi_{SR,0} = e^{-i\tau(G\otimes\mathbb{I}_S\otimes\mathcal{P}_\beta)}\Psi_{ref} \in \mathcal{H}_{ref}$  and belongs to the class of initial states we allow.

## 2.3 Equilibrium states

The uncoupled equilibrium state obtained as the continuous mode limit of  $\propto e^{-\beta H_{\rm S}} \otimes e^{-\beta H_{\rm R}}$  and has the purification

$$\Omega_{SR,\beta,0} = \Omega_{S,\beta} \otimes \Omega_{R}, \tag{2.8}$$

where  $\Omega_R$  is given in (2.4) and (see (1.2))

$$\Omega_{S,\beta} = Z_{S,\beta}^{-1/2} \sum_{j} e^{-\beta E_j/2} \phi_j \otimes \phi_j \in \mathbb{C}^N \otimes \mathbb{C}^N,$$
(2.9)

<sup>&</sup>lt;sup>4</sup>In a more mathematical approach, the reservoir algebra is the Weyl algebra, represented on  $\mathcal{F} \otimes \mathcal{F}$ , generated by thermal Weyl operators  $W_{\beta}(f) = e^{i\varphi_{\beta}(f)}$ .

with  $Z_{S,\beta} = \text{tr}e^{-\beta H_S}$ . Of course  $\Omega_{SR,\beta,0} \in \mathcal{H}_{ref}$ . The interacting equilibrium state  $\Omega_{SR,\beta,\lambda}$ , defined as the continuous mode limit of the density matrix  $\propto e^{-\beta H}$  (the interacting H, (1.1)) is given by

$$\Omega_{\mathrm{SR},\beta,\lambda} = \frac{e^{-\frac{\beta}{2}(L_0 + \lambda G \otimes \mathbb{1}_{\mathrm{S}} \otimes \varphi_{\beta}(g))} \Omega_{\mathrm{SR},\beta,0}}{\|e^{-\frac{\beta}{2}(L_0 + \lambda G \otimes \mathbb{1}_{\mathrm{S}} \otimes \varphi_{\beta}(g))} \Omega_{\mathrm{SR},\beta,0}\|} \in \mathcal{H}_{\mathrm{ref}}.$$
(2.10)

Here,  $L_0$  is the 'uncoupled Liouvillian', explicitly given in (2.13) below. The equilibrium state  $\Omega_{SR,\beta,\lambda}$ , for any  $\lambda \in \mathbb{R}$ , has the important property of 'cyclicity and separability'. Namely, any vector  $\Psi \in \mathcal{H}_{ref}$  can be approximated arbitrarily well by a vector of the form  $B\Omega_{SR,\beta,\lambda}$ , for some operator B which is a linear combination of terms  $G \otimes \mathbb{1}_S \otimes \mathcal{P}_{\beta}$ , where G and  $\mathcal{P}_{\beta}$  are system and reservoir observables  $^5$ . This is the cyclicity of  $\Omega_{SR,\beta,\lambda}$ . Separability means that an arbitrary  $\Psi \in \mathcal{H}_{ref}$  can also be approximated arbitrarily well by a vector of the form  $B'\Omega_{SR,\beta,\lambda}$ , for some operator B' which is a linear combination of terms  $\mathbb{1}_S \otimes G \otimes \mathcal{P}'_{\beta}$ , where G is a system observable and  $\mathcal{P}'_{\beta}$  is an operator acting on  $\mathcal{F} \otimes \mathcal{F}$  which commutes with any reservoir observable  $\mathcal{P}_{\beta}$ .

The cyclicity and separating properties are easily understood, at least for finite dimensional systems. Namely, cyclicity comes from the fact that (in finite dimensions) any equilibirum density matrix  $e^{-\beta H_S}$  has full range (is invertible). The separating property (which is the same as cyclicity relative to the commutant) comes about by a natural isomorphism between observables and operators commuting with observables  $(X \otimes \mathbb{1}_S \leftrightarrow \mathbb{1}_S \otimes X)$ . Explicitly, from (2.9) we see that for any k, l,

$$\phi_k \otimes \phi_l = (G_1 \otimes \mathbb{1}_S) \Omega_{S,\beta} = (\mathbb{1}_S \otimes G_2) \Omega_{S,\beta}, \tag{2.11}$$

for  $G_1 = Z_{\mathrm{S},\beta}^{1/2} e^{\beta E_l/2} |\phi_k\rangle \langle \phi_l|$  and  $G_2 = Z_{\mathrm{S},\beta}^{1/2} e^{\beta E_k/2} |\phi_l\rangle \langle \phi_k|$ . Hence in (2.11) we can reconstruct any basis element  $\phi_k \otimes \phi_l$ . By linear combination, given any  $\Psi \in \mathbb{C}^N \otimes \mathbb{C}^N$ , we can find  $G_1'$  and  $G_2'$  s.t.  $\Psi = (G_1' \otimes \mathbb{I}_{\mathrm{S}})\Omega_{\mathrm{S},\beta} = (\mathbb{I} \otimes G_2')\Omega_{\mathrm{S},\beta}$ . These properties carry over to equilibrium states of infinite dimensional (continuous mode) systems, with the only difference that exact equality might not be possible, but an arbitrarily accurate approximation of  $\Psi$  can be achieved.

Dynamics of the purified state: the Liouvillian. The uncoupled dynamics is generated by the Hamiltonian  $H_0 = H_S + H_R$ , (1.2), (1.3). Its Heisenberg form  $e^{itH_0}(G \otimes a^*(k))e^{-itH_0} = e^{itH_S}Ge^{-itH_S} \otimes e^{i\omega(k)t}a^*(k)$  is implemented in the purification Hilbert space as follows. Let  $\Psi_0 \in \mathcal{H}_{ref}$  be the vector representing the state  $\omega_0$ . Then

$$\omega_0 \left( e^{itH_0} \left( G \otimes a^*(k) \right) e^{-itH_0} \right) = \left\langle \Psi_0, \left( e^{itH_S} G e^{-itH_S} \otimes \mathbb{1}_S \otimes e^{i\omega(k)t} a_\beta^*(k) \right) \Psi_0 \right\rangle$$
$$= \left\langle \Psi_0, e^{itL_0} \left( G \otimes \mathbb{1}_S \otimes a_\beta^*(k) \right) e^{-itL_0} \Psi_0 \right\rangle, \tag{2.12}$$

<sup>&</sup>lt;sup>5</sup>For any  $\epsilon > 0$  there is a B s.t.  $\|\Psi - B\Omega_{SR,\beta,\lambda}\| < \epsilon$ .

where  $L_0$  is called the uncoupled Liouvillian, given by

$$L_{0} = L_{R} + L_{S}$$

$$L_{S} = H_{S} \otimes \mathbb{1}_{S} - \mathbb{1}_{S} \otimes H_{S}$$

$$L_{R} = H_{R} \otimes \mathbb{1}_{R} - \mathbb{1}_{R} \otimes H_{R}.$$
(2.13)

Relation (2.12) is readily verified. Note that  $L_{\rm R}\Omega_{\rm R}=0$  (see (2.4)). Adding the term  $-\mathbb{1}_{\rm S}\otimes H_{\rm S}$  to the system Liouvillian  $L_{\rm S}$  as defined in (2.13) is 'optional'. It serves to ensure the agreeable property  $L_{\rm S}\Omega_{{\rm S},\beta}=0$  (see (2.9)). Thus we have  $L_0\Omega_{{\rm SR},\beta,0}=0$ . The full, interacting dynamics generated by H, (1.1), is implemented as

$$\omega_0(e^{itH}(X \otimes \mathcal{P})e^{-itH}) = \langle \Psi_0, e^{itL_\lambda}(X \otimes \mathbb{1}_S \otimes \mathcal{P}_\beta)e^{-itL_\lambda}\Psi_0 \rangle. \tag{2.14}$$

Here,  $L_{\lambda}$  is the coupled Liouvillian, given by

$$L_{\lambda} = L_{0} + \lambda I$$

$$I = G \otimes \mathbb{1}_{S} \otimes \varphi_{\beta}(g) - J(G \otimes \mathbb{1}_{S} \otimes \varphi_{\beta}(g))J. \tag{2.15}$$

We will not use explicitly the form of  $L_{\lambda}$  in this paper, but let us explain the term  $J(G \otimes \mathbb{I}_{S} \otimes J\varphi_{\beta}(g))J$  in (2.15). This is an operator which commutes with all observables (i.e., with all operators which are linear combinations of the form  $X \otimes \mathbb{I}_{S} \otimes \mathcal{P}_{\beta}$ ). The map J is an 'anti-unitary involution' (the modular conjugation of Tomita Takesaki theory). J has an explicit action which we do not discuss here, as we won't use it directly in this paper (see e.g. [26]). An important property of J is that given any system observable A and any reservoir observable  $\mathcal{P}_{\beta}$ , the operator  $J(A \otimes \mathbb{I}_{S} \otimes \mathcal{P}_{\beta})J$  commutes with all system-reservoir observables  $B \otimes \mathbb{I}_{S} \otimes \mathcal{Q}_{\beta}$ . Adding the commuting term  $J(G \otimes \mathbb{I}_{S} \otimes \varphi_{\beta}(g))J$  in the interaction is optional (meaning that the equality (2.14) still holds if I is defined without adding this term). The reason for this non-uniqueness of the Liouvillian comes from the fact that adding to the generator an operator which commutes with all observables will not alter the dynamics of observables. The choice (2.15) ensures that the coupled equilibrium state (2.10) satisfies

$$L_{\lambda}\Omega_{\mathrm{SR},\beta,\lambda} = 0. \tag{2.16}$$

## 2.4 Representation of the dynamics

The Heisenberg evolution of a system observable X is

$$\alpha_{\lambda}^{t}(X \otimes \mathbb{1}_{R}) = e^{itH}(X \otimes \mathbb{1}_{R})e^{-itH}, \qquad (2.17)$$

where H is the interacting system-reservoir Hamiltonian (1.1). Let  $\omega_0$  be an (initial) system-reservoir state, with purification  $\Psi_0 \in \mathcal{H}_{ref}$ . The vector  $\Psi_0$  can be approximated arbitrarily well by  $B'\Omega_{SR,\beta,\lambda}$  for a suitable B' commuting with all observables. Since the full dynamics is unitary, this approximation is uniform in time. We will hence assume without loss of generality that

$$\Psi_0 = B' \Omega_{SR,\beta,\lambda}. \tag{2.18}$$

Note that if the initial state is of the form  $\rho_S \otimes \omega_{R,\beta}$  then

$$B' = \mathbb{1}_{S} \otimes B'_{S} \otimes \mathbb{1}_{R} + O(\lambda), \quad \text{some } B'_{S} \in \mathcal{B}(\mathcal{H}_{S})$$
 (2.19)

since  $\omega_{SR,\beta,\lambda} = \Omega_{S,\beta} \otimes \Omega_R + O(\lambda)$ . What follows works for all initial states (2.18). We have

$$\omega_{0}(\alpha_{\lambda}^{t}(X \otimes \mathbb{1}_{R})) = \langle \Psi_{0}, e^{itL_{\lambda}}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})e^{-itL_{\lambda}}\Psi_{0} \rangle 
= \langle \Psi_{0}, B'e^{itL_{\lambda}}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})e^{-itL_{\lambda}}\Omega_{SR,\beta,\lambda} \rangle 
= \langle \Psi_{0}, B'e^{itL_{\lambda}}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,\lambda} \rangle.$$
(2.20)

