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# Completely positive Markovian quantum dynamics in the weak-coupling limit

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We obtain exponential decay laws for solutions of density-matrix master equations in the weak-coupling limit: after comparing with results already present in the literature and developing the necessary techniques, we study the crucial aspect of complete positivity under fairly general conditions. We propose a time average that guarantees complete positivity and approximates, in Markovian fashion, the exact dynamics for a plethora of physical applications, no matter which are the spectral properties of the subsystem, or its dimensions. We shall comment on some interesting examples, such as a quantum version of the celebrated Fermi's "golden rule" and some recently proposed entangling projections.

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## I. INTRODUCTION

After the pioneering works in 1974 and 1976 by Davies [1,2], a huge amount of physical information about the irreversibility and the evolution of open quantum mechanical systems has been gained. Alicky [3] showed in 1977 that these efforts were deeply connected to the celebrated Fermi's "golden rule" that now had become mathematically consistent. The conceptual importance of these works is clearly not only academic, as the need for a better understanding of irreversible processes has never been more urgent. Today, so many nanotechnologies are pushing devices towards limits where neither quantum phase coherence, nor dissipation or dephasing, can be neglected [4–6]. Many attempts to improve the theory have been made since then (see, for example, [7,8]), but despite the compelling need, no substantial, fundamental progress, directly applicable to nowadays technologies, has been made so far.

To be more specific, the problem is to understand the dynamics of a subsystem of interest, when the global system is fully coherent. In many cases, the dynamics of the global system can be splitted into a part that leaves the subsystem invariant, plus an interaction between the subsystem and the remaining "uninteresting" degrees of freedom. The problem then arises whether or not the subsystem can be given a Markovian, possibly dissipative, dynamics as a consequence of its interaction with those degrees of freedom. This is generally impossible of course, but it has been shown since the 1970s that a positive answer can be given when the amount of uninteresting degrees of freedom is huge, and the interaction is made small. This last condition is referred to as the "weak-coupling limit."

In [1] the author was able to give a solid physical model of a discrete "atom" (system  $A$ ) interacting with a fermionic particle reservoir at thermal equilibrium (environment  $B$ ). In that case, the subsystem was made of unentangled pairs of atomic states (also referred to as "density matrices") and a fermionic thermal equilibrium state, while all the entangled pairs just constituted the remaining, uninteresting, degrees of freedom. The model was of high conceptual importance, as

the Markovian (and dissipative) dynamics for the subsystem was shown to guarantee the state positivity at all times. This fact gave just enough internal robustness to the model as to be of invaluable practical use, for at any time, the subsystem evolution could be given a strong physical meaning. But the system  $A$  had to be finite dimensional, or at least, its unperturbed Hamiltonian was forced to have discrete spectrum.

Since then, much research has been (and currently is) focusing on the so-called "projection techniques." The name "projection" comes indeed from the fact that, as explained brilliantly in [9], a certain projection superoperator  $P_0$  is introduced:  $P_0$  "is the mathematical expression for the idea of the elimination of degrees of freedom from the complete description of the states of the total system." The effort here is to understand what could be the basic requirement for choosing the subsystem or  $P_0$  in order to guarantee a positive subsystem dynamics. Much information on the general properties of some bipartite subsystems has thus been gained [9–11], which is relevant in the field of (possibly entangled) open quantum systems, where one studies the dynamics of a "small" system  $A$  interacting with a "big" environment  $B$  (not necessarily at thermal equilibrium). Usually, one supposes to be given a generic "phenomenological" Markovian and dissipative dynamics for the global system, and writes down a (Markovian dissipative) master equation for the subsystem. But, as we shall see in the following, the strong interplay between the projection (i.e., subsystem) and the unperturbed global dynamics, severely restricts the possibilities for  $P_0$ , or on the other side, for the global system dynamics. For this reason, although these models are much relevant to nowadays technologies, they all still suffer from the original restriction, that system  $A$  should be finite dimensional, or at least it should have discrete spectral properties, similar to the original Davies' model [1]. We have to say here that alternative important methods have been addressed since a long time (see, for example, Ref. [12]), and still are (see [11]), which are based on stochastic techniques: these models are of course of enormous practical use, but since some randomness has to be put by hand, they are somehow of less fundamental nature.

Unfortunately, the possibility to obtain a "completely positive Markovian subsystem dynamics"—also referred to as quantum dynamical semigroups, or QDSs [13]—through the weak-coupling limit procedure, becomes no more avail-

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able when the system is infinite dimensional. In that case indeed Davies showed that a Markovian approximation, for the subsystem exact projected dynamics, could still be achieved [2], but positivity could not be shown in general, if not up to finite times: not even for the old and “safe” partial tracing over the thermal bath’s degrees of freedom. Although more general, the theory did not share the enormous success of the previous one among physicists, precisely because of this serious limitation. For example, all of the steady state analysis became, physically, completely meaningless.

