

Resonance Dynamics and Decoherence

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Abstract. We present a rigorous analysis of the phenomenon of decoherence for general N -level quantum systems coupled a reservoir modelled by a thermal bosonic quantum environment. We present an explicit form of the dominant reduced dynamics of open systems. We give explicit results for a spin $1/2$ (qubit), including decoherence and thermalization times. Our approach is based on a dynamical theory of quantum resonances. It yields the exact reduced dynamics of the small system and does not involve master equation or van Hove limit approximations. This approach is suitable for a wide variety of systems which are not explicitly solvable, including systems of interacting spins (registers of interacting qubits), for which the coupling between the system and the environment is fixed but small.

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1. Introduction

We consider an open quantum system $S + R$, where S is a “system of interest” and R is an “environment” or “reservoir”. Typically, S is a system under examination in a laboratory, like an atom, a molecule or an aggregate of spins. It is not possible in reality to isolate any physical system entirely from its surroundings R , and only if we take these surroundings into account can we consider the total system as being closed and evolving according to a hamiltonian dynamics. The reservoir R is supposed to be a very *large* quantum system compared to S . An immediate question is how the reservoir influences the dynamics of the small system. Prime examples of effects S shows are *thermalization* and *decoherence*. The former means that, due to its interaction with R , the system S is driven to the equilibrium state at the temperature of R . The effect of decoherence is the subject of this contribution, and we will describe it in detail in the next section.

Typically, we may assume that we know the (relatively simple) *microscopic* structure of S , while our knowledge of R is limited to its *macroscopic* characterization. In other words, we shall assume the energy levels and corresponding states of S to be given to us, as well as the thermodynamic parameters of R (temperature, pressure, chemical potential...). We will always assume that the state space of S is finite-dimensional. Of course, in a true concrete analysis, we will also have to specify the reservoir R on a microscopic level. However, when studying the reduced dynamics of S , only the macroscopic properties of R will be left in the description. The details of the environment do not play any role. In order to avoid introducing the microscopic structure of the environment, often an effective dynamics of the small system S is introduced – however, any trustworthy effective dynamics has to be derived from a full microscopic model, to which certain reduction and/or approximation schemes are applied (e.g. Born- or Born-Markov approximations). Our approach is to start off with a fully microscopic model of $S + R$, to eliminate the degrees of freedom of R and to analyze the remaining reduced description of S . In this process, we do not employ any approximation, however, our results are perturbative in the strength of the coupling between S and R .

We will take reservoirs to be spatially infinitely extended quantum systems. This is not merely a mathematical convenience, but rather a physical necessity that is linked to the very phenomena we want to describe. Indeed, if we try to keep the reservoir very large but finite, then irreversible physical processes will not take place. One can understand this easily heuristically, since for finite systems, hamiltonians have pure point spectrum, and so the dynamics will not drive the system to a final state. On the other hand, we may want to consider reservoirs which are just large, but maybe not infinitely extended, say an oven in a laboratory. The temporal behaviour of such systems is approximated by that of systems with infinitely extended reservoirs on time-scales which are large, but not too large, see e.g. [5].

We focus in this paper on the phenomenon of decoherence. A definition of decoherence is the vanishing of off-diagonal matrix elements of the reduced density matrix of S . A state given by a diagonal density matrix is characterized by classical probabilities, in the sense that averages of observables are obtained by weighing averages in specific states with given probabilities. The quantum nature is contained in the off-diagonal reduced density matrix elements, which are responsible for interference effects typical for quantum mechanics [15]. In this sense, a decohering system undergoes a transition from quantum to classical behaviour.

2. Description of decoherence

The *pure states* of $S + R$ are described by normalized vectors ψ in the Hilbert space $\mathfrak{H} = \mathfrak{H}_S \otimes \mathfrak{H}_R$. An observable A is a (self-adjoint) operator on \mathfrak{H} , its expectation value in the state ψ is $\langle A \rangle = \langle \psi, A\psi \rangle$. The dynamics is determined by the

hamiltonian (energy operator)

$$H = H_S + H_R + \lambda v,$$

where H_S and H_R are the hamiltonians of S and R, $\lambda \in \mathbb{R}$ is a coupling constant and where v represents the interaction between S and R. The dynamical equation is the Schrödinger equation,

$$i\hbar\partial_t\psi = H\psi.$$

We will set for convenience $\hbar = 1$, so that the state vector evolves as $\psi_t = e^{-itH}\psi_0$. Not all states can be represented by a single vector ψ . *Mixed states* are determined by *density matrices* ρ on \mathfrak{H} . These are non-negative (self-adjoint) trace-class operators which are normalized as $\text{Tr}\rho = 1$. The average of an observable A in the mixed state ρ is given by $\langle A \rangle = \text{Tr}(\rho A)$. To any density matrix ρ , we can associate normalized vectors ψ_n and probabilities p_n , $n = 1, 2, \dots$, s.t.

$$\rho = \sum_{n=1}^{\infty} p_n |\psi_n\rangle\langle\psi_n|, \quad (2.1)$$

where $|\psi_n\rangle\langle\psi_n|$ is the rank-one orthonormal projection onto $\mathbb{C}\psi_n$ (spectral decomposition of ρ). Since the evolution of ψ_n is given by $e^{-itH}\psi_n$, it follows from (2.1) that the density matrix ρ evolves according to $\rho_t = e^{-itH}\rho_0 e^{itH}$.

Consider the system S to be finite-dimensional, $\mathfrak{H}_S = \mathbb{C}^N$. An example of a mixed state of S is its equilibrium state at temperature $T = 1/\beta$, given by the density matrix $\rho_{S,\beta} \propto e^{-\beta H_S}$. It is readily seen that one cannot find any vector $\psi \in \mathbb{C}^N$ representing this state, i.e., having the property that $\langle\psi, A\psi\rangle$ equals $\text{Tr}(\rho_{S,\beta}A)$ for all $A \in B(\mathfrak{H}_S)$. However, by enlarging the Hilbert space, such a vector can be found: view $\sqrt{\rho_{S,\beta}}$ as an element of the Hilbert space of Hilbert-Schmidt operators on \mathfrak{H}_S (this space is naturally isomorphic to $\mathfrak{H}_S \otimes \mathfrak{H}_S$). Then clearly $\langle A \rangle = \text{Tr}(\rho_{S,\beta}A) = \langle\sqrt{\rho_{S,\beta}}, A\sqrt{\rho_{S,\beta}}\rangle_{\text{HS}}$, where $\langle\kappa, \sigma\rangle_{\text{HS}} = \text{Tr}(\kappa^*\sigma)$ is the inner product of Hilbert-Schmidt operators.¹

As mentioned in the introduction, the system R is infinitely extended in space. Consequently, even if it has a finite energy density, the total energy H_R is not well defined (is infinite). In fact, it is not even clear which Hilbert space can describe states of the infinitely extended system R. One constructs the system R via the thermodynamic limit. First, one takes a state $\rho_{R,\Lambda}$ of the reservoir constrained to a box $\Lambda \subset \mathbb{R}^3$, with fixed thermodynamic properties (such as temperature, density etc.). For each finite Λ , one knows the Hilbert space and the state. (For instance, a quantum gas in a box Λ is described by the Hilbert space $\oplus_{n \geq 0} L^2(\Lambda^n, d^{3n}x)$ (Fock space), and since Λ is finite, the energy operator has discrete spectrum, so the Gibbs-state density matrix is well defined.) Then the size of the box is made larger and larger, $\Lambda \uparrow \mathbb{R}^3$. This defines averages of (localized) observables A in the infinitely extended state, $E(A) = \lim_{\Lambda \uparrow \mathbb{R}^3} \text{Tr}(\rho_{R,\Lambda}A)$. One can now try to find a Hilbert space \mathfrak{H}_R and a normalized vector $\psi_R \in \mathfrak{H}_R$ such that $E(A) = \langle\psi_R, A\psi_R\rangle$.