In the second equality we moved B' to the left, as it commutes with the observable  $e^{itL_{\lambda}}(X \otimes \mathbb{1}_{\mathbb{S}} \otimes \mathbb{1}_{\mathbb{R}})e^{-itL_{\lambda}}$ . In the third we use the invariance (2.16). Next comes the core analytical tool, the resonance expansion of  $e^{itL_{\lambda}}$ . It is important to realize that this expansion is only correct in the weak sense; one cannot perform it independently on both factors  $e^{\pm itL_{\lambda}}$  in (2.20), <sup>6</sup>. This is why we have to exploit the algebraic structure (existence of B') and eliminate one of the propagators  $e^{-itL_{\lambda}}$  by making it act on the invariant state  $\Omega_{SR,\beta,\lambda}$  in (2.20).

The right side of (2.20) is of the form  $\langle \psi, e^{itL_{\lambda}} \phi \rangle$  for two vectors  $\psi$ ,  $\phi$ . We use the usual resolvent representation of the propagator,

$$\langle \psi, e^{itL_{\lambda}} \phi \rangle = \frac{-1}{2\pi i} \int_{\mathbb{R}_{-i}} e^{itz} \langle \psi, (L_{\lambda} - z)^{-1} \phi \rangle dz.$$
 (2.21)

The integral is over the horizontal contour z = x - i,  $x \in \mathbb{R}$ . Since  $L_{\lambda}$  is self-adjoint,  $(L_{\lambda} - z)^{-1}$  is a well defined, bounded operator. We explain the further analysis of (2.21) in the technically easiest situation (which requires the most regularity, though), namely, when the spectral deformation technique applies. The strategy is to construct a meromorphic continuation in z of the function  $\langle \psi, (L_{\lambda} - z)^{-1} \phi \rangle$ , extending the domain of z from the lower half plane  $\mathbb{C}_{-}$  across the real axis into (parts of) the upper complex half plane. Whether this is possible depends of course on the operator  $L_{\lambda}$  (and the vectors  $\psi, \phi$ ). Define the complex valued function

$$g_{\beta}(u,\Sigma) = \sqrt{\frac{u}{1 - e^{-\beta u}}} |u|^{1/2} \begin{cases} g(u,\Sigma) & u \ge 0 \\ -\bar{g}(-u,\Sigma) & u < 0 \end{cases},$$
 (2.22)

where  $g(u, \Sigma)$  is the form factor g expressed in spherical coordinates. Suppose that

(A) For  $\theta \in \mathbb{R}$ , set  $(T_{\theta}g_{\beta})(u,\Sigma) = g_{\beta}(u-\theta,\Sigma)$ . There exists a  $\theta_0 > 0$  such that  $\theta \mapsto T_{\theta}g_{\beta}$  has an analytic extension (as a function from  $\mathbb{R}$  to  $L^2(\mathbb{R} \times S^2)$ ) to  $0 < \text{Im}\theta < \theta_0$  which is continuous at  $\text{Im}\theta \to 0_+$ .

This is readily seen: weakly,  $e^{itL_{\lambda}} \to |\Omega_{SR,\beta,\lambda}\rangle\langle\Omega_{SR,\beta,\lambda}|$  for  $t \to \infty$  and using this for both propagators in (2.20) would yield the result  $\langle\Omega_{SR,\beta,\lambda},(X\otimes \mathbb{1}_S\otimes \mathbb{1}_R)\Omega_{SR,\beta,\lambda}\rangle|\langle\Omega_{SR,\beta,\lambda},\Psi_0\rangle|^2$  for  $t\to\infty$ . But this is not the correct final state.

This 'translation analyticity' is the technically easiest condition under which one can implement the spectral deformation technique <sup>7</sup>. Denote by  $U_{\theta}$  the action of  $T_{\theta}$  lifted from the single-particle space to Fock space. Then  $U_{\theta}$ ,  $\theta \in \mathbb{R}$ , is a unitary group on  $\mathcal{H}_{ref}$  (see (2.7)) such that

$$\langle \psi, (L_{\lambda} - z)^{-1} \phi \rangle = \langle U_{\theta} \psi, U_{\theta} (L_{\lambda} - z)^{-1} \phi \rangle = \langle \psi_{\bar{\theta}}, (L_{\lambda, \theta} - z)^{-1} \phi_{\theta} \rangle$$
 (2.23)

and (assuming condition (A) above), the right side of (2.23) has an extension to complex values of  $\theta$  (here,  $\bar{\theta}$  is the complex conjugate of  $\theta$  and it shows up in (2.23) since the scalar product is antilinear in its left argument). The first equality in (2.23) is due to unitarity of  $U_{\theta}$  and we define  $\psi_{\theta} = U_{\theta}\psi$ ,  $\phi_{\theta} = U_{\theta}\phi$  and  $L_{\lambda,\theta} = U_{\theta}L_{\lambda}U_{\theta}^*$ . The relation (2.23) stays valid for complex values of  $\theta$  due to the identity theorem of complex analysis (varying the real part of  $\theta$  does not change the inner products, due to unitarity). When  $\theta$  becomes complex,  $L_{\lambda,\theta}$  is not a self-adjoint operator any longer (it is not even a normal operator) and hence generically, its spectrum leaves the real axis as  $\text{Im}\theta \neq 0$ . Take now  $\theta$  with  $\text{Im}\theta = \theta_0 > 0$  fixed.

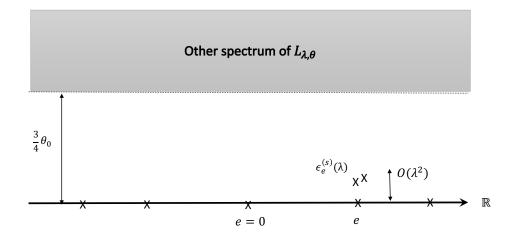


Fig.1: The eigenvalues e of  $L_{0,\theta}$  bifurcate into eigenvalues  $\epsilon_e^{(s)}(\lambda)$  of  $L_{\lambda,\theta}$  for nonzero  $\lambda$ .

By analytic perturbation theory and the fact that  $L_{0,\theta} = L_0 + \theta N$ , where N is the number operator, having spectrum  $\mathbb{N} \cup \{0\}$ , one shows the following result [16, 4, 26]:

In a strip  $\{z \in \mathbb{C} : 0 \leq \operatorname{Im} z < \theta_0/2\}$ , the spectrum of the operator  $L_{\lambda,\theta} = L_{0,\theta} + \lambda I_{\theta}$  (c.f. (2.15)) consists of eigenvalues which are independent of  $\theta$  (for  $\lambda$  not too large compared to  $\theta$ ). All other spectrum of  $L_{\lambda,\theta}$  is located within  $\{z \in \mathbb{C} : \operatorname{Im} z > 3\theta_0/4\}$ .

The reservoir correlation function can be written as  $C_{\beta}(t) = \int_{\mathbb{R}} du \, e^{iut} \int_{S^2} d\Sigma \, |g_{\beta}(u,\Sigma)|^2$  and translation analyticity implies exponential decay of the correlation function.

The situation is depicted in Fig.1. For  $\lambda = 0$ , the eigenvalues coincide (including multiplicity) with those of  $L_{\rm S}$ . More precisely, the (rank  $m_e$ ) spectral projection associated to the eigenvalue e of  $L_{0,\theta}$  is given by

$$P_e = P(L_S = e) \otimes P_R, \tag{2.24}$$

where  $P(L_{\rm S}=e)$  is the eigenprojection of  $L_{\rm S}$  associated to the eigenvalue e and  $P_{\rm R}=|\Omega_{\rm R}\rangle\langle\Omega_{\rm R}|$ . Since e is an isolated eigenvalue of  $L_{0,\theta}$ , analytic perturbation theory implies that for small  $\lambda$ , e splits into  $\leq m_e$  eigenvalues  $\epsilon_e^{(s)}(\lambda)$ ,  $s=1,2,\ldots$  (the added up multiplicity equaling  $m_e$ ), which are analytic at  $\lambda=0$  and have the expansion

$$\epsilon_e^{(s)}(\lambda) = e + \lambda^2 a_e^{(s)} + O(\lambda^4). \tag{2.25}$$

The corrections  $a_e^{(s)}$  can be calculated by perturbation theory <sup>8</sup>. They are the eigenvalues of the *level shift operator* (second order analytic perturbation theory)

$$\Lambda_e = -P_e I P_e^{\perp} (L_0 - e + i0)^{-1} I P_e. \tag{2.26}$$

Using (2.23) in (2.21) yields

$$\left\langle \psi, e^{itL} \phi \right\rangle = \frac{-1}{2\pi i} \sum_{e \in \operatorname{spec}(L_{S})} \sum_{s=1}^{m_{e}} \oint_{\Gamma_{e}^{(s)}} e^{itz} \left\langle \psi_{\bar{\theta}}, (L_{\lambda, \theta} - z)^{-1} \phi_{\theta} \right\rangle dz + O\left(e^{-\frac{3}{4}\theta_{0}t}\right). \tag{2.27}$$