In this work we follow the path set by Davies, in supposing the global system is undergoing a fully coherent (Hamiltonian) dynamics, and propose a master equation for the subsystem, on the basis of time-symmetry considerations. At this point, we will introduce an object, called “completed collision time,” which represents a safe overestimation of the subsystem relaxation times, as well as a safe underestimation of the global system recurrence time. This will be a key physical step, that is amply justified from the following well-known fact (see, for example, [13–15] among many others): the “semigroup” or Markovian approximation is physically meaningful only when neither we observe the subsystem at short times (where probabilities of excited states have a parabolic time dependence), nor we observe it long enough to see Poincaré recurrence cycles. Indeed these cycles are present, and explicitly appear in the subsystem exact dynamics, whenever the global dynamics is Hamiltonian. This time will scale with the coupling constant, and will serve us to “dynamically diagonalize” our time-symmetrized master equation, thereby eliminating in symmetric fashion most of the off-diagonal terms in the generator. We will then be able to show that our master equation will correctly describe the exact subsystem dynamics in the weak-coupling limit, it will be defined irrespective of the subsystem dimensions or spectral properties, and it will guarantee positivity for the dynamics, for a plethora of different projections and/or subsystems. The number of possible projections is indeed huge enough to incorporate the partial trace over the bath, together with some more recently proposed “entangling” projections [9,10], and some others by us, that furnish a quantum version for the Fermi’s “golden rule” (QFGR).

This deserves a comment: there are many proposed quantum generalization of the well-known Fermi’s “golden rule” [7,14], which are robust and physically and mathematically meaningful. All these generalizations consider a bipartite system (this in fact is the only way to propose the standard Fermi’s “golden rule” in mathematical terms, see [3]): nevertheless, the original idea by Fermi, although mathematically ill posed, did not come from any sort of (rather sophisticated) projection on some bipartite system. Stated in modern terms, Fermi’s idea was rather to take a global system and project on the space of density matrices, that are diagonal in the basis of the unperturbed Hamiltonian. His motivations referred to the fact that the system eigenvalues are “robust” against dissipation, and thus constitute the relevant degrees of freedom. Just along these lines, no environment will be present in our model of the QFGR, and the relevant degrees of freedom will be “box-diagonal” density matrices for a “box-diagonal” unperturbed Hamiltonian. The possibility to obtain a semigroup (a dissipative and Markov-

ian dynamics) comes exactly by the fact that the unperturbed Hamiltonian has continuous spectrum, thus conferring our QFGR version an autonomous relevance.

It is worth noting that the explicit form for our master equation in this case will share some very similar and interesting formal properties with some recently appeared master equations coming from the theory of entangled open quantum systems [8,10]. These, as ours, are linear homogeneous equations for a “composed” density matrix, which turn into a linear homogeneous system of equations for each component. Needless to say, these kind of equations are currently showing an enormous potential, and will be shown here to be taken into account by our general theory. But contrary to our QFGR, these models are all based on bipartite systems.

Two final introductory remarks. First, we have to say that, contrary to what is sometimes believed, a “diagonal” super-operator *does not* imply that the dynamics is free from quantum effects: first of all, diagonal refers to some basis, say, for example, that induced by some unperturbed Hamiltonian  $H_0$ . Then, talking in Heisenberg picture, it is true that a diagonal generator will leave a subset of observables—those commuting with  $H_0$ —invariant (and this would be a remarkable property). But the subsystem *needs not* be formed only by such a subset, and nontrivial commutation relations could well be observed within the subsystem evolution, even for “diagonal” generators. With respect to this, our theory is highly nontrivial, as it fully keeps track of quantum effects and does not, to any extent, constitute a sort of semiclassical limit. This is at variance, for example, with many widely used Green’s functions truncation schemes, where one takes “ $n$ -point” quantum correlations functions into account, but only up to some finite  $n$  (from this point of view, the weak-coupling and the Green’s function theories are applied in completely different contexts, a fact that is often misunderstood). Rather, the fact that a generator is diagonal in the unperturbed basis will be shown to be strictly linked with its algebraic properties, such as that of the positivity of its generated dynamics.

Finally, we have to say that we have made explicit use of Hilbert spaces instead of the (much more natural environment of) Banach spaces. This is justified by the fact that the Banach space  $\mathcal{T}(\mathcal{H})$  of trace class operators on a Hilbert space  $\mathcal{H}$  can be equipped with a scalar product, and the resulting completion is a Hilbert space (that of Hilbert-Schmidt operators on  $\mathcal{H}$ ). Our choice only comes from simplicity in the proofs involved, as we can make use a huge amount of spectral theory, but, of course, is still a rather serious limitation. Nevertheless we feel that our message could be extended to Banach spaces, and we are currently obtaining promising results in this direction. This indicates that the physical content of what we discuss here should survive the mathematical formalism, substantially unmodified. We also want to assure the less mathematically inclined (or more physically motivated) reader that our theorems, although mathematical statements, will be critically discussed within a fully self-contained physical contest, that will offer, so to say, the physical arguments that led us to the proofs. These will instead be reported in the appendixes, and are directed to the more mathematically oriented readers.