¹This is a manifestation of a general fact: a state over a C^* -algebra can be represented by a vector state in a Hilbert space. This is the so-called Gelfand-Naimark-Segal representation [3].

This is a difficult task in general, but explicit expressions for Hilbert spaces and vectors have been found in the important cases of infinitely extended ideal quantum gases in thermal equilibrium.² We understand that this construction has been carried out, and that the state of R is represented on the Hilbert space \mathfrak{H}_R by a vector (or a density matrix). We give a more detailed explanation of this procedure at the end of this section. For now we carry on with a more qualitative discussion.

Given the density matrix of the total system, ρ_t , how can we extract the dynamics of S? Define the *reduced density matrix* of S by

$$\bar{\rho}_t := \text{Tr}_R(\rho_t),$$

where the trace is taken over \mathfrak{H}_R only (partial trace). This is a density matrix on \mathfrak{H}_S , and it satisfies

$$\text{Tr}_S(\bar{\rho}_t A_S) = \text{Tr}_{S+R}(\rho_t (A_S \otimes \mathbb{1}_R))$$

for all observables $A_S \in B(\mathfrak{H}_S)$. The reduced density matrix contains all information to describe the evolution of expectation values of observables of S alone. The degrees of freedom of R and the effects of the interaction between S and R are encoded in $\bar{\rho}_t$, which acts on the Hilbert space of the system S only.

Let $\{\varphi_j\}_{j=1}^N$ be a fixed basis of \mathfrak{H}_S and denote the matrix elements of $\bar{\rho}_t$ as $[\bar{\rho}_t]_{m,n} := \langle \varphi_m, \bar{\rho}_t \varphi_n \rangle$. A definition of decoherence is the vanishing of off-diagonal reduced density matrix elements in the limit of large times,

$$\lim_{t \rightarrow \infty} [\bar{\rho}_t]_{m,n} = 0, \quad \forall m \neq n. \quad (2.2)$$

This is a *basis dependent* notion of disappearance of correlations,

$$\bar{\rho}_t = \sum_{m,n} c_{m,n}(t) |\varphi_m\rangle \langle \varphi_n| \longrightarrow \sum_m p_m(t) |\varphi_m\rangle \langle \varphi_m|, \quad (2.3)$$

as $t \rightarrow \infty$. Most often, the basis considered is the energy basis, consisting of eigenvectors of H_S . A mixture of states φ_j of the form $\sum_{m,n} c_{m,n} |\varphi_m\rangle \langle \varphi_n|$ is called an incoherent mixture if all ‘‘off-diagonals’’ vanish, $c_{m,n} = 0$ for $m \neq n$. Else it is called a coherent mixture of the φ_j . The process (2.3) is thus a transition of a coherent to an incoherent mixture. Hence the name decoherence.

2.1. An explicitly solvable model of decoherence

Consider S to be an N -level system, coupled to a reservoir R of thermal bosons at temperature $T = 1/\beta$ through an *energy-conserving interaction* (see [14] for the qubit case, $N = 2$, and [11] for general N).

The Hilbert space and hamiltonian of S are given by $\mathfrak{H}_S = \mathbb{C}^N$ and $H_S = \text{diag}(E_1, \dots, E_N)$, respectively, and the interaction operator is $v = G \otimes \varphi(g)$, where $G = \text{diag}(\gamma_1, \dots, \gamma_N)$. Here,

$$\varphi(g) = \frac{1}{\sqrt{2}} [a^*(g) + a(g)], \quad (2.4)$$

²For bosons, this is known as the Araki-Woods construction, for fermions it is the Araki-Wyss construction, [1, 2, 13].

where the $a^\#(g)$ are the usual bosonic creation and annihilation operators, smeared out with a *form factor* $g \in L^2(\mathbb{R}^3, d^3k)$ (momentum space representation): $a(g) = \int_{\mathbb{R}^3} \overline{g(k)} a(k) d^3k$, $a^*(g) = \int_{\mathbb{R}^3} g(k) a^*(k) d^3k$, $[a(k), a^*(l)] = \delta(k-l)$.

Since $[H_S, H] = [H_S, H_S + H_R + v] = 0$ the energy of the small system is conserved. This model is exactly solvable. The solution is given by

$$[\bar{\rho}_t]_{m,n} = [\bar{\rho}_0]_{m,n} e^{-it(E_m - E_n) + i\alpha_{m,n}(t)}, \quad (2.5)$$

where

$$\alpha_{m,n}(t) = (\gamma_m^2 - \gamma_n^2)S(t) + i(\gamma_m - \gamma_n)^2\Gamma(t) \quad (2.6)$$

$$\Gamma(t) = \int_{\mathbb{R}^3} |g(k)|^2 \coth(\beta|k|/2) \frac{\sin^2(|k|t/2)}{|k|^2} d^3k \quad (2.7)$$

$$S(t) = \frac{1}{2} \int_{\mathbb{R}^3} |g(k)|^2 \frac{|k|t - \sin(|k|t)}{|k|^2} d^3k. \quad (2.8)$$

The parameter β in the above expression for $\Gamma(t)$ is the inverse temperature of the reservoir. We immediately see that

1. The populations are constant, $[\bar{\rho}_t]_{m,m} = [\bar{\rho}_0]_{m,m}$ for all m and all t .
2. If $\gamma_m = \gamma_n$ for some $m \neq n$, then the corresponding off-diagonal matrix element does not decay (decoherence-free subspaces).
3. Full decoherence (2.2) occurs if and only if $\Gamma(t) \rightarrow \infty$ as $t \rightarrow \infty$. Whether this happens or not depends on the *infrared behaviour* (small k) of the form factor, as well as on the *space dimension*. Let the infrared behaviour be characterized by $g(k) \sim |k|^p$ as $|k| \sim 0$. We obtain in three space-dimensions

$$\lim_{t \rightarrow \infty} \frac{\alpha_{m,n}(t)}{t} = \frac{1}{2}(\gamma_m^2 - \gamma_n^2) \langle g, |k|^{-1}g \rangle + i(\gamma_m - \gamma_n)^2 \begin{cases} 0 & \text{if } p > 0 \\ \text{const.} & \text{if } p = -1/2 \\ +\infty & \text{if } p < -1/2 \end{cases}$$

For $p = -1/2$ the off-diagonal matrix elements decay exponentially quickly, $|\bar{\rho}_t]_{m,n}| \sim e^{-\text{const.}t(\gamma_m - \gamma_n)^2}$ and for $p < -1/2$ the decay is quicker. For $p > 0$ the function $h(k) := |g(k)|^2 \coth(\beta|k|/2) |k|^{-2}$ is integrable on \mathbb{R}^3 . We write $\sin^2(|k|t/2) = \frac{1}{2}(1 - \cos(|k|t))$ and obtain from (2.7)

$$\Gamma(t) = \frac{1}{2} \int_{\mathbb{R}^3} \frac{|g(k)|^2}{|k|^2} \coth(\beta|k|/2) d^3k - \text{Re}(\widehat{F}(t)),$$

where \widehat{F} is the Fourier transform of the function

$$F(r) = \frac{1}{4} \coth(\beta|r|/2) \int_{S^2} |g(|r|, \sigma)|^2 d\sigma,$$

defined for and integrable on $r \in \mathbb{R}$ ($d\sigma$ is the uniform measure on the sphere S^2). From the Riemann-Lebesgue lemma we know that $\lim_{t \rightarrow \infty} \widehat{F}(t) = 0$, so

$$\lim_{t \rightarrow \infty} \Gamma(t) = \frac{1}{2} \int_{\mathbb{R}^3} \frac{|g(k)|^2}{|k|^2} \coth(\beta|k|/2) d^3k \neq 0, \quad \text{for } p > 0.$$

That is, for $p > 0$ we do not have full decoherence.