To arrive at (2.27), we have deformed the contour of integration z = x - i into  $z = x + \frac{3}{4}i\theta_0$ , thereby (by the residue theorem) creating the contour integrals  $\oint_{\Gamma_e^{(s)}}$ , where  $\Gamma_e^{(s)}$  is a circle centered at  $\epsilon_e^{(s)}(\lambda)$ , not containing any other eigenvalue of  $L_{\lambda,\theta}$ . The remainder decays at rate  $-\frac{3}{4}\theta_0$  due to the factor  $e^{itz}$ . Consider the situation where all of the  $\epsilon_e^{(s)}$  are distinct (for  $\lambda \neq 0$ ). The integrand in (2.27) has a simple pole at  $z = \epsilon_e^{(s)}$  in the interior of  $\Gamma_e^{(s)}$  and so we have

$$\frac{-1}{2\pi i} \oint_{\Gamma_e^{(s)}} e^{itz} (L_{\lambda,\theta} - z)^{-1} dz = e^{it\epsilon_e^{(s)}(\lambda)} \left(\frac{-1}{2\pi i}\right) \oint_{\Gamma_e^{(s)}} (L_{\lambda,\theta} - z)^{-1} dz \equiv e^{it\epsilon_e^{(s)}(\lambda)} \Pi_e^{(s)}, \quad (2.28)$$

where  $\Pi_e^{(s)} = \Pi_e^{(s)}(\lambda, \theta)$  is the (Riesz) spectral projection associated to the eigenvalue  $\epsilon_e^{(s)}(\lambda)$  of  $L_{\lambda,\theta}$ . Combining (2.20), (2.27) and (2.28) yields

$$\omega_0 \left( \alpha_{\lambda}^t (X \otimes \mathbf{1}_{R}) \right) = \sum_{e \in \operatorname{spec}(L_S)} \sum_{s=1}^{m_e} e^{\mathrm{i}t\epsilon_e^{(s)}} \left\langle [(B')^* \Psi_0]_{\bar{\theta}}, \Pi_e^{(s)} \left( X \otimes \mathbf{1}_{S} \otimes \mathbf{1}_{R} \right) [\Omega_{SR,\beta,\lambda}]_{\theta} \right\rangle + O\left(\lambda e^{-\frac{3}{4}\theta_0 t}\right). \tag{2.29}$$

<sup>&</sup>lt;sup>8</sup> In principle, there are  $O(\lambda)$  correction terms given by  $P_eI_\theta P_e$ , but this operator vanishes for the interactions we consider.

Note that the remainder is proportional to  $\lambda$  as the integral over the zeroth order term vanishes. If the initial state is of the form  $\rho_{\rm S} \otimes \omega_{{\rm S},\beta}$ , then the remainder in (2.29) is actually  $O(\lambda^2)$ , due to (2.19) (see Proposition 4.2 of [25]).

Our next step is to 'eliminate' the  $\theta$  dependence of the main term in (2.29). Consider first e = 0. Due to (2.16) and since  $[\Omega_{SR,\beta,\lambda}]_{\theta} = U_{\theta}\Omega_{SR,\beta,\lambda}$  is analytic in  $\theta$ , we have  $L_{\lambda,\theta}[\Omega_{SR,\beta,\lambda}]_{\theta} = 0$ . It follows that  $L_{\lambda,\theta}$  has an eigenvalue  $\epsilon_0^{(1)} = 0$  for all  $\lambda, \theta$ . We use s = 1 to label it. The associated eigenprojection is

$$\Pi_0^{(1)} = |[\Omega_{SR,\beta,\lambda}]_{\theta}\rangle\langle[\Omega_{SR,\beta,\lambda}]_{\bar{\theta}}|. \tag{2.30}$$

In the sum (2.29), the term e = 0, s = 1 equals

$$\langle [(B')^* \Psi_0]_{\theta}, [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle \langle [\Omega_{SR,\beta,\lambda}]_{\bar{\theta}}, (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle$$

$$= \langle \Psi_0, B' \Omega_{SR,\beta,\lambda} \rangle \langle \Omega_{SR,\beta,\lambda}, (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) \Omega_{SR,\beta,\lambda} \rangle$$

$$= \operatorname{tr}_S(\rho_{S,\beta,\lambda} X). \tag{2.31}$$

The first equality in (2.31) holds by the identity principle of complex analysis. The final equality follows from (recall (2.18))  $\langle \Psi_0, B'\Omega_{SR,\beta,\lambda} \rangle = \langle \Psi_0, \Psi_0 \rangle = 1$  and from the definition of  $\rho_{S,\beta,\lambda}$  as the reduction to the system of the full, interacting system-reservoir equilibrium state. Above, we are able to arrive at the result (2.31), which is non-perturbative in  $\lambda$ , since we know to begin with that  $L_{\lambda}\Omega_{SR,\beta,\lambda} = 0$ .

For the other terms in the sum (2.29), associated with nonzero resonance energies, we use regular analytic perturbation theory in  $\lambda$  (as we do not know an *a priori* expression for them). Consider the situation where each  $\Lambda_e$  is diagonalizable, i.e.,

$$\Lambda_e = \sum_{s=1}^{m_e} a_e^{(s)} Q_e^{(s)}, \tag{2.32}$$

where  $a_e^{(s)}$  and  $Q_e^{(s)}$  are the eigenvalues and rank-one eigenprojections, neither depending on  $\theta$ . We have

$$Q_e^{(s)} \subset P(L_S = e)$$
 and  $\sum_{s=1}^{m_e} Q_e^{(s)} = P(L_S = e).$  (2.33)

The relation  $L_{\lambda}\Omega_{SR,\beta,\lambda} = 0$  implies that  $\Lambda_0\Omega_{S,\beta} = 0$ . Assuming that all the eigenvalues of  $\Lambda_0$  are simple then yields

$$Q_0^{(1)} = |\Omega_{S,\beta}\rangle\langle\Omega_{S,\beta}|. \tag{2.34}$$

Analytic perturbation theory gives the following expansion for  $\Pi_e^{(s)}$ , the spectral projection of  $L_{\lambda,\theta}$  associated to  $\epsilon_e^{(s)}$ 

$$\Pi_e^{(s)}(\theta,\lambda) = Q_e^{(s)} \otimes |\Omega_{\mathcal{R}}\rangle \langle \Omega_{\mathcal{R}}| + O(\lambda). \tag{2.35}$$

Consider a term in (2.29) with (e, s) fixed (not equal to (0, 1)). We have

$$\begin{aligned}
&\langle [(B')^* \Psi_0]_{\bar{\theta}}, \Pi_e^{(s)} (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle \\
&= \langle \Psi_0, B' (Q_e^{(s)} \otimes |\Omega_R\rangle \langle \Omega_R|) (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) \Omega_{SR,\beta,\lambda} \rangle + O(\lambda) \\
&= \langle \Psi_0, B' (Q_e^{(s)} \otimes \mathbb{1}_R) (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) (\Omega_{S,\beta} \otimes \Omega_R) \rangle + O(\lambda).
\end{aligned} (2.36)$$

In the first equality of (2.36) we have used the approximation (2.35) and that  $U_{\theta}\Omega_{\rm R} = \Omega_{\rm R}$ . In the second equality we made use of  $(\mathbb{1}_{\rm S} \otimes \mathbb{1}_{\rm S} \otimes |\Omega_{\rm R}\rangle\langle\Omega_{\rm R}|)\Omega_{{\rm SR},\beta,\lambda} = \Omega_{{\rm S},\beta} \otimes \Omega_{\rm R} + O(\lambda^2)$  (see (2.8) and (2.10)). If the initial condition is of the form  $\rho_{\rm S} \otimes \omega_{{\rm R},\beta}$ , then (2.19) holds and it is not hard to see that since  $\langle \Omega_{\rm R}|I|\Omega_{\rm R}\rangle = 0$ , the remainder in (2.36) is actually  $O(\lambda^2)$ . Due to the cyclicity of  $\Omega_{{\rm S},\beta}$ , there are uniquely defined operators  $\mathcal{Q}_e^{(s)}$  acting on system observables, satisfying

$$\left(\mathcal{Q}_{e}^{(s)}(X) \otimes \mathbb{1}_{S}\right)\Omega_{S,\beta} = Q_{e}^{(s)}(X \otimes \mathbb{1}_{S})\Omega_{S,\beta}, \quad \forall X.$$
 (2.37)

The  $Q_e^{(s)}$  are a family of disjoint projection operators (as the  $Q_e^{(s)}$  are). The main term on the right side of (2.36) is then

$$\langle \Psi_{0}, B' \left( Q_{e}^{(s)} \otimes \mathbb{1}_{R} \right) \left( X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R} \right) \left( \Omega_{S,\beta} \otimes \Omega_{R} \right) \rangle 
= \langle \Psi_{0}, \left( \mathcal{Q}_{e}^{(s)}(X) \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R} \right) B' \left( \Omega_{S,\beta} \otimes \Omega_{R} \right) \rangle 
= \omega_{0} \left( \mathcal{Q}_{e}^{(s)}(X) \otimes \mathbb{1}_{R} \right) + O(\lambda)$$
(2.38)

To arrive at (2.38), we have used that B' commutes with all observables, so we can move it to the right of  $\mathcal{Q}_e^{(s)}(X) \otimes \mathbb{1}_{\mathcal{S}} \otimes \mathbb{1}_{\mathcal{R}}$  and we also take into account that

$$B'(\Omega_{S,\beta} \otimes \Omega_R) = B'\Omega_{SR,\beta,\lambda} + O(\lambda) = \Psi_0 + O(\lambda). \tag{2.39}$$

The  $O(\lambda)$  term in (2.39) comes about by replacing the uncoupled equilibrium  $\Omega_{S,\beta} \otimes \Omega_R$  by the coupled one,  $\Omega_{SR,\beta,\lambda}$ . The initial state  $\Psi_0$  emerges in (2.39) due to (2.18). Again, for initial states  $\rho_S \otimes \omega_{R,\beta}$ , the remainder in (2.38), (2.39) is actually  $O(\lambda^2)$ , due to (2.19). Combining (2.38) with (2.36), (2.31) and (2.29) shows the expansion

$$\omega_0 \left( \alpha_{\lambda}^t (X \otimes \mathbf{1}_{R}) \right) = \operatorname{tr}_{S} \left( \rho_{S,\beta,\lambda} X \right) + \sum_{(e,s) \neq (0,1)} e^{\mathrm{i}t\epsilon_{e}^{(s)}} \omega_0 \left( \mathcal{Q}_{e}^{(s)}(X) \otimes \mathbb{1}_{R} \right) + O(\lambda e^{-\gamma(\lambda)t}) + O(\lambda e^{-\frac{3}{4}\theta_0 t}).$$

$$(2.40)$$

Since  $\gamma(\lambda) < \frac{3}{4}\theta_0$  the second error term in (2.40) is smaller than the first one. Equation (2.40) is the basic result of the resonance theory for system observables. Again, as explained during the derivation, for initial states  $\rho_S \otimes \omega_{R,\beta}$  the  $\lambda$  in both remainders in (2.40) are actually  $\lambda^2$ .