The paper is organized as follows: in the next section we begin with a warm up to clarify notations and state some

physical example to motivate our theory, which we then present. In Sec. III we discuss a time symmetrized Markovian generator and make contact with some preliminary results by one of us, reported in [16]; in Sec. IV we propose our dynamically time averaged generator; finally in Sec. IV we find some fairly general class of projections that make our generator into a Lindblad form [13], thus obtaining a generator of a (completely positive markovian) quantum dynamical semigroup. We will also discuss some (already cited) important applications, such as our quantum version of the Fermi's "golden rule" and some recently appeared entangling projection [9]. Then we shall conclude, and report our proofs in the Appendixes.

**II. GENERAL FRAMEWORK**

Let us briefly run through some well-known examples that will serve us to better state what we aim at, clarify notation, and motivate the general theory.

**A. Partial trace**

This is also referred to as "tracing away the bath degrees of freedom." Let  $\mathcal{H}=\mathcal{H}_A \otimes \mathcal{H}_B$  be the tensor product of two Hilbert spaces, representing a coupled system-environment pair. Let  $\mathcal{B}$  be the space of trace-class operators on  $\mathcal{H}$  and  $\mathcal{B}_0$  the space of trace-class operators on  $\mathcal{H}_A$ . These are Banach spaces, but they can be completed with the scalar product  $\langle A, B \rangle = \text{Tr}(A^\dagger B)$  to the Hilbert spaces [respectively,  $\mathcal{H}.S.(\mathcal{H})$  and  $\mathcal{H}.S.(\mathcal{H}_A)$ ] of Hilbert-Schmidt operators on the respective Hilbert spaces: we shall always work within these spaces, which we shall denote with the same letters  $\mathcal{B}$  and  $\mathcal{B}_0$ . Now define the linear map, called the "partial trace,"  $\bar{P}_0: \mathcal{B} \rightarrow \mathcal{B}_0$  uniquely determined by

$$\text{Tr}[\bar{P}_0(\rho)X_A] = \text{Tr}[\rho(X_A \otimes 1_B)] \tag{1}$$

for arbitrary  $\rho \in \mathcal{B}$  and bounded operator  $X_A$  on  $\mathcal{H}_A$ . If a state  $\sigma \in \mathcal{H}.S.(\mathcal{H}_B)$  is given on  $\mathcal{H}_B$ , then  $P_0\rho = \bar{P}_0(\rho) \otimes \sigma$  is a projection in  $\mathcal{B}$  with image  $\mathcal{B}_0$ , and is called "the partial trace." Then we have a direct sum decomposition

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1, \tag{2}$$

where  $\mathcal{B}_i = P_i(\mathcal{B})$  and we have put  $P_1 = 1 - P_0$ .

Now suppose we are given a Hamiltonian of the form  $H = H_0 + \lambda H_1$  with  $H_0 = H_A \otimes 1 + 1 \otimes H_B$  and  $H_1 = \sum_n \Phi_n \otimes \Psi_n$  (take all operators Hermitian). Call  $Z$  the generator of the one parameter group  $U_t$  of unitarities, on the global system  $\mathcal{B}$ , defined by the von Neumann equation

$$\partial_t \rho = -i[H_0, \rho] = Z\rho. \tag{3}$$

Then we have

$$U_t \rho = e^{Zt} \rho = e^{-iH_0 t} \rho e^{iH_0 t}. \tag{4}$$

And one obtains the all important (superoperator) commutation property

$$[Z, P_0] = 0. \tag{5}$$

This is telling us that the relevant degrees of freedom [the

subsystem  $\mathcal{B}_0 = P_0(\mathcal{B})$  do not interact with the irrelevant ones (the "superpolarization space"  $\mathcal{B}_1$ ] by means of the unperturbed dynamics  $U_t$ . This is a fundamental assumption that intrinsically links the projection  $P_0$  to the way the dynamics is splitted into a perturbation and an unperturbed one, and that should always be checked to avoid drastic mistakes: if this hypothesis is not verified, the whole theory of the weak-coupling limit simply breaks down.