This is a non-demolition model (H_S conserved), in which processes of absorption and emission of quanta of the reservoir by the system S are suppressed. To enable such processes one needs interactions v which do not commute with H_S . In the latter case, one typically expects that *thermalization* takes place. The phenomenon of thermalization can be described as follows.

Let $\rho(\beta, \lambda)$ be the equilibrium state of the total system at temperature $T = 1/\beta$ (where λ is the coupling constant measuring the strength of interaction between S and R) and let $\rho_{t=0}$ be any initial density matrix (on \mathfrak{H}). Thermalization means that

$$\text{Tr}_{S+R}(\rho_t A) \longrightarrow \text{Tr}_{S+R}(\rho(\beta, \lambda) A), \quad \text{as } t \rightarrow \infty, \quad (2.9)$$

where A is any observable of the total system S + R. The convergence (2.9) implies that

$$\bar{\rho}_t \longrightarrow \bar{\rho}_\infty(\beta, \lambda) := \text{Tr}_R(\bar{\rho}(\beta, \lambda)),$$

as $t \rightarrow \infty$. An expansion of $\bar{\rho}_\infty(\beta, \lambda)$ in the coupling constant λ gives

$$\bar{\rho}_\infty(\beta, \lambda) = \bar{\rho}_\infty(\beta, 0) + O(\lambda),$$

where $\bar{\rho}_\infty(\beta, 0)$ is the *Gibbs state* of the system S. The Gibbs state (density matrix) is diagonal in the energy basis (diagonalizing H_S), however, the correction term $O(\lambda)$ is not, in general (see e.g. [11] for explicit calculations for the qubit). This shows the following effect.

Even if S is initially in an incoherent superposition of energy eigenstates it will acquire some “residual coherence” of order $O(\lambda)$ in the process of thermalization. This leads us to defining decoherence in thermalizing systems as being the decay of off-diagonals of $\bar{\rho}_t$ to their (non-zero) limit values, i.e., to the corresponding off-diagonals of $\bar{\rho}_\infty(\beta, \lambda)$.

In examining the vast literature on this topic (some references are [7, 14, 15, 16]) we have only encountered either models with energy-conserving interactions (which are explicitly solvable), or models with markovian approximations with uncontrolled errors (master equations, Lindblad dynamics). The goal of our work is to describe decoherence for systems which may also exhibit thermalization, in a rigorous fashion (controlled perturbation expansion).

2.2. Description of the infinitely extended reservoir R

Before taking the thermodynamic limit, as outlined above, the reservoir confined to a box Λ is described by the bosonic Fock space

$$\mathfrak{H}_{R,\Lambda} = \bigoplus_{n \geq 0} L^2_{\text{sym}}(\Lambda^n, d^{3n}x), \quad (2.10)$$

where the subindex “sym” means that we take symmetric square-integrable functions only (indistinguishable Bose particles). The hamiltonian is that of non-interacting particles, given by $H_{R,\Lambda} = \bigoplus_{n \geq 0} H_{R,\Lambda}^{(n)}$, with $H_{R,\Lambda}^{(n)} = \sum_{j=1}^n \sqrt{-\partial_{x_j}^2}$ (with periodic boundary conditions). The density matrix $\rho_{R,\beta,\Lambda} = Z_{R,\beta,\Lambda}^{-1} e^{-\beta H_{R,\Lambda}}$ is a well defined trace-class operator on the space (2.10), and the normalization factor $Z_{R,\beta,\Lambda}$ is chosen so that $\text{Tr}(\rho_{R,\beta,\Lambda}) = 1$. One calculates [1, 13] $E_\beta(a^\#(f)) := \lim_{\Lambda \uparrow \mathbb{R}^3} \text{Tr}(\rho_{R,\beta,\Lambda} a^\#(f)) = 0$, where $a^\#$ stands for either a or a^* , and

$$E_\beta(a^*(f)a(g)) := \lim_{\Lambda \uparrow \mathbb{R}^3} \text{Tr}(\rho_{R,\beta,\Lambda} a^*(f)a(g)) = \left\langle g, \frac{1}{e^{\beta|k|} - 1} f \right\rangle, \quad (2.11)$$

where the square-integrable f, g are represented in Fourier transform in the inner product on the right hand side.³ All products of creation and annihilation operators can be calculated using the Wick theorem [3], so (2.11) (plus the vanishing of averages of $a(f)$ and $a^*(f)$) determines the infinitely extended thermal state E_β of R completely. We consider here only reservoir equilibrium states below critical density, i.e., in absence of Bose-Einstein condensate.

The Araki-Woods Hilbert space representation is given by

$$\mathfrak{H}_R = \mathcal{F} \otimes \mathcal{F}, \quad (2.12)$$

where $\mathcal{F} = \bigoplus_{n \geq 0} L^2_{\text{sym}}(\mathbb{R}^{3n}, d^{3n}x)$,

$$\psi_R = \Omega \otimes \Omega, \quad (2.13)$$

the product of the Fock vacua in \mathcal{F} , and

$$a_\beta^*(g) = a^* \left(\frac{e^{\beta|k|}}{e^{\beta|k|} - 1} g \right) \otimes \mathbb{1} + \mathbb{1} \otimes a \left(\frac{1}{e^{\beta|k|} - 1} \bar{g} \right),$$

where \bar{g} is the complex conjugate of g , and where the $a^\#$ are the ordinary Fock creation and annihilation operators on \mathcal{F} . We also set $a_\beta(g) := [a_\beta^*(g)]^*$. It is easy to check that

$$E_\beta(a^*(f)a(g)) = \langle \psi_R, a_\beta^*(f)a_\beta(g)\psi_R \rangle.$$

This last equation shows us that we have successfully represented the thermal state of the infinitely extended R as a vector state on a concrete Hilbert space.

³Of course, one has to restrict this to functions for which the r.h.s. is well defined.

3. Dynamical resonance theory: Results

Let S be an N -level system, $\mathfrak{H}_S = \mathbb{C}^N$, with energies $\{E_j\}_{j=1}^N$, and let R be the free massless Bose field, spatially infinitely extended in \mathbb{R}^3 in equilibrium at temperature $T = 1/\beta$, as described at the end of Section 2.

The interaction operator is obtained by taking the thermodynamic limit of $\lambda v_\Lambda = \lambda G \otimes \varphi(g_\Lambda)$. Here, $G = G^* \in B(\mathfrak{H}_S)$ is a self-adjoint $N \times N$ matrix and $\varphi(g_\Lambda)$ is the smoothed-out field operator (2.4) acting on $\mathfrak{H}_{R,\Lambda}$, (2.10), and $g_\Lambda(x) = \chi_\Lambda(x)g(x)$ is the function g , cut off by being set equal to zero outside Λ . It is customary to abbreviate this description by simply writing

$$v = \lambda G \otimes \varphi(g), \quad (3.1)$$

and the thermodynamic limit is understood to be taken automatically.

We denote the average of observables $A \in B(\mathfrak{H}_S)$ at time t by

$$\langle A \rangle_t := \text{Tr}_S(\bar{\rho}_t A), \quad (3.2)$$

and the ergodic average is denoted by

$$\langle\langle A \rangle\rangle_\infty := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle A \rangle_t dt.$$

Our approach is based on a dynamical resonance theory, where resonances are treated in a setting of *spectral deformation* (see Section 4). This leads to the following regularity requirement which we assume to be fulfilled throughout this paper.