#### **2.5** Proof of (1.15)

Suppose that the initial state is disentangled,  $\omega_0 = \omega_S \otimes \omega_{R,\beta}$ , where  $\omega_S$  is given by a general system density matrix  $\rho$  and  $\omega_{R,\beta}$  is the reservoir equilibrium (or a local perturbation thereof). The remainders in (2.40) are then  $O(\lambda^2)$ . The dynamical map  $\rho \mapsto V_t \rho$  is defined by

$$\operatorname{tr}_{S}((V_{t}\rho)X) = \omega_{0}(\alpha_{\lambda}^{t}(X \otimes \mathbb{1}_{R})), \qquad \forall X.$$
(2.41)

The result (2.40) then implies

$$V_t \rho = \rho_{S,\beta,\lambda} + W_t \rho + O(\lambda^2 e^{-\gamma(\lambda)t}), \qquad (2.42)$$

where  $W_t$  is the map on density matrices defined by duality. It is given by (1.16) in which the sum is over  $j = (e, s) \neq (0, 1)$ . In particular, the  $\mathcal{P}_e^{(s)}$  are determined uniquely by

$$\operatorname{tr}(\mathcal{P}_e^{(s)}\rho)X = \operatorname{tr}\rho(\mathcal{Q}_e^{(s)}X), \qquad \forall \rho, X.$$
(2.43)

Recall the definition (2.37), in which the  $Q_e^{(s)}$  are spectral projections of the level shift operators (2.32). They form a family of disjoint projections,  $Q_e^{(s)}Q_{e'}^{(s')} = \delta_{e,e'}\delta_{s,s'}Q_e^{(s)}$  and satisfy (see (2.33))  $\sum_{(e,s)\neq(0,1)}Q_e^{(s)} = \mathbb{1}_S\otimes\mathbb{1}_S - |\Omega_{S,\beta}\rangle\langle\Omega_{S,\beta}|$ . Accordingly, it follows from (2.37) that

$$\mathcal{Q}_{e}^{(s)}\mathcal{Q}_{e'}^{(s')} = \delta_{e,e'}\delta_{s,s'}\mathcal{Q}_{e}^{(s)} \tag{2.44}$$

and  $\forall X \in \mathcal{B}(\mathcal{H}_S)$ ,

$$\sum_{(e,s)\neq(0,1)} \mathcal{Q}_e^{(s)} X = X - \operatorname{tr}(\rho_{S,\beta,0} X) \mathbb{1}_S.$$
 (2.45)

The duality (2.43) then translates into the corresponding properties (1.17) of the family  $\mathcal{P}_e^{(s)}$ .

## 3 Derivation of the main results

## **3.1** Proof of (1.24)

Define the operator  $\mathcal{M}(\lambda)$ , acting on system observables, by its spectral decomposition

$$\mathcal{M}(\lambda) = \sum_{(e,s)\neq(0,1)} \epsilon_e^{(s)}(\lambda) \ \mathcal{Q}_e^{(s)}, \tag{3.1}$$

where the sum is over all e, s except (e, s) = (0, 1). Note that if  $\epsilon_e^{(s)}(\lambda) \neq 0$  for  $(e, s) \neq (0, 1)$  (this is typically the case and holds in particular if the Fermi Golden Rule (1.22) is satisfied), then we have <sup>9</sup>

$$\ker \mathcal{M}(\lambda) = \operatorname{ran} \mathcal{Q}_0^{(1)} = \{ \mathbb{C}\rho_{S,\beta,0} \}^{\perp} \equiv \{ X : \operatorname{tr}(\rho_{S,\beta,0}X) = 0 \}.$$
 (3.2)

<sup>&</sup>lt;sup>9</sup>Note that  $Q_0^{(1)}(X \otimes \mathbb{1}_S)\Omega_{S,\beta} = (\operatorname{tr}\rho_{S,\beta,0}X)\Omega_{S,\beta}$ , so by (2.37)  $Q_0^{(1)}(X) = \operatorname{tr}(\rho_{S,\beta,0}X)\mathbb{1}_S$ .

Using the definition (3.1), the power series expansion of the exponential and (2.44), we obtain

$$e^{it\mathcal{M}(\lambda)} = \sum_{(e,s)\neq(0,1)} e^{it\epsilon_e^{(s)}(\lambda)} \mathcal{Q}_e^{(s)} + 1 - \sum_{(e,s)\neq(0,1)} \mathcal{Q}_e^{(s)}$$

$$= \sum_{(e,s)\neq(0,1)} e^{it\epsilon_e^{(s)}(\lambda)} \mathcal{Q}_e^{(s)} + tr(\rho_{S,\beta,0} \cdot). \tag{3.3}$$

Combining (3.3) with (2.40) (with error  $\propto \lambda^2$  due to the form of the initial condition) gives

$$\omega_0 \left( \alpha_{\lambda}^t (X \otimes \mathbf{1}_{\mathbf{R}}) \right) = \operatorname{tr}_{\mathbf{S}} \left( (\rho_{\mathbf{S}, \beta, \lambda} - \rho_{\mathbf{S}, \beta, 0}) X \right) + \omega_0 \left( e^{it \mathcal{M}(\lambda)} (X) \otimes \mathbb{1}_{\mathbf{R}} \right) + O(\lambda^2 e^{-\gamma(\lambda)t}). \tag{3.4}$$

The first term on the right side is  $O(\lambda^2)$ , hence

$$\omega_0(\alpha_\lambda^t(X \otimes \mathbf{1}_R)) = \omega_0(e^{it\mathcal{M}(\lambda)}(X) \otimes \mathbb{1}_R) + O(\lambda^2), \tag{3.5}$$

where the remainder is uniform in t. Equation (3.5) gives an approximation of the Heisenberg system dynamics by the semigroup  $e^{it\mathcal{M}(\lambda)}$ , up to a precision  $O(\lambda^2)$ , for all times. Notice that the state  $\omega_{S,\beta} \otimes \omega_{R,\beta}$ , where  $\omega_{S,\beta}$  is given by the system equilibrium state  $\rho_{S,\beta,0}$ , is invariant under this dynamics (see (3.2)). We now show that if we truncate the generator  $\mathcal{M}(\lambda)$  by taking into account only the part up to  $O(\lambda^2)$  in the eigenvalues  $\epsilon_e^{(s)}(\lambda)$  in (3.1), then we obtain a CPT semigroup. Using that <sup>10</sup>

$$e^{it\epsilon_e^{(s)}(\lambda)} = e^{it(e+\lambda^2 a_e^{(s)})} + O(\lambda^4 t e^{-\lambda^2 t(\gamma_{FGR} + O(\lambda^2))}), \tag{3.6}$$

we obtain

$$\left( e^{it\mathcal{M}(\lambda)}(X) \otimes \mathbb{1}_{S} \right) \Omega_{S,\beta} = \sum_{e,s} e^{it\epsilon_{e}^{(s)}} Q_{e}^{(s)}(X \otimes \mathbb{1}_{S}) \Omega_{S,\beta}$$

$$= e^{it(L_{S} + \lambda^{2}\Lambda)} (X \otimes \mathbb{1}_{S}) \Omega_{S,\beta} + O\left(\lambda^{4} t e^{-\lambda^{2} t (\gamma_{FGR} + O(\lambda^{2}))}\right), \quad (3.7)$$

where the 'total' level shift operator is defined to be

$$\Lambda = \bigoplus_{e \in \operatorname{spec}(L_{S})} \Lambda_{e}, \tag{3.8}$$

with  $\Lambda_e$  given in (2.32). We now define the group  $\delta_{\lambda}^t$ , acting on system observables, by

$$\left(\delta_{\lambda}^{t}(X) \otimes \mathbb{1}_{S}\right) \Omega_{S,\beta} = e^{it(L_{S} + \lambda^{2}\Lambda)} (X \otimes \mathbb{1}_{S}) \Omega_{S,\beta}. \tag{3.9}$$

Combining (3.5) and (3.7) we get, for  $\gamma_{FGR} > 0$ ,

$$\omega_0(\alpha_\lambda^t(X \otimes \mathbf{1}_R)) = \omega_0(\delta_\lambda^t(X) \otimes \mathbb{1}_R) + O(\lambda^2). \tag{3.10}$$

 $<sup>\</sup>overline{ ^{10}\text{We have } \mathrm{e}^{\mathrm{i}t\epsilon(\lambda)} = \mathrm{e}^{\mathrm{i}t(e+\lambda^2a+O(\lambda^4))} } = \mathrm{e}^{\mathrm{i}t(e+\lambda^2a)} + \mathrm{e}^{\mathrm{i}t(e+\lambda^2a)} [\mathrm{e}^{\mathrm{i}tO(\lambda^4)} - 1] \text{ and } |\mathrm{e}^{\mathrm{i}tO(\lambda^4)} - 1| = |\mathrm{i}O(\lambda^4) \int_0^t e^{\mathrm{i}sO(\lambda^4)} ds| \leq C\lambda^4 t e^{t\lambda^4c}, \text{ for some } C, c > 0 \text{ independent of } \lambda, t.$ 

By duality, we have  $\operatorname{tr}_{S}(\rho \, \delta_{\lambda}^{t}(X)) = \operatorname{tr}_{S}((e^{t\mathcal{G}}\rho)X)$  for all system density matrices  $\rho$  and all system observables X. We have  $e^{\operatorname{i}tL_{S}}(X \otimes \mathbb{1}_{S})\Omega_{S,\beta} = (e^{\operatorname{i}tH_{S}}X e^{-\operatorname{i}tH_{S}} \otimes \mathbb{1}_{S})\Omega_{S,\beta}$ , which follows simply from  $e^{-\operatorname{i}tL_{S}}\Omega_{S,\beta} = \Omega_{S,\beta}$ . This gives a contribution  $-\operatorname{i}[H_{S},\cdot]$  to the generator  $\mathcal{G}$ . For nonzero  $\lambda$ , we then get  $\mathcal{G}\rho = -\operatorname{i}[H_{S},\rho] + \lambda^{2}K\rho$ , with K satisfying (1.27), see also Appendix A.