At this point we introduce the perturbation superoperator  $A\rho = -i[H_1, \rho]$  so that we can state with precision what we aim at: we simply would like to know something about the projection at current time  $t$  of the unitary group describing the exact global Hamiltonian dynamics. That is, we want to study

$$\rho_t = P_0 e^{(Z+\lambda A)t} P_0 \rho = W_t^\lambda \rho \tag{6}$$

for a given initial condition  $\rho$  in  $\mathcal{B}$ . In passing, we have defined the subsystem evolution operator  $W_t^\lambda = P_0 e^{(Z+\lambda A)t} P_0$  (which of course is not a one parameter group of unitary transformations).

**B. Diagonal matrices in a closed quantum system**

This is close to the philosophy followed by Fermi. Let  $\mathcal{H} = \mathbb{C}^n$  be the  $n$ -dimensional Hilbert space over the complex field: then trace class operators are just  $n \times n$  matrices. Let these matrices form the total state space  $\mathcal{B}$ , and let a Hamiltonian  $H_0$  be given. Let  $|\alpha\rangle$  denote its eigenbasis, denote with  $\mathcal{B}_0$  the space of diagonal elements of  $\mathcal{B}$  in such basis, and define the projection  $P_0$  on  $\mathcal{B}_0$  by

$$P_0(\rho) = \sum_{\alpha=1}^n |\alpha\rangle \langle \alpha| \rho |\alpha\rangle \langle \alpha|. \tag{7}$$

Then as before one defines  $Z$  through  $H_0$  and gives a perturbation  $A$  through some Hermitian  $H_1$ . Obviously  $[Z, P_0] = 0$ , and the diagonal part of the evolution at time  $t$  of the initial state  $\rho$  in  $\mathcal{B}$  is  $\rho_t = P_0 e^{(Z+\lambda A)t} P_0 \rho = W_t^\lambda \rho$ .

**C. General theory**

We are ready to state the general theory: we suppose that  $P_0$  is a (not necessarily orthogonal) projection on a Hilbert space  $\mathcal{B}$ , put  $P_1 = 1 - P_0$  and  $\mathcal{B}_i = P_i \mathcal{B}$ , so that

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1. \tag{8}$$

We suppose that  $Z$  is the (skew-adjoint) generator of a strongly continuous one parameter group of unitarities  $U_t$  on  $\mathcal{B}$  with

$$U_t P_0 = P_0 U_t \tag{9}$$

for all  $t \in \mathbb{R}$ , or equivalently

$$[Z, P_0] = 0, \tag{10}$$

and put  $Z_i = P_i Z$ . We suppose that  $A$  is a bounded perturbation of  $Z$  and put  $A_{ij} = P_i A P_j$ . We shall always suppose, for simplicity, that no first-order terms are present for the subsystem. That is, we shall take  $A_{00} = 0$  all throughout. We let  $U_t^\lambda$  be the one parameter group generated by  $Z + \lambda A_{11}$  and let

$V_t^\lambda$  be the one parameter group generated by  $(Z + \lambda A)$ . Then putting

$$W_t^\lambda = P_0 V_t^\lambda P_0 \quad (11)$$

one obtains an exact and closed equation for the projected dynamics:

$$W_t^\lambda = U_t + \lambda^2 \int_{s=0}^t \int_{u=0}^s U_{t-s} A_{01} U_{s-u}^\lambda A_{10} W_u^\lambda ds du. \quad (12)$$

This is nothing but the integrated form of the well-known master equation constructed by Nakajima, Prigogine, Resibois, and Zwanzig [17,18].

It is a good moment here to note that, strictly speaking,  $P_0$  does not coincide with the physical subsystem: rather, the subsystem should be identified with the *image* of  $P_0$ , that is with  $\mathcal{B}_0$ . We will see that dissipative effects will be depending also upon the complete features of  $P_0$  itself, so *not only the relevant degrees of freedom  $\mathcal{B}_0$  determine the semigroup dynamics: also the way we look at them, with  $P_0$ , does influence the evolution.* With this in mind, we shall use the terms “subsystem” or “ $P_0$ ” equivalently, when there is no room for misinterpretations.

### III. TIME-SYMMETRIC MARKOVIAN APPROXIMATION

Changing variables to  $x=s-u$ ,  $\sigma=\lambda^2 u$  and introducing the time rescaled interaction picture dynamics  $W_\tau^{\lambda,i} = U_{-\lambda^{-2}\tau} W_{\lambda^{-2}\tau}^\lambda$ , one is led to [2]

$$W_\tau^{\lambda,i} = 1 + \int_{\sigma=0}^{\tau} U_{-\lambda^{-2}\sigma} K(\lambda, \tau - \sigma) U_{\lambda^{-2}\sigma} W_\sigma^{\lambda,i} d\sigma, \quad (13)$$

where

$$K(\lambda, \tau) = \int_0^{\lambda^{-2}\tau} U_{-x} A_{01} U_x^\lambda A_{10} dx. \quad (14)$$