(A) The function

$$g_\beta(u, \sigma) := \sqrt{\frac{u}{1 - e^{-\beta u}}} |u|^{1/2} \begin{cases} g(u, \sigma) & \text{if } u \geq 0 \\ e^{i\phi} \bar{g}(-u, \sigma) & \text{if } u < 0 \end{cases}$$

is such that $\vartheta \mapsto g_\beta(u + \vartheta, \sigma)$ has an analytic continuation, as a map $\mathbb{C} \rightarrow L^2(\mathbb{R} \times S^2, du \times d\sigma)$, into $\{|\vartheta| < \tau\}$, for some $\tau > 0$. Here, ϕ is an arbitrary fixed phase. (See [6] for the usefulness and physical interpretation of this phase.)

Examples of admissible g are $g(k) = g_1(\sigma)|k|^p e^{-|k|^2}$, where $p = -1/2 + n$, $n = 0, 1, 2, \dots$, and $g_1(\sigma) = e^{i\phi} \bar{g}_1(\sigma)$. They include the physically most important cases, see also [14]. We point out that it is possible to weaken condition (A) considerably, at the expense of a mathematically more involved treatment, as mentioned in [11, 12]. The following result is the main result of [11]. We give an outline of the proof in Section 4.

Theorem 3.1 (Evolution of observables [11]). *There is a $\lambda_0 > 0$ s.t. the following statements hold for $|\lambda| < \lambda_0$, $t \geq 0$, and $A \in B(\mathfrak{H}_S)$.*

1. $\langle\langle A \rangle\rangle_\infty$ exists.
2. We have

$$\langle A \rangle_t - \langle\langle A \rangle\rangle_\infty = \sum_{\varepsilon \neq 0} e^{it\varepsilon} R_\varepsilon(A) + O(\lambda^2 e^{-\tau t}), \quad (3.3)$$

where the ε are “resonance energies”, $0 \leq \text{Im}\varepsilon < \tau/2$, and $R_\varepsilon(A)$ are linear functionals of A which depend on the initial state $\rho_{t=0}$.

3. Let e be an eigenvalue of the operator $H_S \otimes \mathbb{1}_S - \mathbb{1}_S \otimes H_S$ (acting on $\mathfrak{H}_S \otimes \mathfrak{H}_S$). For $\lambda = 0$ each ε coincides with one of the e and we have the following expansion for small λ

$$\varepsilon \equiv \varepsilon_e^{(s)} = e - \lambda^2 \delta_e^{(s)} + O(\lambda^4).$$

The $\delta_e^{(s)}$ satisfy $\text{Im}\delta_e^{(s)} \leq 0$. They are eigenvalues of so-called level shift operators Λ_e , and $s = 1, \dots, \nu(s) \leq \text{mult}(e)$ labels the eigenvalue splitting. Furthermore, we have

$$R_\varepsilon(A) = \sum_{(m,n) \in I_e} \kappa_{m,n} A_{m,n} + O(\lambda^2), \quad (3.4)$$

with $I_e = \{(m,n) \mid E_m - E_n = e\}$, and where $A_{m,n}$ is the (m,n) -matrix element of A and the numbers $\kappa_{m,n}$ depend on the initial state.

Discussion. Relation (3.3) gives a detailed picture of the dynamics of averages of observables. The resonance energies ε and the functionals R_ε can be calculated for concrete models, to arbitrary precision (in the sense of rigorous perturbation theory in λ). See Section 3.1 for explicit expressions for the qubit. In the absence of interaction ($\lambda = 0$) we have $\varepsilon = e \in \mathbb{R}$. Depending on the interaction each resonance energy ε may migrate into the upper complex plane, or it may stay on the real axis, as $\lambda \neq 0$. The averages $\langle A \rangle_t$ approach their ergodic means $\langle\langle A \rangle\rangle_\infty$ if and only if $\text{Im}\varepsilon > 0$ for all $\varepsilon \neq 0$. In this case the convergence takes place on the time scale $[\text{Im}\varepsilon]^{-1}$. Otherwise $\langle A \rangle_t$ oscillates. A sufficient condition for decay is that $\text{Im}\delta_e^{(s)} < 0$ (and λ small).

There are two kinds of processes which drive the decay: energy-exchange processes and energy preserving ones. The former are induced by interactions enabling processes of absorption and emission of field quanta with energies corresponding to the Bohr frequencies of S (this is the “Fermi Golden Rule Condition”). Energy preserving interactions suppress such processes, allowing only for a phase change of the system during the evolution (“phase damping”).

Even if the initial density matrix, $\rho_{t=0}$, is a product of the system and reservoir density matrices, the density matrix ρ_t at any subsequent moment of time $t > 0$ is *not* of product form. The evolution creates entanglement between the system and reservoir. Our technique does not require $\rho_{t=0}$ to be a product state [11].

Our next goal is to use Theorem 3.1 to describe in detail the decay of reduced density matrix elements. According to Theorem 3.1 the dynamics is governed by the resonance energies $\varepsilon_e^{(s)}$ whose lowest order contributions $\delta_e^{(s)}$ are eigenvalues of level shift operators Λ_e . In what follows we assume that all eigenvalues $\delta_e^{(s)}$ are simple. We denote the corresponding eigenvector by $\eta_e^{(s)}$, and the eigenvector associated to the adjoint operator Λ_e^* with eigenvalue $\overline{\delta_e^{(s)}}$ is denoted by $\tilde{\eta}_e^{(s)}$. They

are normalized as $\langle \eta_e^{(s)}, \tilde{\eta}_e^{(s)} \rangle = 1$. The assumption of simplicity of the spectrum of Λ_e is not necessary at all for our method, it is simply made to make the exposition somewhat simpler. Let $\{\varphi_n\}$ be an orthonormal basis of \mathbb{C}^N diagonalizing the Hamiltonian of S , $H_S \varphi_n = E_n \varphi_n$. The matrix element $[\bar{\rho}_t]_{m,n}$ is obtained by choosing the observable $A = |\varphi_n\rangle\langle\varphi_m|$ in (3.2). We denote the difference of two eigenvalues of H_S by $E_{m,n} = E_m - E_n$. A closer analysis of the functionals R_ε yields the following result, the proof of which we give in Section 5.

Theorem 3.2 (Dominant dynamics). *There is a constant λ_1 s.t. if $0 < |\lambda| < \lambda_1$, then for all m, n and all $t \geq 0$*

$$\begin{aligned} [\bar{\rho}_t]_{m,n} - \langle |\varphi_n\rangle\langle\varphi_m| \rangle_\infty = \\ \sum_{\{s: \varepsilon_{E_{n,m}}^{(s)} \neq 0\}} e^{it\varepsilon_{E_{n,m}}^{(s)}} \sum_{\{k,l: E_{l,k} = E_{n,m}\}} \sigma_{m,n;k,l}^{(s)} [\bar{\rho}_0]_{k,l} + O(\lambda^2 e^{-t\gamma_{m,n}}), \end{aligned} \quad (3.5)$$

where $\gamma_{m,n} = \min\{\text{Im}\varepsilon_e^{(s)} : \varepsilon_e^{(s)} \neq 0 \text{ and } e \neq E_{n,m}\}$. The mixing constants $\sigma_{m,n;k,l}^{(s)}$ are given by

$$\sigma_{m,n;k,l}^{(s)} = \left\langle \tilde{\eta}_{E_{n,m}}^{(s)}, \varphi_n \otimes \varphi_m \right\rangle \left\langle \varphi_l \otimes \varphi_k, \eta_{E_{n,m}}^{(s)} \right\rangle,$$

$\eta_{E_{n,m}}^{(s)}$ and $\tilde{\eta}_{E_{n,m}}^{(s)}$ being the resonance eigenvectors introduced above.