Since  $(L_S + \lambda^2 \Lambda)\Omega_{S,\beta} = 0$  we have  $\delta_{\lambda}^t(\mathbb{1}_S) = \mathbb{1}_S$ . It remains to prove that  $\delta_{\lambda}^t$  is completely positive.

#### 3.1.1 Proof that $\delta_{\lambda}^{t}$ is CP

It follows from (3.10) that

$$\lim_{\lambda \to 0} \omega_0 \left( \alpha_{\lambda}^{t/\lambda^2} \circ \alpha_0^{-t/\lambda^2} (X \otimes \mathbf{1}_{R}) \right) = \omega_0 \left( \sigma^t(X) \otimes \mathbb{1}_{R} \right), \tag{3.11}$$

where  $\sigma^t$  is defined by

$$(\sigma^{t}(X) \otimes \mathbb{1}_{S})\Omega_{S,\beta} = e^{it\Lambda}(X \otimes \mathbb{1}_{S})\Omega_{S,\beta}.$$
(3.12)

Since limits of CP maps are CP, we know from (3.11) that  $\sigma^t$  is CP. Next,  $\delta^t_{\lambda}$  is the composition of two CP maps,

$$\delta_{\lambda}^{t} = \left( e^{itH_{S}} \cdot e^{-itH_{S}} \right) \circ \sigma^{\lambda^{2}t},$$

and hence it is CP itself. This shows (1.24).

### **3.2** Proof of (1.29)

#### 3.2.1 The renormalized quantities

The reduced system equilibrium density matrix  $\rho_{S,\beta,\lambda}$  is defined by the relation

$$\operatorname{tr}(\rho_{S,\beta,\lambda}X) = \omega_{SR,\beta,\lambda}(X \otimes \mathbb{1}_R), \qquad \forall X \tag{3.13}$$

where  $\omega_{SR,\beta,\lambda}$  is the coupled system-reservoir equilibrium state whose purification is (2.10). We introduce the renormalized system Hamiltonian  $\widetilde{H}_S(\lambda)$  by the relation (1.28). This defines  $\widetilde{H}_S(\lambda)$  only up to an additive term  $\propto \mathbb{1}_S$ . Of course, we would like the property  $\widetilde{H}_S(0) = H_S$ , which will determine this additive term. Without loss of generality, we suppose that min spec $H_S = 0$  (the smallest eigenvalue of  $H_S$  is normalized to be at the origin). Let  $\widetilde{E}_0(\lambda)$  be the smallest eigenvalue of  $\widetilde{H}_S(\lambda)$ . We have from (1.28) that  $\operatorname{tr}(e^{-\beta \widetilde{H}_S(\lambda)}) \|\rho_{S,\beta,\lambda}\| = e^{-\beta \widetilde{E}_0(\lambda)}$ , where  $\|\rho_{S,\beta,\lambda}\|$  is the operator norm of the density matrix. Then we impose the normalization  $\widetilde{E}_0(\lambda) = 0$ , which amounts to  $\operatorname{tr}(e^{-\beta \widetilde{H}_S(\lambda)}) = 1/\|\rho_{S,\beta,\lambda}\|$  and so we define

$$\widetilde{H}_{S}(\lambda) = -\frac{1}{\beta} \ln \frac{\rho_{S,\beta,\lambda}}{\|\rho_{S,\beta,\lambda}\|}.$$
 (3.14)

By simple perturbation theory we have  $\rho_{S,\beta,\lambda} = \rho_{S,\beta,0} + O(\lambda^2)$ . It follows from (3.14) that

$$\widetilde{H}_{S}(\lambda) = H_{S} + O(\lambda^{2}),$$
(3.15)

where  $H_{\rm S}$  is the original, uncoupled system Hamiltonian (1.2). The spectral representation of the renormalized Hamiltonian is

$$\widetilde{H}_{S}(\lambda) = \sum_{j=1}^{N} \widetilde{E}_{j} |\widetilde{\phi}_{j}\rangle\langle\widetilde{\phi}_{j}|, \qquad (3.16)$$

where  $\widetilde{E}_j$  and  $\widetilde{\phi}_j$  depend on  $\lambda$  and satisfy

$$|E_j - \widetilde{E}_j(\lambda)| = O(\lambda^2), \qquad \|\phi_j - \widetilde{\phi}_j(\lambda)\| = O(\lambda^2).$$
 (3.17)

In analogy with (2.13) we introduce the Liouvillians

$$\widetilde{L}_{0} = \widetilde{L}_{S} + L_{R} 
\widetilde{L}_{S} = \widetilde{H}_{S} \otimes \mathbb{1}_{S} - \mathbb{1}_{S} \otimes \mathcal{C}\widetilde{H}_{S} \mathcal{C} 
L_{R} = H_{R} \otimes \mathbb{1}_{R} - \mathbb{1}_{R} \otimes H_{R}$$
(3.18)

where C is the operator taking complex conjugation of coordinates in the basis of eigenvectors  $\{\phi_j\}$  of  $H_S$ . A purification of  $\rho_{S,\beta,\lambda}$  is given by the vector  $(\widetilde{Z}$  is a normalization constant)

$$\widetilde{\Omega}_{S,\beta,\lambda} = \widetilde{Z}^{-1/2} \sum_{j=1}^{N} e^{-\beta \widetilde{E}_j/2} \widetilde{\phi}_j \otimes C\widetilde{\phi}_j.$$
 (3.19)

Namely, for any system observable X, we have

$$\operatorname{tr}_{\mathbf{S}}(\rho_{\mathbf{S},\beta,\lambda}X) = \langle \widetilde{\Omega}_{\mathbf{S},\beta,\lambda}, (X \otimes \mathbb{1}_{\mathbf{S}})\widetilde{\Omega}_{\mathbf{S},\beta,\lambda} \rangle. \tag{3.20}$$

We also define

$$\widetilde{\Omega}_0 = \widetilde{\Omega}_{S,\beta,\lambda} \otimes \Omega_R,$$
(3.21)

where  $\Omega_{\rm R}$  is the vacuum (2.4). It is clear from the definitions (3.18), (3.19) and (3.21) that

$$\widetilde{L}_{S}\widetilde{\Omega}_{S,\beta,\lambda} = 0$$
 and  $\widetilde{L}_{0}\widetilde{\Omega}_{0} = 0.$  (3.22)

Given an eigenvalue  $\tilde{e}$  of  $\tilde{L}_0$  (the eigenvalues of  $\tilde{L}_0$  and of  $\tilde{L}_S$  are the same), we denote by  $\tilde{P}_{\tilde{e}}$  the associated spectral projection and we define the level shift operators (compare with (2.26), (3.8))

$$\widetilde{\Lambda}_{\widetilde{e}} = -\widetilde{P}_{\widetilde{e}} I \widetilde{P}_{\widetilde{e}}^{\perp} (\widetilde{L}_0 - \widetilde{e} + i0)^{-1} I \widetilde{P}_{\widetilde{e}}, \quad \widetilde{\Lambda} = \bigoplus_{\widetilde{e} \in \text{spec}(\widetilde{L}_S)} \Lambda_{\widetilde{e}}.$$
(3.23)

<sup>&</sup>lt;sup>11</sup>The correction linear in  $\lambda$  vanishes, since in our models, the interaction is linear in the field (c.f. (1.1)) and  $\langle \Omega_{\rm R}, \varphi_{\beta}(g)\Omega_{\rm R} \rangle = 0$ .

A perturbation theory argument based on (3.15) shows that  $\widetilde{\Lambda}_{\tilde{e}} - \Lambda_e = O(\lambda^2)$ . Assuming that the  $\Lambda_e$  have the expansion (2.32) (where all  $a_e^{(s)}$  are distinct, for simplicity), the operator  $\widetilde{\Lambda}_{\tilde{e}}$  has a similar expansion,

$$\widetilde{\Lambda}_{\widetilde{e}} = \sum_{s=1}^{m_e} \widetilde{a}_{\widetilde{e}}^{(s)} \widetilde{Q}_{\widetilde{e}}^{(s)}, \tag{3.24}$$

where  $\widetilde{a}^{(s)}_{\widetilde{e}}$  and  $\widetilde{Q}^{(s)}_{\widetilde{e}}$  are the eigenvalues and rank-one eigenprojections, satisfying

$$a_e^{(s)} = \tilde{a}_{\tilde{e}}^{(s)} + O(\lambda^2), \qquad \tilde{Q}_{\tilde{e}}^{(s)} = Q_e^{(s)} + O(\lambda^2).$$
 (3.25)

One also shows that (compare with (2.34), and see [18], Proposition 3.2)

$$\widetilde{\Lambda}_0 \widetilde{\Omega}_0 = 0$$
, i.e.,  $\widetilde{a}_0^{(1)} = 0$ ,  $\widetilde{Q}_0^{(1)} = |\widetilde{\Omega}_0\rangle\langle\widetilde{\Omega}_0|$ . (3.26)

#### 3.2.2 The resonance expansion

The vector  $\widetilde{\Omega}_0$  is cyclic and separating and furthermore, one can find an operator D', which commutes with all system-reservoir observables  $^{12}$ , and which satisfies

$$\widetilde{\Omega}_0 = D'\Omega_{SR,\beta,\lambda}, \qquad D' = \mathbb{1} + O(\lambda).$$
 (3.27)