This form separates an “interacting” and “slowly varying” part  $K(\lambda, \tau)$  from the “rapidly oscillating” free-evolution  $U_{\lambda^{-2}\sigma}$  to second order in the coupling constant  $\lambda$ . Now in the weak-coupling limit  $\lambda \rightarrow 0$ , the slowly varying integral kernel  $K(\lambda, \tau)$  converges to

$$K_D = \int_0^\infty U_{-x} A_{01} U_x A_{10} dx, \quad (15)$$

where  $K_D$  is the celebrated Davies’ superoperator. Substituting  $K_D \sim K(\lambda, \tau)$  in Eq. (13) and moving back to the “Schrödinger picture” we obtain the Markovian approximation for our subsystem dynamics

$$W_t^\lambda \sim \bar{W}_t^\lambda = e^{(Z_0 + \lambda^2 K_D)t}. \quad (16)$$

Indeed in [2] an important theorem shows that under reasonable and general conditions the approximation holds in the weak-coupling limit, up to  $\lambda^{-2}$ -rescaled times, independently of the subsystem dimensions or spectral properties. Unfortunately, although  $K_D$  is defined irrespective of the subsystem spectral properties, it does not guarantee positivity of the generated dynamics.

However, uniqueness of  $K_D$ , that is, of the semigroup approximation, is by no means to be expected: already in case  $\mathcal{B}_0$  is finite dimensional (or more generally when  $Z_0$  has discrete spectrum) one can define a time average of  $K_D$  (which takes the diagonal part of  $K_D$  in the  $Z$  supereigenbasis), and show that the generated dynamics is still asymptotic to the exact one in the weak limit. In the infinite dimensional case this averaging map is not generally defined, but still no physical argument would imply uniqueness.

With respect to this, we shall now propose a time-symmetrized Markov approximation: changing variable in Eq. (12) to

$$\begin{cases} \sigma = \frac{\lambda^2}{2}(s+u), \\ r = s-u, \end{cases} \quad (17)$$

and working again in the time-rescaled interaction picture, we obtain

$$W_\tau^{\lambda,i} = 1 + \int_{\sigma=0}^{\tau} U_{-\lambda^{-2}\sigma} \int_{r=0}^{\lambda^{-2}g(\tau,\sigma)} U_{-r/2} A_{01} U_r^\lambda A_{01} \times U_{-r/2} U_{\lambda^{-2}\sigma} W_{(\sigma+\lambda^2 r/2)}^{\lambda,i} d\sigma dr \quad (18)$$

with  $g(\tau, \sigma) = |\tau/2 - |\sigma - \tau/2||$ . Now we argue as follows: by direct inspection we see that in the weak-coupling limit  $\lambda \rightarrow 0$ , the function  $\lambda^{-2}g(\tau, \sigma)$ , defining the integration domain for the  $r$  variable, converges to

$$\lambda^{-2}g(\tau, \sigma) \rightarrow +\infty \quad (19)$$

for each  $\sigma \in (0, \tau)$ . But at the same time, the time-rescaled interaction picture dynamics moves slowly with respect to the  $r$  variable (again when  $\lambda \sim 0$ ), and this fact makes us guess that we can further approximate

$$W_{(\sigma+\lambda^2 r/2)}^{\lambda,i} \sim W_\sigma^{\lambda,i} \quad (20)$$

in the dynamics (18). Then, the “frozen” integral in the  $r$ -variable factors, and our integral equation can then be easily seen to turn into the Markovian subsystem evolution

$$\tilde{W}_t^\lambda = e^{(Z_0 + \lambda^2 K_R)t}, \quad (21)$$

with

$$K_R = \int_0^\infty U_{-x/2} A_{01} U_x A_{10} U_{-x/2} dx. \quad (22)$$

Here  $K_R$  is the superoperatorial and projected version of what Rossi proposes in [16], that also includes the second-order energy renormalization effects.

In fact, let us consider  $Z\rho = -i[H_0, \rho]$  and  $A\rho = -i[H', \rho]$  for self-adjoint  $H_0$  and (bounded)  $H'$  on a Hilbert space  $\mathcal{H}$ . Denoting  $A(t) = U_{-t} A U_t$  and  $H'(t) = e^{-iH_0 t} H' e^{iH_0 t}$ , we factor  $K_R = P_0 \tilde{K}_R P_0$  where

$$\begin{aligned} \tilde{K}_R \rho &= \int_0^\infty dx A\left(\frac{x}{2}\right) A\left(-\frac{x}{2}\right) \rho \\ &= - \int_0^\infty dx \left[ H' \left(-\frac{x}{2}\right), \left[ H' \left(\frac{x}{2}\right), \rho \right] \right], \end{aligned} \quad (23)$$

which in fact makes contact with the explicit form given in [16].