Discussion. The group of matrix elements $[\bar{\rho}_t]_{m,n}$ associated to the same energy difference $e = E_n - E_m$ evolve in a coupled way, while groups belonging to different e evolve independently, in the regime of Theorem 3.2. It is clear that the eigenvalue $e = 0$ is always degenerate ($\varphi_k \otimes \varphi_k$ is always an associated eigenvector, for all k). One easily sees that if $e = E_n - E_m$ is simple then $\sigma_{m,n;k,l}^{(s)}$ vanishes unless $(k, l) = (m, n)$, in which case $\sigma_{m,n;k,l}^{(s)} = 1$ equals one (this follows simply from the fact that η_e and $\tilde{\eta}_e$ belong to the spectral subspace associated to e). The main term of the r.h.s. of (3.5) is then simply $e^{it\varepsilon_{E_{n,m}}}$, so

$$[\bar{\rho}_t]_{m,n} - \langle |\varphi_n\rangle\langle\varphi_m| \rangle_\infty = e^{it\varepsilon_{E_{n,m}}} [\bar{\rho}_0]_{m,n} + O(\lambda^2 e^{-t\gamma_{m,n}}).$$

The usefulness of Theorem 3.2 is that it relates $[\bar{\rho}_t]_{m,n}$ to the initial conditions $[\bar{\rho}_0]_{k,l}$. We can understand how to arrive at Theorem 3.2 from Theorem 3.1 in the following way. The expansion (3.4) implies that the main term of $R_\varepsilon(|\varphi_n\rangle\langle\varphi_m|)$ is non-vanishing only if ε bifurcates out of $e = E_n - E_m$. This means that all contributions to the sum in (3.3) with ε not bifurcating out of $E_n - E_m$ are of order λ^2 , and decaying according to $e^{it\varepsilon}$. These terms, plus the $O(\lambda^2 e^{-\tau t})$ term in (3.3), constitute the remainder term in (3.5).

The constants $\gamma_{m,n}$ are typically of order λ^2 (they may be of higher order if the so-called Fermi Golden Rule condition for efficient coupling is not satisfied [9]). Expansion (3.5) is thus useful in the regime

$$\lambda^2 e^{-t\lambda^2 \min\{\text{Im}\delta_e^{(s)} : e \neq E_{n,m}\}} \ll e^{-t\lambda^2 \max\{\text{Im}\delta_{E_{n,m}}^{(s)} : s=1, \dots, \nu(E_{n,m})\}}.$$

In other words, given any finite maximal time of interest t_{\max} , there is a λ_1 s.t. if $0 < |\lambda| < \lambda_1$, expansion (3.5) is valid, and the remainder term is negligible for all $0 \leq t \leq t_{\max}$. The expansion (3.5) thus isolates the dominant dynamics.

3.1. Application: thermalization versus decoherence time for a qubit

A qubit, or spin 1/2, is described by the Hilbert-space of pure states \mathbb{C}^2 . The hamiltonian is $H_S = \text{diag}(E_1, E_2)$ (in the canonical basis of \mathbb{C}^2). We set $\Delta = E_2 - E_1 > 0$. The coupling operator is given by the self-adjoint operator

$$v = \begin{bmatrix} a & c \\ \bar{c} & b \end{bmatrix} \otimes \varphi(g),$$

where $\varphi(g)$ is given in (2.4). The operator $H_S \otimes \mathbb{1} - \mathbb{1} \otimes H_S$ has four eigenvalues, $e \in \{-\Delta, 0, 0, \Delta\}$. One calculates the resonance energies associated to these e to be (see also Theorem 3.1 and the next subsection)

$$\begin{aligned} \varepsilon_0^{(1)}(\lambda) &= 0 \\ \varepsilon_0^{(2)}(\lambda) &= i\lambda^2|c|^2\xi(\Delta) + O(\lambda^4) \\ \varepsilon_\Delta(\lambda) &= \Delta + \lambda^2 R + \frac{i}{2}\lambda^2 [|c|^2\xi(\Delta) + (b-a)^2\xi(0)] + O(\lambda^4) \\ \varepsilon_{-\Delta}(\lambda) &= \overline{-\varepsilon_\Delta(\lambda)} \end{aligned}$$

where we have set

$$\xi(\eta) := \pi \int_{\mathbb{R}^3} \coth\left(\frac{\beta|k|}{2}\right) |g(k)|^2 \delta(\eta - |k|) d^3k$$

and (P.V. denoting the principal value)

$$R = \frac{b^2 - a^2}{2} \langle g, |k|^{-1}g \rangle + \frac{|c|^2}{2} \text{P.V.} \int_{\mathbb{R} \times S^2} u^2 \coth\left(\frac{\beta|k|}{2}\right) \frac{|g(|u|, \sigma)|^2}{u - \Delta} du d\sigma. \quad (3.6)$$

The corresponding resonance eigenvectors (defined before Theorem 3.2) are as follows, where $\{\varphi_1, \varphi_2\}$ is the canonical orthonormal basis of \mathbb{C}^2 , and where $\varphi_{i,j} = \varphi_i \otimes \varphi_j$:

$$\eta_0^{(1)} = \varphi_{1,1} + \varphi_{2,2}, \quad \tilde{\eta}_0^{(1)} = \frac{1}{1 + e^{-\beta\Delta}} [\varphi_{1,1} + e^{-\beta\Delta} \varphi_{2,2}],$$

$$\eta_0^{(2)} = \varphi_{1,1} - e^{\beta\Delta} \varphi_{2,2}, \quad \tilde{\eta}_0^{(2)} = \frac{1}{1 + e^{\beta\Delta}} [\varphi_{1,1} - \varphi_{2,2}],$$

and $\eta_\Delta = \tilde{\eta}_\Delta = \varphi_{2,1}$, $\eta_{-\Delta} = \tilde{\eta}_{-\Delta} = \varphi_{1,2}$. Note that $\eta_0^{(1)}$ is just the (not normalized) trace state on S. The mixing constants $\sigma_{m,n;k,l}^{(s)}$ (see Theorem 3.2) are thus

$$\begin{aligned}\sigma_{1,2;1,2}^{(1)} = \sigma_{2,1;2,1}^{(1)} &= 1, \\ \sigma_{1,1;1,1}^{(2)} &= \langle \eta_0^{(2)}, \varphi_{1,1} \rangle \langle \varphi_{1,1}, \eta_0^{(2)} \rangle = \frac{1}{1 + e^{\beta\Delta}}, \\ \sigma_{1,1;2,2}^{(2)} = \sigma_{2,2;1,1}^{(2)} &= \langle \eta_0^{(2)}, \varphi_{1,1} \rangle \langle \varphi_{2,2}, \eta_0^{(2)} \rangle = \frac{-1}{1 + e^{-\beta\Delta}}, \\ \sigma_{2,2;2,2}^{(2)} &= \langle \eta_0^{(2)}, \varphi_{2,2} \rangle \langle \varphi_{2,2}, \eta_0^{(2)} \rangle = \frac{1}{1 + e^{-\beta\Delta}}.\end{aligned}$$

We shall assume that the Fermi Golden Rule is satisfied: $\xi(\Delta) \neq 0$. Then zero is a simple resonance eigenvalue, $\varepsilon_0^{(1)} = 0$, and consequently, for $e = 0$ the term $s = 1$ is not present in the sum (3.5). Theorem 3.1 thus gives the following dominant dynamics:

$$[\bar{\rho}_t]_{1,1} - \langle |\varphi_1\rangle \langle \varphi_1| \rangle_\infty \sim e^{it\varepsilon_0^{(2)}(\lambda)} \left\{ \frac{[\bar{\rho}_0]_{1,1}}{1 + e^{\beta\Delta}} - \frac{[\bar{\rho}_0]_{2,2}}{1 + e^{-\beta\Delta}} \right\}, \quad (3.7)$$

$$[\bar{\rho}_t]_{1,2} - \langle |\varphi_2\rangle \langle \varphi_1| \rangle_\infty \sim e^{it\varepsilon_\Delta(\lambda)} [\bar{\rho}_0]_{1,2}. \quad (3.8)$$

The dynamics for $[\bar{\rho}_t]_{2,2}$ and $[\bar{\rho}_t]_{2,1}$ are easily obtained also directly from Theorem 3.1, or by using that $[\bar{\rho}_t]_{1,1} + [\bar{\rho}_t]_{2,2} = 1$ (since $\text{Tr } \bar{\rho}_t = 1$) and the fact that $\bar{\rho}_t$ is self-adjoint. We point out that since the system S+R approaches its (joint) equilibrium as $t \rightarrow \infty$, we have $\langle |\varphi_1\rangle \langle \varphi_1| \rangle_\infty = \frac{e^{\beta\Delta}}{1 + e^{\beta\Delta}} + O(\lambda^2)$ and $\langle |\varphi_2\rangle \langle \varphi_1| \rangle_\infty = O(\lambda^2)$ (Gibbs distribution). This law can also be recovered by setting $t = 0$ in (3.7), (3.8) and using that $[\bar{\rho}_0]_{2,2} = 1 - [\bar{\rho}_0]_{1,1}$.