(The existence of a bounded D' belonging to the commutant of the operator algebra, and which satisfies (3.27) to arbitrary precision, is guaranteed by the separating property of  $\Omega_{SR,\beta,\lambda}$ . However, (3.27) is an equality, not an approximation. The equality can be obtained due to the special form of the vectors involved, see [18].) We take initial conditions of the form

$$\Psi_0 = B'\widetilde{\Omega}_0 = B'D'\Omega_{SR,\beta,\lambda},\tag{3.28}$$

where B' belongs to the commutant (as before) and where the second equality follows from (3.27). Varying over B', the vectors  $\Psi_0$  form a dense set. We repeat the argument in (2.20),

$$\omega_0 \left( \alpha_{\lambda}^t (X \otimes \mathbb{1}_{\mathbb{R}}) \right) = \left\langle \Psi_0, e^{itL_{\lambda}} (X \otimes \mathbb{1}_{\mathbb{S}} \otimes \mathbb{1}_{\mathbb{R}}) e^{-itL_{\lambda}} \Psi_0 \right\rangle$$
$$= \left\langle \Psi_0, B'D' e^{itL_{\lambda}} (X \otimes \mathbb{1}_{\mathbb{S}} \otimes \mathbb{1}_{\mathbb{R}}) \Omega_{\operatorname{SR},\beta,\lambda} \right\rangle. \tag{3.29}$$

Then we perform again the spectral deformation, (2.23) and deform the contour of integration, to arrive at (compare with (2.29))

$$\omega_{0}\left(\alpha_{\lambda}^{t}(X \otimes \mathbf{1}_{R})\right) = \sum_{e \in \operatorname{spec}(L_{S})} \sum_{s=1}^{m_{e}} e^{it\epsilon_{e}^{(s)}} \left\langle \left[ (D'B')^{*}\Psi_{0} \right]_{\bar{\theta}}, \Pi_{e}^{(s)} \left( X \otimes \mathbf{1}_{S} \otimes \mathbf{1}_{R} \right) \left[ \Omega_{SR,\beta,\lambda} \right]_{\theta} \right\rangle + O\left(\lambda e^{-\frac{3}{4}\theta_{0}t}\right). \tag{3.30}$$

 $<sup>^{12}</sup>$ Some care has to be taken here as D' is not a bounded operator, but the technicalities of this difficulty are not too severe to overcome, see Lemma 3.4 of [18].

The term e = 0, s = 1 is (see (2.30))

$$\langle [(D'B')^*\Psi_0]_{\bar{\theta}}, [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle \langle [\Omega_{SR,\beta,\lambda}]_{\bar{\theta}}, (X \otimes \mathbf{1}_S \otimes \mathbf{1}_R) [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle$$

$$= \operatorname{tr}_S(\rho_{S,\beta,\lambda}X)$$

$$= \langle \widetilde{\Omega}_0, (X \otimes \mathbb{1}_S \otimes \mathbb{1}_R) \widetilde{\Omega}_0 \rangle$$

$$= \langle (B')^*\Psi_0, |\widetilde{\Omega}_0 \rangle \langle \widetilde{\Omega}_0 | (X \otimes \mathbb{1}_S \otimes \mathbb{1}_R) \widetilde{\Omega}_0 \rangle. \tag{3.31}$$

We use here that  $\langle [(D'B')^*\Psi_0]_{\bar{\theta}}, [\Omega_{SR,\beta,\lambda}]_{\theta} \rangle = 1$  and  $\langle (B')^*\Psi_0, \widetilde{\Omega}_0 \rangle = 1$ . In the other terms,  $(e,s) \neq (0,1)$ , in the sum in (3.30), we replace D' by 1 (see (3.27)), use the approximation (2.35) and retain only the part  $e + \lambda^2 a_e^{(s)}$  in the resonance energies (see (3.6)). Then (3.30) and (3.31) give

$$\omega_{0}\left(\alpha_{\lambda}^{t}(X \otimes \mathbf{1}_{R})\right) = \left\langle (B')^{*}\Psi_{0}, |\widetilde{\Omega}_{0}\rangle\langle\widetilde{\Omega}_{0}|\left(X \otimes \mathbf{1}_{S} \otimes \mathbf{1}_{R}\right)\widetilde{\Omega}_{0}\right\rangle$$

$$+ \sum_{(e,s)\neq(0,1)} e^{it(e+\lambda^{2}a_{e}^{(s)})} \left\langle (B')^{*}\Psi_{0}, Q_{e}^{(s)}\left(X \otimes \mathbf{1}_{S} \otimes \mathbf{1}_{R}\right)\Omega_{SR,\beta,\lambda}\right\rangle$$

$$+O\left((\lambda+\lambda^{4}t) e^{-\lambda^{2}t(\gamma_{FGR}+O(\lambda^{2}))}\right)$$

$$+O\left(\lambda e^{-\frac{3}{4}\theta_{0}t}\right).$$

$$(3.32)$$

Next, since  $e + \lambda^2 a_e^{(s)} = \widetilde{e} + \lambda^2 \widetilde{a}_{\widetilde{e}}^{(s)} + O(\lambda^2)$  and  $Q_e^{(s)} = \widetilde{Q}_{\widetilde{e}}^{(s)} + O(\lambda^2)$  (see (3.25)), we replace in (3.32)  $e + \lambda^2 a_e^{(s)}$  and  $Q_e^{(s)}$  by  $\widetilde{e} + \lambda^2 \widetilde{a}_{\widetilde{e}}^{(s)}$  and  $\widetilde{Q}_{\widetilde{e}}^{(s)}$ , incurring an error  $O((\lambda + \lambda^2 t) e^{-\lambda^2 t \gamma_{\text{FGR}}})$  (proceed similarly as in (3.6)). But now,

$$\sum_{(\tilde{e},s)\neq(0,1)} e^{it(\tilde{e}+\lambda^2 \tilde{a}_{\tilde{e}}^{(s)})} \widetilde{Q}_{\tilde{e}}^{(s)} = e^{it(\tilde{L}_S + \lambda^2 \tilde{\Lambda})} P(\tilde{\Lambda} \neq 0)$$
(3.33)

and  $P(\widetilde{\Lambda}=0)=|\widetilde{\Omega}_0\rangle\langle\widetilde{\Omega}_0|$ , where  $P(\widetilde{\Lambda}\neq0)$  and  $P(\widetilde{\Lambda}=0)$  are spectral (Riesz) projections. (See also (3.23) and (3.26).) Therefore, the two main terms on the right side of (3.32) yield the operator  $e^{it(\widetilde{L}_S+\lambda^2\widetilde{\Lambda})}$ , namely,

$$\omega_{0}\left(\alpha_{\lambda}^{t}(X \otimes \mathbf{1}_{R})\right) = \left\langle (B')^{*}\Psi_{0}, e^{it(\widetilde{L}_{S} + \lambda^{2}\widetilde{\Lambda})}\left(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R}\right)\widetilde{\Omega}_{0} \right\rangle + O\left(\left(\lambda + \lambda^{2}t\right)e^{-\lambda^{2}t(\gamma_{FGR} + O(\lambda^{2}))}\right). \tag{3.34}$$

By cyclicity of  $\widetilde{\Omega}_{S,\beta,\lambda}$ , the relation

$$e^{it(\widetilde{L}_{S} + \lambda^{2}\widetilde{\Lambda})} (X \otimes \mathbb{1}_{S}) \widetilde{\Omega}_{S,\beta,\lambda} = (\tau_{\lambda}^{t}(X) \otimes \mathbb{1}_{S}) \widetilde{\Omega}_{S,\beta,\lambda}$$
(3.35)

defines uniquely a group (in t),  $\tau_{\lambda}^{t}$ , acting on system observables. Using (3.35) and commuting B' through the observable and using  $B'\widetilde{\Omega}_{0} = \Psi_{0}$ , we obtain for the first term on

the right side of (3.34) simply the expression  $\langle \Psi_0, (\tau_{\lambda}^t(X) \otimes \mathbb{1}_S \otimes \mathbb{1}_R) \Psi_0 \rangle = \omega_0(\tau_{\lambda}^t(X) \otimes \mathbb{1}_R)$ . So (3.34) yields

$$\omega_0\left(\alpha_\lambda^t(X\otimes \mathbf{1}_R)\right) = \omega_0\left(\tau_\lambda^t(X)\otimes \mathbb{1}_R\right) + O\left(\left(\lambda + \lambda^2 t\right) e^{-\lambda^2 t(\gamma_{FGR} + O(\lambda^2))}\right). \tag{3.36}$$

For initial states  $\omega_0 = \omega_S \otimes \omega_{R,\beta}$ , where  $\omega_S$  is given by a density matrix  $\rho$  and  $\omega_{R,\beta}$  is the reservoir equilibrium (or a local perturbation thereof), we get

$$\omega_0\left(\alpha_\lambda^t(X\otimes \mathbf{1}_R)\right) = \operatorname{tr}_S\left(\rho\tau_\lambda^t(X)\right) + O\left(\left(\lambda + \lambda^2 t\right) e^{-\lambda^2 t(\gamma_{FGR} + O(\lambda^2))}\right). \tag{3.37}$$

By duality, we define uniquely  $M(\lambda)$ , an operator acting on system density matrices, by

$$\operatorname{tr}_{S}(\rho \tau_{\lambda}^{t}(X)) = \operatorname{tr}((e^{tM(\lambda)}\rho)X), \tag{3.38}$$

and (1.29) follows from (3.37), (3.38).

That  $\tau_{\lambda}^{t}(\mathbb{1}_{S}) = \mathbb{1}_{S}$  is clear from the definition (3.35), as  $(\widetilde{L}_{S} + \lambda^{2}\widetilde{\Lambda})\widetilde{\Omega}_{S,\beta,\lambda} = 0$ . We show below in Section 3.2.3 that for  $\lambda, t$  fixed,  $\tau_{\lambda}^{t}$  is a CP map.