Clearly, starting from the interactions  $A_{ij}$ , the superoperator  $K_R$  is built in a much more time-symmetric fashion than  $K_D$ , as can be directly seen by inspection of Eq. (22). Of course, all our arguments here are but a physical motivation, and we must prove that our Markovian approximation indeed is consistent with the exact dynamics, at least up to  $\lambda^{-2}$ -rescaled times. From what we have stated here, we see that the main difficulty is to justify the fact that the convergence  $W_{(\sigma+\lambda^2 r/2)}^{\lambda,i} \rightarrow W_\sigma^{\lambda,i}$  is faster than the convergence  $g(\tau, \sigma) \rightarrow \infty$ , when  $\lambda \rightarrow 0$ , or alternatively, that the subsystem evolves slowly compared to a  $\lambda^{-2}$ -time scale, in the weak-coupling limit.

This problem presents surprising difficulties when  $\mathcal{B}$  is a general Banach space, but as we have said, it can be attacked with a spectral analysis when we suppose  $\mathcal{B}$  to be a Hilbert space, and the final answer is positive.

The idea is precisely to compare our Markov semigroup approximation with that of Davies (outlined before), and show compatibility when  $\lambda \rightarrow 0$ . Compatibility of our semigroup with the exact projected dynamics would then follow automatically, thanks to the work by Davies in [2]. What we do is to estimate the greatest difference between the two semigroups at times from zero up to time  $\lambda^{-2}\bar{\tau}$ , where  $\bar{\tau}$  is some initially, arbitrarily chosen, positive reference time. Then we show that this difference goes to zero in the weak-coupling limit. So we state the following:

*Theorem III.1.* Suppose that

$$\int_0^\infty \|A_{01} U_t A_{10}\| dt < \infty. \quad (24)$$

Then for every  $\bar{\tau} > 0$

$$\lim_{\lambda \rightarrow 0} \left\{ \sup_{0 \leq t \leq \lambda^{-2}\bar{\tau}} \|\bar{W}_t^\lambda - \tilde{W}_t^\lambda\| \right\} = 0. \quad (25)$$

We defer the proof to Appendix A, for the mathematically inclined readers, while we now think we have completely justified and commented the theorem from a physical point of view. But we still have to understand the physical meaning of the all-important hypothesis (24): the integrand  $\|A_{01} U_t A_{10}\|$  has a very simple interpretation as the “subsystem-to-superpolarization space supercorrelation function.” In fact, reading it from right to left, we start in our subsystem  $\mathcal{B}_0$ , interact and go into the “superpolarization space”  $\mathcal{B}_1$ , evolve with the unperturbed  $U_t$ , and finally interact a second time to land back into our subsystem  $\mathcal{B}_0$ . The norm is just the mathematical tool to evaluate how big such a superamplitude is. Our hypothesis is thus telling us that everything works fine if these correlations fall faster than  $1/t$  as the time  $t$  increases. That is, the superpolarization space  $\mathcal{B}_1$  is so huge that even though the global dynamics is

fully coherent and Hamiltonian, information leaves the subsystem very fast, at least from a given time on. This hypothesis obviously excludes from a Markovian approximation any finite (and even countably infinite) dimensional global system: in this case, the only things that one is going to see in its subsystems are nothing but some projected forms of never-damping Bloch oscillations. This explains the need to use an infinite-dimensional bath with continuous spectrum in Sec. II A, and the impossibility to observe dissipation in Sec. II B.

Unfortunately we are not finished yet, as the superoperator  $K_R$  does not generate a positive semigroup. But the effort we have done so far in symmetrizing the well-known usual Markovian approximation  $K_D$  will be completely paid in a moment: the idea is that  $K_R$  is, as  $K_D$ , highly nondiagonal in the  $Z_0$  eigenbasis. But contrary to  $K_D$ , the upper triangular part of  $K_R$  in such a basis perfectly mirrors its lower triangular part. So if now we could somehow remove the off diagonal terms in a simple symmetric fashion, we should be done in obtaining a fully diagonal superoperator. Needless to say in fact, a diagonal superoperator must be intrinsically linked with positivity features of its generated dynamics. But the term “diagonal part” must be handled with caution, as strictly speaking, it is a measure zero sector when the subsystem Hamiltonian spectrum is continuous. We shall thus here propose a “dynamic” version of the averaging map in [1], that extracts a diagonal “cloud” from  $K_R$  whose width goes to zero only in the limit  $\lambda \rightarrow 0$ . Let us see how.

#### IV. SPECTRAL DIAGONALIZATION AND COMPLETED COLLISION TIME

In [1] an averaging map is introduced: for an operator  $K: \mathcal{B}_0 \rightarrow \mathcal{B}_0$ , we put

$$K^\natural = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T dq U_{-q} K U_q, \quad (26)$$

whenever the right-hand side is defined. Then Davies shows in [2] that if  $\mathcal{B}_0$  is finite dimensional, then the operation  $\natural$  is well defined and completely recovers the exact subsystem dynamics in the weak limit.