The *thermalization time* (decay of diagonals) is $\tau_{\text{th}} := [\text{Im}\varepsilon_0^{(2)}(\lambda)]^{-1}$, and the *decoherence time* (decay of off-diagonals) is $\tau_{\text{dec}} := [\text{Im}\varepsilon_\Delta(\lambda)]^{-1}$. Their ratio is

$$\frac{\tau_{\text{th}}}{\tau_{\text{dec}}} = \frac{1}{2} \left[1 + \frac{(b-a)^2}{|c|^2} \frac{\xi(0)}{\xi(\Delta)} \right] + O(\lambda^2).$$

Note that we have $\xi(0) > 0$ for infra-red behaviour $g(k) \sim |k|^{-1/2}$ as $|k| \sim 0$ and $\xi(0) = 0$ for more regular infra-red behaviour. Moreover, $\xi(0) \sim T$ and $\xi(\Delta) \sim \text{const.} > 0$, as the temperature $T \sim 0$.

Spin-Boson model. The Hamiltonian of S is given by [4, 8]

$$H_S = -\frac{1}{2}\hbar\Delta_0\sigma_x + \frac{1}{2}\epsilon\sigma_z,$$

where the σ are Pauli matrices, Δ_0 is the bare tunneling matrix element, and ϵ is the bias. The coupling operator is

$$v = \sigma_z \otimes \varphi(g).$$

This determines the matrix elements a, b, c in the general formulation, and we obtain

$$\frac{(b-a)^2}{|c|^2} = 16 \frac{\epsilon^2}{\hbar^2 \Delta_0^2}.$$

This shows for instance that the thermalization time will become smaller relative to the decoherence time if the bias ϵ is decreased, or if the tunneling parameter Δ_0 is increased.

Explicit form of the level shift operators. For the sake of completeness, we include the explicit form of the level shift operators Λ_e , $e = 0, \pm\Delta$. By definition,

$$\Lambda_e = P_e I \bar{P}_e (\bar{L}_0 - e + i0)^{-1} \bar{P}_e I P_e,$$

where P_e is the spectral projection onto the eigenspace of $H_S \otimes \mathbb{1} - \mathbb{1} \otimes H_S$ associated to the eigenvalue e , $\bar{P}_e = \mathbb{1} - P_e$, \bar{L}_0 is the operator L_0 restricted to $\text{Ran } \bar{P}_e$, and where I is the interaction operator, see [11] and Section 4. The explicit form of Λ_e has been calculated in [11] for a general N -level system coupled to the thermal bose environment (Proposition 5.1 of [11]).⁴ The explicit form of Λ_0 , expressed in the basis $\{\varphi_1 \otimes \varphi_1, \varphi_2 \otimes \varphi_2\}$ of $\text{Ran } P_0$ is

$$\Lambda_0 = \frac{i}{2} \frac{|c|^2 \xi(\Delta)}{e^{\beta\Delta} - 1} \begin{bmatrix} 1 & -1 \\ -e^{\beta\Delta} & e^{\beta\Delta} \end{bmatrix}.$$

The dimension of $\text{Ran } P_{\pm\Delta}$ is one, so $\Lambda_{\pm\Delta}$ reduces simply to a number,

$$\Lambda_{\pm\Delta} = R \pm \frac{i}{2} [|c|^2 \xi(\Delta) + (b-a)^2 \xi(0)],$$

where R is given in (3.6). Knowing the explicit form of the level shift operators, the expansions of the resonance energies and resonance eigenvectors are now easy to obtain.

4. Outline of resonance approach

Consider any observable $A \in B(\mathfrak{H}_S)$. We have

$$\begin{aligned} \langle A \rangle_t &= \text{Tr}_S [\bar{\rho}_t A] \\ &= \text{Tr}_{S+R} [\rho_t A \otimes \mathbb{1}_R] \\ &= \langle \psi_0, e^{itL_\lambda} [A \otimes \mathbb{1}_S \otimes \mathbb{1}_R] e^{-itL_\lambda} \psi_0 \rangle. \end{aligned} \quad (4.1)$$

In the last step, we pass to the *representation Hilbert space* of the system (the GNS Hilbert space), where the initial density matrix is represented by the vector ψ_0 (in particular, the Hilbert space of the small system becomes $\mathfrak{H}_S \otimes \mathfrak{H}_S$), see also after equation (2.1) and Section 2.2. For this outline we take the initial state to be one represented by the product vector $\psi_0 = \psi_{S,\infty} \otimes \psi_R$, where $\psi_{S,\infty}$ is the trace

⁴In the present work, we take the generator of dynamics to be the Liouville operator associated to the reference state $\psi_0 = \psi_{S,\infty} \otimes \psi_R$, see Section 4. In [11] the Liouville operator is taken with respect to the reference vector $\psi_{S,\beta} \otimes \psi_R$. Those two choices are related by a simple transformation, and all physical results are independent of the particular choice of reference state.

state of S, $\langle \psi_{S,\infty}, (A_S \otimes \mathbb{1}_S) \psi_{S,\infty} \rangle = \frac{1}{N} \text{Tr}(A_S)$, and where ψ_R is the equilibrium state of R at a fixed inverse temperature $0 < \beta < \infty$, (2.13). (This form of the initial state is not necessary for our method to work, see [11].) The dynamics is implemented by the group of automorphisms $e^{itL_\lambda} \cdot e^{-itL_\lambda}$. The self-adjoint generator L_λ is called the *Liouville operator*. It is of the form $L_\lambda = L_0 + \lambda W$, where $L_0 = L_S + L_R$ represents the uncoupled Liouville operator, and λW is the interaction (represented in the GNS Hilbert space).

We borrow a trick from the analysis of open systems far from equilibrium: there is a (non-self-adjoint) generator K_λ s.t.

$$\begin{aligned} e^{itL_\lambda} A e^{-itL_\lambda} &= e^{itK_\lambda} A e^{-itK_\lambda} \text{ for all observables } A, t \geq 0, \text{ and} \\ K_\lambda \psi_0 &= 0. \end{aligned}$$

There is a standard way of constructing K_λ given L_λ and the reference vector ψ_0 . K_λ is of the form $K_\lambda = L_0 + \lambda I$, where the interaction term undergoes a certain modification ($W \rightarrow I$), c.f. [11]. As a consequence, formally, we may replace the propagators in (4.1) by those involving K . The resulting propagator which is directly applied to ψ_0 will then just disappear due to the invariance of ψ_0 . One can carry out this procedure in a rigorous manner, obtaining the following resolvent representation [11]

$$\langle A \rangle_t = -\frac{1}{2\pi i} \int_{\mathbb{R}-i} \langle \psi_0, (K_\lambda(\omega) - z)^{-1} [A \otimes \mathbb{1}_S \otimes \mathbb{1}_R] \psi_0 \rangle e^{itz} dz, \quad (4.2)$$

where $K_\lambda(\omega) = L_0(\omega) + \lambda I(\omega)$, I is representing the interaction, and $\omega \mapsto K_\lambda(\omega)$ is a spectral deformation (translation) of K_λ . The latter is constructed as follows. There is a deformation transformation $U(\omega) = e^{-i\omega D}$, where D is the (explicit) self-adjoint generator of translations [11, 10] transforming the operator K_λ as

$$K_\lambda(\omega) = U(\omega) K_\lambda U(\omega)^{-1} = L_0 + \omega N + \lambda I(\omega). \quad (4.3)$$