Evolution of observables X commuting with  $H_S$ . We treat the general term in the sum of (3.32) as follows,

$$e^{ite}Q_{e}^{(s)}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,\lambda} = Q_{e}^{(s)} e^{itL_{S}}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,\lambda} 
= Q_{e}^{(s)} e^{itL_{S}}(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,0} + O(\lambda) 
= Q_{e}^{(s)}(X_{t} \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,0} + O(\lambda) 
= Q_{e}^{(s)}(X_{t} \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R})\Omega_{SR,\beta,\lambda} + O(\lambda).$$
(3.39)

Here, we have set

$$X_t \equiv e^{itH_S} X e^{-itH_S}. \tag{3.40}$$

The first equality in (3.39) is due to (2.33). The third one comes from  $e^{-itL_S}\Omega_{SR,\beta,0} = \Omega_{SR,\beta,0}$  and the remaining ones follow from  $\Omega_{SR,\beta,\lambda} - \Omega_{SR,\beta,0} = O(\lambda)$ . We now use (3.39) in the sum over  $(e,s) \neq (0,1)$  in (3.32) and arrive at

$$\omega_{0}\left(\alpha_{\lambda}^{t}(X \otimes \mathbf{1}_{R})\right) = \left\langle (B')^{*}\Psi_{0}, |\widetilde{\Omega}_{0}\rangle\langle\widetilde{\Omega}_{0}|\left(X \otimes \mathbb{1}_{S} \otimes \mathbb{1}_{R}\right)\widetilde{\Omega}_{0}\right\rangle + \sum_{(e,s)\neq(0,1)} e^{\mathrm{i}t\lambda^{2}a_{e}^{(s)}}\left\langle (B')^{*}\Psi_{0}, Q_{e}^{(s)}\left(X_{t} \otimes \mathbf{1}_{S} \otimes \mathbf{1}_{R}\right)\Omega_{\mathrm{SR},\beta,\lambda}\right\rangle + O\left((\lambda + \lambda^{4}t) e^{-\lambda^{2}t(\gamma_{\mathrm{FGR}} + O(\lambda^{2}))}\right) + O\left(\lambda e^{-\frac{3}{4}\theta_{0}t}\right).$$
(3.41)

For the invariant observables in question, we have  $X_t = X$  for all t. We replace in the last sum  $e^{it\lambda^2 a_e^{(s)}}$  by  $e^{it\lambda^2 \tilde{a}_{\tilde{e}}^{(s)}}$ , thus incurring an error of  $O(\lambda^4 t \, e^{-\lambda^2 t (\gamma_{FGR} + O(\lambda^2))})$ . Now we define the group  $\tau_{d,\lambda}^t$ , acting on system observables, by

$$e^{it\lambda^{2}\widetilde{\Lambda}}(X\otimes \mathbb{1}_{S})\widetilde{\Omega}_{S,\beta,\lambda} = (\tau_{d,\lambda}^{t}(X)\otimes \mathbb{1}_{S})\widetilde{\Omega}_{S,\beta,\lambda}. \tag{3.42}$$

Combining (3.42) with (3.41) then yields, for all X s.t.  $[X, H_S] = 0$ ,

$$\omega_0\left(\alpha_{\lambda}^t(X\otimes \mathbf{1}_{\mathrm{R}})\right) = \omega_0\left(\tau_{\mathrm{d},\lambda}^t(X)\otimes \mathbb{1}_{\mathrm{R}}\right) + O\left(\left(\lambda + \lambda^4 t\right) e^{-\lambda^2 t(\gamma_{\mathrm{FGR}} + O(\lambda^2))}\right). \tag{3.43}$$

It is clear from (3.42) and (3.26) that  $\tau_{d,\lambda}^t(\mathbb{1}_S) = \mathbb{1}_S$ . We show below in Section 3.2.3 that  $\tau_{d,\lambda}^t$  is completely positive. Again by duality, and for an initial condition  $\omega_0 = \operatorname{tr}_S(\rho \cdot) \otimes \omega_{R,\beta}$ , equation (3.43) becomes

$$\operatorname{tr}_{S}(V_{t}\rho)X = \operatorname{tr}_{S}(e^{t\lambda^{2}M_{d}(\lambda)}\rho)X + O\left((\lambda + \lambda^{4}t)e^{-\lambda^{2}t(\gamma_{FGR} + O(\lambda^{2}))}\right), \tag{3.44}$$

valid  $\forall X$  s.t.  $[X, H_S] = 0$ . Taking  $X = |\varphi_k\rangle\langle\varphi_k|$  we obtain equation (1.32).

#### 3.2.3 Proof that $\tau_{\lambda}^{t}$ and $\tau_{\mathrm{d},\lambda}^{t}$ are CP

The idea is to view  $\tau_{\lambda}^{t}$  as a weak coupling dynamics and proceed as in Subsection 3.1.1. To do this, introduce the Liouvillian

$$\widetilde{L}_{\mu} = \widetilde{L}_0 + \mu \lambda I, \tag{3.45}$$

where  $\widetilde{L}_0$  is given in (3.18) and the interaction I is (2.15). Here we consider  $\mu \in \mathbb{R}$  as the interaction constant, and  $\lambda$  is viewed as part of the interaction operator. (Recall that  $\widetilde{L}_0$  also depends on  $\lambda$ .) The eigenvalues of the unperturbed  $\widetilde{L}_{\mu}|_{\mu=0}$  are the same as those of  $\widetilde{L}_0$  and the levels shift operators associated to (3.45) are given by (3.23) with I replaced by  $\lambda I$  (they give the quadratic corrections in  $\mu$  to the spectrum). In other words,  $\lambda^2 \widetilde{\Lambda}$ , with  $\widetilde{\Lambda}$  given in (3.23), is the (complete) level shift operator of  $\widetilde{L}_{\mu}$ . We define the dynamics  $\widetilde{\gamma}_{\mu}^t$  by

$$\omega_0(\widetilde{\gamma}_{\mu}^t(X\otimes\mathcal{P})) = \left\langle \Psi_0, \, e^{it\widetilde{L}_{\mu}}(X\otimes\mathbb{1}_S\otimes\mathcal{P}_{\beta}) \, e^{-it\widetilde{L}_{\mu}}\Psi_0 \right\rangle. \tag{3.46}$$

In (3.46), X and  $\mathcal{P}$  are system and reservoir observables, with  $\mathcal{P}_{\beta}$  being the representation in the purification space, see also (2.3). The equilibrium (KMS) state associated to  $\widetilde{L}_{\mu}$  is given by (compare with (2.10))

$$\widetilde{\Omega}_{SR,\beta,\mu} = \frac{e^{-\frac{\beta}{2}(\widetilde{L}_0 + \mu\lambda G \otimes \mathbb{1}_S \otimes \varphi_{\beta}(g))} \Omega_{SR,\beta,0}}{\|e^{-\frac{\beta}{2}(\widetilde{L}_0 + \mu\lambda G \otimes \mathbb{1}_S \otimes \varphi_{\beta}(g))} \Omega_{SR,\beta,0}\|}$$
(3.47)

(and depends on  $\lambda$  as well). This is a cyclic and separating vector and the initial condition can be written as  $\Psi_0 = B'D'\widetilde{\Omega}_{\mathrm{SR},\beta,\mu}$  (c.f. (3.28)). We then obtain (c.f. (3.29))

$$\omega_0(\widetilde{\gamma}_{\lambda}^t(X\otimes \mathbb{1}_{\mathbf{R}})) = \left\langle \Psi_0, B'D' e^{\mathrm{i}t\widetilde{L}_{\mu}}(X\otimes \mathbb{1}_{\mathbf{S}}\otimes \mathbb{1}_{\mathbf{R}})\widetilde{\Omega}_{\mathrm{SR},\beta,\mu} \right\rangle$$
(3.48)

(with B', D' depending on both  $\lambda$  and  $\mu$ ). Proceeding to perform the spectral deformation and resonance expansion in the same manner as we did in Sections 2.4 –3.1, we obtain (analogous to (3.5)),

$$\omega_0(\widetilde{\gamma}_{\mu}^{t/\mu^2}(X \otimes \mathbf{1}_{\mathbf{R}})) = \left\langle (B')^* \Psi_0, \, e^{it(\widetilde{L}_0 + \mu^2 \lambda^2 \widetilde{\Lambda})} (X \otimes \mathbb{1}_{\mathbf{S}} \otimes \mathbb{1}_{\mathbf{R}}) \widetilde{\Omega}_0 \right\rangle + O(\mu^2), \tag{3.49}$$

with a remainder term uniform in t. It follows that

$$\lim_{\mu \to 0} \omega_0 \left( \widetilde{\gamma}_{\mu}^{t/\mu^2} \circ \widetilde{\gamma}_0^{-t/\mu^2} (X \otimes \mathbf{1}_{\mathrm{R}}) \right) = \left\langle (B')^* \Psi_0, \, \mathrm{e}^{\mathrm{i}t\lambda^2 \widetilde{\Lambda}} \left( X \otimes \mathbb{1}_{\mathrm{S}} \otimes \mathbb{1}_{\mathrm{R}} \right) \widetilde{\Omega}_0 \right\rangle$$
$$= \omega_0 \left( \left( \tau_{\mathrm{d},\lambda}^t (X) \otimes \mathbb{1}_{\mathrm{R}} \right) \right). \tag{3.50}$$

Consequently,  $\tau_{\mathrm{d},\lambda}^t$  is CP. Since  $\tau_{\lambda}^t = \tau_{\mathrm{d},\lambda}^t \circ (\mathrm{e}^{\mathrm{i}t\widetilde{H}_\mathrm{S}} \cdot \mathrm{e}^{-\mathrm{i}t\widetilde{H}_\mathrm{S}})$  it follows that  $\tau_{\lambda}^t$  is CP as well.

Acknowledgements. The author thanks Martin Könenberg for his collaborations on which the present work builds, and for carefully proofreading the current manuscript, and Roberto Floreanini for valuable comments. The author was supported by the Simons Foundation and the Centre de Recherches Mathématiques, through the Simons-CRM scholar-in-residence program, as well as by an NSERC Discovery Grant and an NSERC Discovery Accelerator Supplement grant.