Unfortunately, as said before, the spectral average  $\natural$  is not generally defined when the system Hamiltonian has continuous spectrum. We thus introduce a spectral averaging: we note that the integral over time in Eq. (26) can be extended to the entire real line by putting a  $T$ -related damping term inside the integral:

$$K^\natural = \lim_{T \rightarrow +\infty} \frac{1}{\sqrt{\pi T}} \int_{-\infty}^{\infty} dq e^{-q^2/T^2} U_{-q} K U_q. \quad (27)$$

The factor  $\sqrt{\pi}$  is needed for the two definitions of  $\natural$  to coincide when  $\mathcal{B}_0$  is finite dimensional: then the spectral decomposition

$$Z_0 = \sum_{\alpha} i\omega_{\alpha} Q_{\alpha} \quad (28)$$

gives

$$\begin{aligned}
 K^{\natural} &= \lim_{T \rightarrow +\infty} \frac{1}{2T} \int_{-T}^T dq e^{i(\omega_{\alpha} - \omega_{\beta})q} \sum_{\alpha\beta} Q_{\alpha} K Q_{\beta} \\
 &= \lim_{T \rightarrow +\infty} \frac{1}{\sqrt{\pi T}} \int_{-\infty}^{\infty} dq e^{-q^2/T^2} e^{i(\omega_{\alpha} - \omega_{\beta})q} \sum_{\alpha\beta} Q_{\alpha} K Q_{\beta} \\
 &= \sum_{\alpha} Q_{\alpha} K Q_{\alpha}
 \end{aligned} \tag{29}$$

for both definitions (26) and (27).

We may ask ourselves about the physical origin of this new object  $T$ : it appears that the higher its value, the finer is our ability to separate the system characteristic frequencies. This is exactly what happens when we tune our radio on a given frequency: the more we wait, the more precise we are in counting the transmitted oscillations, and thus the finer we are in resolving the wanted frequency. So this  $T$  looks similar to a subsystem observation time: we have to wait an infinite amount of time to resolve the system frequencies *exactly*, but it is everyday experience that we only have a *finite* (but long enough) observation time at our disposal. The idea is then to make use of such observation time  $T$  to compare with the subsystem relaxation times, and the global system recurrence times. It could be referred to as an “observation time” (but also, as we shall see later on, “completed collision time”): it is somewhat proportional to our instrumental uncertainty, or lack of precision, on the energy measurements we perform, since we study the system evolution only up to finite times. This way of understanding the origin of  $T$  is consistent with the fact that when  $Z_0$  has discrete spectrum, then the averaging map (26) is well defined. In fact, while we raise  $T$ , thus raising our energy measurements precision, we meet a finite value for  $T$  over which we are precise enough to unambiguously distinguish among the different system frequencies. This is not the case when the system frequencies (those of  $Z_0$ ) form a continuous set, as there is no finite value for  $T$  beyond which the system energy levels are distinguishable. In any case, our precision in measuring them becomes higher as we are able to increase  $T$ .

After having so understood the physical origin of  $T$  we could as well introduce a  $T$ -smoothed version of  $\tilde{K}_R$  [see Eq. (23) for notation],

$$\tilde{K}^T = \int_0^{\infty} dx e^{-(x/2)^2/T^2} A\left(\frac{x}{2}\right) A\left(-\frac{x}{2}\right), \tag{30}$$

which of course converges to the previous one in the limit  $T \rightarrow \infty$ , and put  $K^T = P_0 \tilde{K}^T P_0$ . Then we have yet another expression for the spectral average of  $K_R$ :

$$K_R^{\natural} = \lim_{T \rightarrow +\infty} K_T. \tag{31}$$

where we have defined

$$\begin{aligned}
 K_T &= \frac{1}{\sqrt{\pi T}} \int_{-\infty}^{\infty} dq e^{-q^2/T^2} U_{-q} K^T U_q \\
 &= \frac{1}{\sqrt{\pi T}} \int_{-\infty}^{\infty} dt_1 e^{-t_1^2/2T^2} A_{01}(t_1) \\
 &\quad \times \int_{-\infty}^{t_1} dt_2 e^{-t_2^2/2T^2} A_{10}(t_2),
 \end{aligned} \tag{32}$$