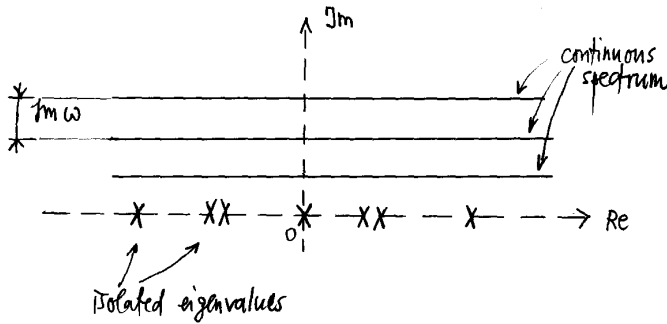


FIGURE 1. Spectrum of $K_0(\omega)$

Here, $N = N_1 \otimes \mathbb{1} + \mathbb{1} \otimes N_1$ is the total number operator of \mathfrak{H}_R , (2.12), and where N_1 is the usual number operator on \mathcal{F} . N has spectrum $\mathbb{N} \cup \{0\}$, where 0 is a simple eigenvalue (vacuum eigenvector ψ_R). For real values of ω , $U(\omega)$ is a group of unitaries. The spectrum of $K_\lambda(\omega)$ depends on $\text{Im } \omega$ and moves according to the value of $\text{Im } \omega$, whence the name ‘‘spectral deformation’’. Even though $U(\omega)$ becomes unbounded for complex ω , the r.h.s. of (4.3) is a well defined closed operator on a dense domain, analytic in ω at zero. Analyticity is used in the derivation of (4.2) and this is where the analyticity condition (A) before Theorem 3.1 comes into play. The operator $I(\omega)$ is infinitesimally small with respect to the number operator N . Hence we use perturbation theory in λ to examine the spectrum of $K_\lambda(\omega)$.

The point of the spectral deformation is that the (important part of the) spectrum of $K_\lambda(\omega)$ is much easier to analyze than that of K_λ , because the deformation uncovers the resonances of K_λ . We have (see Figure 1)

$$\text{spec}(K_0(\omega)) = \{E_i - E_j\}_{i,j=1,\dots,N} \bigcup_{n \geq 1} \{\omega n + \mathbb{R}\},$$

because $K_0(\omega) = L_0 + \omega N$, L_0 and N commute, and the eigenvectors of $L_0 = L_S + L_R$ are $\varphi_i \otimes \varphi_j \otimes \psi_R$. The continuous spectrum is bounded away from the isolated eigenvalues by a gap of size $\text{Im } \omega$. For values of the coupling parameter λ small compared to $\text{Im } \omega$, we can follow the displacements of the eigenvalues by using analytic perturbation theory. (Note that for $\text{Im } \omega = 0$, the eigenvalues are imbedded into the continuous spectrum, and analytic perturbation theory is not valid!

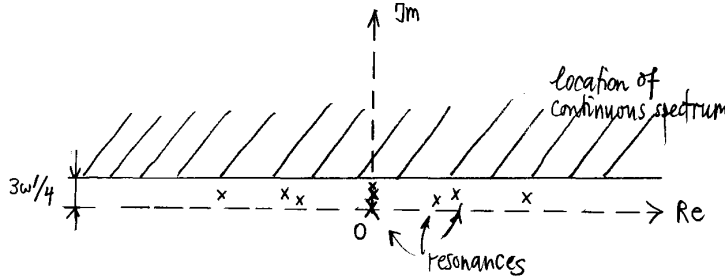


FIGURE 2. Spectrum of $K_\lambda(\omega)$. Resonances $\varepsilon_e^{(s)}$ are uncovered.

Theorem 4.1. (See Fig. 2.) Fix $\text{Im } \omega$ s.t. $0 < \text{Im } \omega < \tau$ (where τ is as in Condition (A) given after (3.2)). There is a constant $c_0 > 0$ s.t. if $|\lambda| \leq c_0/\beta$ then, for all ω with $\text{Im } \omega > \omega'$, the spectrum of $K_\lambda(\omega)$ in the complex half-plane $\{\text{Im } z < \omega'/2\}$ is independent of ω and consists purely of the distinct eigenvalues

$$\{\varepsilon_e^{(s)} : e \in \text{spec}(L_S), s = 1, \dots, \nu(e)\},$$

where $1 \leq \nu(e) \leq \text{mult}(e)$ counts the splitting of the eigenvalue e . Moreover, $\lim_{\lambda \rightarrow 0} |\varepsilon_e^{(s)}(\lambda) - e| = 0$ for all s , and we have $\text{Im} \varepsilon_e^{(s)} \geq 0$. Also, the continuous spectrum of $K_\lambda(\omega)$ lies in the region $\{\text{Im} z \geq 3\omega'/4\}$.

Next we separate the contributions to the path integral in (4.2) coming from the singularities at the resonance energies and from the continuous spectrum. We deform the path of integration $z = \mathbb{R} - i$ into the line $z = \mathbb{R} + i\omega'/2$, thereby picking up the residues of poles of the integrand at $\varepsilon_e^{(s)}$ (all e, s). Let $\mathcal{C}_e^{(s)}$ be a small circle around $\varepsilon_e^{(s)}$, not enclosing or touching any other spectrum of $K_\lambda(\omega)$. We introduce the generally non-orthogonal Riesz spectral projections

$$Q_e^{(s)} = Q_e^{(s)}(\omega, \lambda) = -\frac{1}{2\pi i} \int_{\mathcal{C}_e^{(s)}} (K_\lambda(\omega) - z)^{-1} dz. \quad (4.4)$$

It follows from (4.2) that

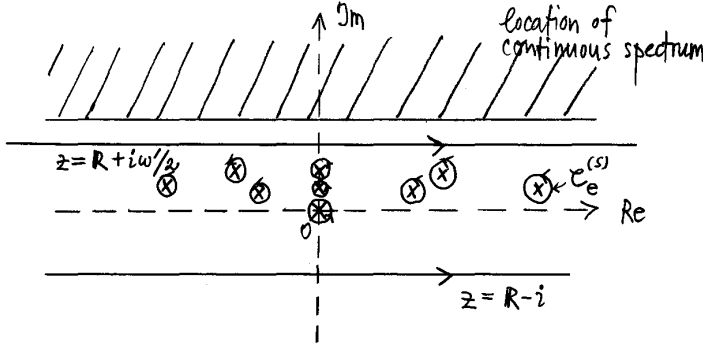


FIGURE 3. Contour deformation: $\int_{\mathbb{R}-i} dz = \sum_{e,s} \int_{\mathcal{C}_e^{(s)}} dz + \int_{\mathbb{R}+i\omega'/2} dz$

$$\langle A \rangle_t = \sum_e \sum_{s=1}^{\nu(e)} e^{it\varepsilon_e^{(s)}} \left\langle \psi_0, Q_e^{(s)} [A \otimes \mathbb{1}_S \otimes \mathbb{1}_R] \psi_0 \right\rangle + O(\lambda^2 e^{-\omega't/2}). \quad (4.5)$$

Note that the imaginary parts of all resonance energies $\varepsilon_e^{(s)}$ are smaller than $\omega'/2$, so that the remainder term in (4.5) is not only small in λ , but it also decays faster than all of the terms in the sum! (See also Figure 3.)