## A Explicit form of the generator K

We define the generator  $\mathcal{G}$  acting on system density matrices by

$$\operatorname{tr}_{S}(\rho \, \delta_{\lambda}^{t}(X)) = \operatorname{tr}_{S}((e^{t\mathcal{G}}\rho) \, X), \tag{A.1}$$

valid for all system observables and density matrices X and  $\rho$ . Here,  $\delta_{\lambda}^{t}$  is given in (3.9). We show that

$$G\rho = -i[H_S, \rho] + \lambda^2 K\rho, \tag{A.2}$$

where  $[\cdot,\cdot]$  is the commutator and (denoting by  $\{\cdot,\cdot\}$  the anti-commutator)

$$K\rho = \hat{h}(0) \sum_{k,\ell=1}^{N} \left( P_{k}GP_{k}\rho P_{\ell}GP_{\ell} - \frac{1}{2} \left\{ P_{\ell}GP_{\ell} P_{k}GP_{k}, \rho \right\} \right) + \sum_{k,\ell:k\neq\ell} \hat{h}(E_{k} - E_{\ell}) \left( P_{\ell}GP_{k}\rho P_{k}GP_{\ell} - \frac{1}{2} \left\{ P_{k}GP_{\ell}GP_{k}, \rho \right\} \right) - \mathrm{i} \left[ H_{\mathrm{LS}}, \rho \right]$$
(A.3)

and

$$H_{\rm LS} = \frac{1}{\pi} \sum_{k,\ell=1}^{N} \left( \text{P.V.} \int_{\mathbb{R}} \frac{\widehat{h}(u)}{E_k - E_\ell - u} \ du \right) P_k G P_\ell G P_k. \tag{A.4}$$

Here, h(u) is the Fourier transform of the correlation function,

$$\widehat{h}(u) = \int_{\mathbb{R}} e^{-itu} \,\omega_{R,\beta} \big( \varphi(g) \varphi(g_t) \big) dt, \qquad u \in \mathbb{R}$$
(A.5)

where g(k) is the form factor and  $g_t(k) = e^{i\omega(k)t}g(k)$ . We have the expression  $(u \in \mathbb{R}, \omega \geq 0)$ 

$$\widehat{h}(u) = J(|u|) \left| \frac{e^{\beta u}}{e^{\beta u} - 1} \right|, \ J(\omega) = \frac{\pi}{2} \omega^2 \int_{S^2} |g(\omega, \Sigma)|^2 d\Sigma$$

(spherical coordinates). J is called the reservoir spectral density and  $\hat{h}(0)$  is understood as the limit  $u \to 0$  of  $\hat{h}(u)$ , (A.5). The first two terms in (A.3) constitute the 'dissipator' and the commutator is with the 'Lamb shift' Hamiltonian  $H_{LS}$ , representing a correction to the system energies. K is the usual 'Davies generator' [1, 7, 8]. It is manifestly CPT due to the results [14, 20].

In order to show (A.2)-(A.4) we first calculate  $\mathcal{G}_*$ , defined by  $e^{t\mathcal{G}_*}X = \delta_{\lambda}^t(X)$ , i.e.,

$$((\mathcal{G}_*X) \otimes \mathbf{1}_S)\Omega_{S,\beta} = i(L_S + \lambda^2 \Lambda)(X \otimes \mathbf{1}_S)\Omega_{S,\beta}. \tag{A.6}$$

The definitions of  $L_{\rm S}$  and  $\Lambda$  are (2.13) and (3.8), (2.26) and the system Gibbs state  $\Omega_{{\rm S},\beta}$  is defined in (2.9). For any system operators X,Y and Z we have

$$(Y \otimes \mathbb{1}_{S}) J(Z \otimes \mathbb{1}_{S}) J(X \otimes \mathbb{1}_{S}) \Omega_{S,\beta} = ((YXe^{-\beta H_{S}/2}Z^{*}e^{\beta H_{S}/2}) \otimes \mathbb{1}_{S})\Omega_{S,\beta}.$$
(A.7)

Formula (A.7) is readily verified.<sup>13</sup> It is then clear that  $iL_S(X \otimes \mathbf{1}_S)\Omega_{S,\beta} = (i[H_S, X] \otimes \mathbf{1}_R)\Omega_{S,\beta}$ . This gives a contribution  $-i[H_S, \cdot]$  to  $\mathcal{G}$ . To calculate the contribution coming from  $i\lambda^2\Lambda$ , we consider the situation where all nonzero eigenvalue differences  $e = E_k - E_\ell$  are simple (the general case is done in the same way). Then the projections in (2.26) are rank one for  $e \neq 0$ ,  $P_e = P_k \otimes P_\ell \otimes |\Omega_R\rangle\langle\Omega_R|$ , where  $P_k = |\phi_k\rangle\langle\phi_k|$  (see (1.2)). The projection onto the eigenvalue e = 0 of  $L_S$  has dimension N,  $P_{e=0} = \sum_{j=1}^N P_j \otimes P_j \otimes |\Omega_R\rangle\langle\Omega_R|$ . By expanding  $\Lambda_e$ , (2.26), using the form (2.15) of the interaction I we arrive at the expressions (A.3), (A.4).

## References

- [1] R. Alicki, K. Lendi: Quantum Dynamical Semigroups and Applications, Lect. Notes Phys. 717, Springer Verlag 2007
- [2] R. Alicki: The Markov Master Equations and the Fermi Golden Rule, International Journal of Theoretical Physics, 16, No.5, 351-355 (1977)
- [3] H. Araki, E.J. Woods: Representation of the canonical commutation relations describing a nonrelativistic infinite free bose gas, J. Math. Phys. 4, 637-662 (1963)
- [4] V. Bach, J. Fröhlich, I.M. Sigal: Return to equilibrium, J. Math. Phys. 41, 3985-4060 (2000)

<sup>&</sup>lt;sup>13</sup>Use that  $J(Z \otimes \mathbb{1}_S)J$  commutes with  $X \otimes \mathbb{1}_S$  and  $J\Omega_{S,\beta} = \Omega_{S,\beta}$  and  $J(Z \otimes \mathbb{1}_S)\Omega_{S,\beta} = e^{-\beta H_S/2}(Z \otimes \mathbb{1}_S)\Omega_{S,\beta}$ .

- [5] F. Benatti, R. Floreanini: Open Quantum Dynamics: Complete Positivity and Entanglement, Int. J. Mod. Phys. **B19** 3063 (2005)
- [6] F. Benatti, M. Fannes, R. Floreanini, D. Petritis (Eds): Quantum Information, Computation and Cryptography, Springer Lecture Notes in Physics 808, 2010
- [7] H.-P. Breuer, F. Petruccione: The theory of open quantum systems, Oxford University Press 2002
- [8] D. Chruściński, S. Pascazio: A Brief History of the GKLS Equation, Open Systems & Information Dynamics, Vol. 24, No. 03, 1740001 (2017)
- [9] E.B. Davies: Markovian Master Equations, Commun. Math. Phys. 39, 9-110 (1974)
- [10] E.B. Davies: Markovian Master Equations, II, Math. Ann. **219**, 147-158 (1976)
- [11] R. Dümke, H. Spohn: The Proper Form of the Generator in the Weak Coupling Limit, Z. Physik B, **34**, 419-422 (1979)
- [12] P. Facchi, S. Pascazio: Deviations from exponential law and Van Hove's  $\lambda^2 t$  limit, Physica A **271** 133-146 (1999)
- [13] P. Facchi, M. Ligabò, K. Yuasa: On the Derivation of the GKLS Equation for Weakly Coupled Systems, Open Systems & Information Dynamics 24, No.4
- [14] V. Gorini, A. Kossakowski, E.C.G. Sudarshan: Completely positive dynamical semigroups of N-level systems, J. Math. Phys. 17, 821 (1976)
- [15] S. Haroche, J.-M. Raimond: Exploring the Quantum. Atoms, Cavities and Photons, Oxford University Press 2006
- [16] V. Jakšić, C.-A. Pillet: On a model for quantum friction. II. Fermi's golden rule and dynamics at positive temperature, Comm. Math. Phys. 176, no. 3, 619-644 (1996)
- [17] V. Jakšić, C.-A. Pillet: From resonances to master equations, Ann. Inst. H. Poincaré 67, no.4, 425-445 (1997)
- [18] M. Könenberg, M. Merkli: Completely positive dynamical semigroups and quantum resonance theory, Lett. Math. Phys. 107, Issue 7, 1215-1233 (2017)
- [19] M. Könenberg, M. Merkli: On the irreversible dynamics emerging from quantum resonances, J. Math. Phys. 57, 033302 (2016)
- [20] G. Lindblad: On the generators of quantum dynamical semigroups, Comm. Math. Phys. 48, No.2, 119-130 (1976)
- [21] M. Merkli: The ideal quantum gas, Lecture Notes in Mathematics, 1880, 183-233 (2006)

- [22] M. Merkli, G.P. Berman, R.T. Sayre, S. Gnanakaran, M. Könenberg, A.I. Nesterov, H. Song: Dynamics of a Chlorophyll Dimer in Collective and Local Thermal Environments, J. Math. Chem. 54(4), 866-917 (2016)
- [23] M. Mohseni, Y. Omar, G.S. Engel, and M.B. Plenio (Eds): Quantum Effects in Biology, Cambridge University Press, 2014
- [24] M. Merkli, G.P. Berman, F. Borgonovi, K. Gebresellasie: Evolution of Entanglement of Two Qubits Interacting through Local and Collective Environments, Quantum Information & Computation 11, no. 5 & 6, 390-419 (2011)
- [25] M. Merkli, I.M. Sigal, G.P. Berman: *Decoherence and Thermalization*, Phys. Rev. Lett. **98**, 130401 (2007)
- [26] M. Merkli, I.M. Sigal, G.P. Berman: Resonance Theory of Decoherence and Thermalization, Annals of Physics 323, 373-412 (2008)
- [27] À. Rivas: Refined weak-coupling limit: Coherence, entanglement, and non-Markovianity, Phys. Rev. A 95, 042104, 10pp (2017)
- [28] À. Rivas, A.D.K. Plato, S. F. Huelga, M. B. Plenio: *Markovian master equations: a critical study*, New J. Phys. **12** 113032, 38pp, (2010)
- [29] A. Rivas, S. F. Huelga, M.B. Plenio: Quantum non-Markovianity: characterization, quantification and detection, Reports on Progress in Physics 77, no.9, 094001, 26pp (2014)
- [30] G. Schaller, T. Brandes: Preservation of positivity by dynamical coarse graining, Phys. Rev. A 78, 022106, 17pp (2008)
- [31] S. Tasaki, K. Yuasa, P. Facchi, G. Kimura, H. Nakazato, I. Ohba and S. Pascazio: On the Assumption of Initial Factorization in the Master Equation for Weakly Coupled Systems I: General Framework, Annals of Physics 322 631-656 (2007)
- [32] L. Van Hove: Quantum-mechanical perturbations giving rise to a statistical transport equation, Physica 21, Issue 1-5, 517-540 (1955)
- [33] N.G. Van Kampen: Stochastic behavior of quantum systems, Chapter XVII of Stochastic Processes in Physics and Chemistry, North-Holland Personal Library, 3rd edition, 422-456, 2007
- [34] K. Yuasa, S. Tasaki, P. Facchi, G. Kimura, H. Nakazato, I. Ohba and S. Pascazio: On the Assumption of Initial Factorization in the Master Equation for Weakly Coupled Systems II: Solvable Models, Annals of Physics **322** 657-676 (2007)