Finally, we notice that all terms in (4.5) with $\varepsilon_e^{(s)} \neq 0$ will vanish in the ergodic mean limit, so

$$\langle \langle A \rangle \rangle_\infty = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle A \rangle_t dt = \sum_{s: \varepsilon_0^{(s)}=0} \left\langle \psi_0, Q_0^{(s)} [A \otimes \mathbb{1}_R \otimes \mathbb{1}_R] \psi_0 \right\rangle.$$

The identification of the linear functionals

$$R_{\varepsilon_e^{(s)}}(A) = \left\langle \psi_0, Q_e^{(s)} [A \otimes \mathbb{1}_S \otimes \mathbb{1}_R] \psi_0 \right\rangle \quad (4.6)$$

(c.f. (3.3)) is useful for concrete calculations, as well as in the proof of Theorem 3.2. This concludes the outline of the proof of Theorem 3.1.

5. Proof of Theorem 3.2

The proof is based on expansion (3.3) together with formula (4.6). We have $[\bar{\rho}_t]_{m,n} = \text{Tr}(\bar{\rho}_t |\varphi_n\rangle\langle\varphi_m|)$, and it follows that

$$\begin{aligned} & [\bar{\rho}_t]_{m,n} - \langle\langle |\varphi_n\rangle\langle\varphi_m| \rangle\rangle_\infty \\ &= \sum_{\{e,s:\varepsilon_e^{(s)} \neq 0\}} e^{it\varepsilon_e^{(s)}} \left\langle \psi_0, Q_e^{(s)} [|\varphi_n\rangle\langle\varphi_m| \otimes \mathbb{1}_S] \psi_0 \right\rangle + O(\lambda^2 e^{-\omega't/2}). \end{aligned} \quad (5.1)$$

We leave out the trivial $\mathbb{1}_R$. Remembering that $\psi_0 = \psi_{S,\infty} \otimes \psi_R$, where $\psi_{S,\infty}$ is the trace state of S , represented by the vector $\frac{1}{\sqrt{N}} \sum_{j=1}^N \varphi_j \otimes \varphi_j$, we see that

$$[|\varphi_n\rangle\langle\varphi_m| \otimes \mathbb{1}_S] \psi_0 = \frac{1}{\sqrt{N}} \varphi_n \otimes \varphi_m \otimes \psi_R. \quad (5.2)$$

We shall treat in here the case where all resonance eigenvalues $\varepsilon_e^{(s)}$ are simple (the general case is dealt with in a similar fashion). Thus $Q_e^{(s)} = \frac{|\chi_e^{(s)}\rangle\langle\tilde{\chi}_e^{(s)}|}{\langle\chi_e^{(s)}|\tilde{\chi}_e^{(s)}\rangle}$ is a rank-one projection, with $K_\lambda(\omega)\chi_e^{(s)} = \varepsilon_e^{(s)}\chi_e^{(s)}$, $K_\lambda(\omega)^*\tilde{\chi}_e^{(s)} = \varepsilon_e^{(s)}\tilde{\chi}_e^{(s)}$ and with the normalization $\langle\chi_e^{(s)}|\tilde{\chi}_e^{(s)}\rangle = 1$. We expand the resonance eigenvectors in powers of λ ,

$$\chi_e^{(s)} = \eta_e^{(s)} \otimes \psi_R + O(\lambda), \quad \tilde{\chi}_e^{(s)} = \tilde{\eta}_e^{(s)} \otimes \psi_R + O(\lambda), \quad (5.3)$$

where $\eta_e^{(s)}$, $\tilde{\eta}_e^{(s)}$ are eigenvectors of the level shift operator Λ_e associated to the eigenvalue $\delta_e^{(s)}$ and its complex conjugate, respectively (see also before Theorem 3.2 and [11]). Λ_e acts on the eigenspace $P(L_S = e)$, and $\eta_e^{(s)}, \tilde{\eta}_e^{(s)} \in \text{Ran } P(L_S = e)$. We obtain

$$Q_e^{(s)} = |\eta_e^{(s)}\rangle\langle\tilde{\eta}_e^{(s)}| \otimes |\psi_R\rangle\langle\psi_R| + R_1(\lambda),$$

where R_1 satisfies $\langle\psi_R|R_1(\lambda)|\psi_R\rangle = O(\lambda^2)$. (This term is of order λ^2 and not only λ since the average of the interaction (3.1) vanishes in the vacuum state.) Combining (5.2) and (5.3) and setting $\varphi_{m,n} = \varphi_m \otimes \varphi_n$, we arrive at

$$\begin{aligned} & \left\langle \psi_0, Q_e^{(s)} [|\varphi_n\rangle\langle\varphi_m| \otimes \mathbb{1}_S] \psi_0 \right\rangle \\ &= \frac{\delta_{e=E_{n,m}}}{\sqrt{N}} \left\langle \psi_0, \eta_e^{(s)} \otimes \psi_R \right\rangle \left\langle \tilde{\eta}_e^{(s)}, \varphi_{n,m} \right\rangle + O(\lambda^2) \\ &= \frac{\delta_{e=E_{n,m}}}{\sqrt{N}} \sum_{\{l,k:E_{l,k}=e\}} \left\langle \psi_0, \varphi_{l,k} \otimes \psi_R \right\rangle \left\langle \varphi_{l,k}, \eta_e^{(s)} \right\rangle \left\langle \tilde{\eta}_e^{(s)}, \varphi_{n,m} \right\rangle + O(\lambda^2). \end{aligned}$$

(The δ is the Kronecker delta here.) The initial values are recovered from the first scalar product on the r.h.s.,

$$\frac{1}{\sqrt{N}} \left\langle \psi_0, \varphi_{l,k} \otimes \psi_R \right\rangle = \left\langle \psi_0, [|\varphi_l\rangle\langle\varphi_k| \otimes \mathbb{1}_S] \psi_0 \right\rangle = [\bar{\rho}_0]_{k,l}.$$

This shows that

$$\left\langle \psi_0, Q_e^{(s)} [|\varphi_n\rangle\langle\varphi_m| \otimes \mathbb{1}_S] \psi_0 \right\rangle = \delta_{e, E_{n,m}} \sum_{\{l,k: E_{l,k}=E_{n,m}\}} \sigma_{m,n;k,l} [\bar{\rho}_0]_{k,l} + O(\lambda^2), \quad (5.4)$$

where the “mixing coefficients” $\sigma_{m,n;k,l}^{(s)}$ are defined in Theorem 3.2. We use expression (5.4) in (5.1),

$$\begin{aligned} & [\bar{\rho}_t]_{m,n} - \langle\langle |\varphi_n\rangle\langle\varphi_m| \rangle\rangle_\infty \\ &= \sum_{\{e,s:\varepsilon_e^{(s)} \neq 0\}} e^{it\varepsilon_e^{(s)}} \left[\delta_{e, E_{n,m}} \sum_{\{l,k: E_{l,k}=E_{n,m}\}} \sigma_{m,n;k,l}^{(s)} [\bar{\rho}_0]_{k,l} + O(\lambda^2) \right] + O(\lambda^2 e^{-\omega' t/2}). \end{aligned} \quad (5.5)$$

The main term in the sum selects $e = E_{n,m}$ and only the summation over $s : \varepsilon_{E_{n,m}}^{(s)} \neq 0$ remains. This yields the dominant part in the r.h.s. of formula (3.5). The remainder is

$$\sum_{\{e:e \neq E_{n,m}, s:\varepsilon_e^{(s)} \neq 0\}} e^{it\varepsilon_e^{(s)}} O(\lambda^2) + O(\lambda^2 e^{-\omega' t/2}),$$

which is $O(\lambda^2 e^{-t\gamma_{m,n}})$, as indicated in Theorem 3.2. This concludes the proof of Theorem 3.2.

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