and in the last line we have changed variable to  $t_1 = q + x/2$  and  $t_2 = q - x/2$ . This last expression deserves some comments: first, it is probably the most symmetric thing that one could imagine to build from basic objects—such as  $P_0$ ,  $Z$ , and  $A$ —starting from the Nakajima-Zwanzig memory term in Eq. (12). Second, unlike our preliminary  $K_R$  in Eq. (22),  $K_T$  becomes more and more diagonal in the  $Z$  eigenbasis, as is evident by the procedure we use to obtain it. Third, the Gaussian smoothing—sometimes referred to as homogeneous broadening—seems not to be there by chance, or in other words, an exponential decay—also referred to as inhomogeneous broadening—would *not* allow one to so easily pass from the first line to the second in Eq. (32). In fact, the Gaussian is the only distribution  $\Phi$ , such that

$$\Phi(q^2 + (x/2)^2) = \Phi((t_1^2 + t_2^2)/2) \tag{33}$$

for  $t_1 = q + x/2$  and  $t_2 = q - x/2$ .

Now the important thing to note is that the limit  $T \rightarrow 0$  is well defined, as said above, only when  $\mathcal{B}_0$  is finite dimensional, or more generally when  $Z_0$  has discrete spectrum, but, for finite values of  $T$ ,  $K_T$  and  $\tilde{K}_T$  are always well defined, no matter which are the spectral properties of  $Z_0$  nor the dimension of  $\mathcal{B}_0$ , and moreover we can write  $\tilde{K}_T$  explicitly as

$$\begin{aligned}
 \tilde{K}_T \rho &= \frac{1}{\sqrt{\pi T}} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 e^{-t_1^2 + t_2^2/2T^2} [H'(t_1), [H'(t_2)]] \\
 &= -i[H_T^{(2)}, \rho] - [\mathcal{L}_T, [\mathcal{L}_T, \rho]],
 \end{aligned} \tag{34}$$

where both

$$H_T^{(2)} = \frac{i}{2\sqrt{\pi T}} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 e^{-t_1^2 + t_2^2/2T^2} [H'(t_1), H'(t_2)] \tag{35}$$

and

$$\mathcal{L}_T = \sqrt{\frac{1}{2\sqrt{\pi T}}} \int_{-\infty}^{\infty} dt e^{-t^2/2T^2} H'(t) \tag{36}$$

are self-adjoint operators on  $\mathcal{H}$ . This puts  $\tilde{K}_T$  in explicit Lindblad form, and shows that  $Z + \lambda^2 \tilde{K}_T$  is a generator of a (completely positive) quantum dynamical semigroup (QDS) for any finite value of  $T$  (see [13]). This is possible thanks to the symmetric definition of  $K_R$ : a similar treatment of  $K_D$  would not allow one to reach these conclusions, and this explains the effort we have made so far to justify the semigroup generated by  $K_R$  in the weak limit. Of course we are not yet completely done as far as positivity is concerned: one would like to show positivity for the projected  $K_T$  rather than

for the unphysical  $\tilde{K}_T$  (we will comment on this later). We shall see in the sequel that under fairly general conditions on  $P_0$ ,  $K_T$  generates a completely positive QDS whenever  $\tilde{K}_T$  does.

Another key issue concerns the weak limit: if  $T$  is kept fixed, than of course the generated semigroup fails to describe the exact evolution when  $\lambda \rightarrow 0$ , while all of our approximations hold only in that case. The idea is then to allow a  $\lambda$  dependence

$$T(\lambda) \sim |\lambda|^{-\xi} \tilde{T}, \quad \lambda \rightarrow 0 \tag{37}$$

(we shall soon be more precise on this asymptotic behavior, thanks to our next theorem). This dispenses us to actually compute the limit  $\lim_{T \rightarrow \infty} K_T$ , that would not be defined in general, before performing the weak-limit  $\lambda \rightarrow 0$ , and simply merges the weak-coupling and the collision limits together. The physical origin of  $T$  again helps us to understand the content of this rather abstract procedure: when we decrease  $\lambda$  we have to increase the time variable with  $\lambda^{-2}t$ , and so also the time  $T$  needed to observe the system, and resolve its frequencies, increases. From the mathematical point of view, constructing the averaging map together as the weak-limit  $\lambda \rightarrow 0$  is performed, allows  $K_T = K_{T(\lambda)}$  to be well defined, and to generate a completely positive QDS, every step of the way, and as we now state, to correctly describe the exact dynamics in the weak limit.

Now we recall that we defined as

$$\tilde{W}_t^\lambda = e^{(Z_0 + \lambda^2 K_R)t} \tag{38}$$

the semigroup dynamics generated by  $K_R$  and we give the following:

*Theorem IV.1.* Suppose an ‘‘observation time’’  $T(\lambda)$  is given, with the asymptotic behavior reported in Eq. (37) for some  $\tilde{T} > 0$  and real  $\xi$ , and call

$$\hat{W}_t^\lambda = e^{(Z_0 + \lambda^2 K_{T(\lambda)})t} \tag{39}$$

the generated dynamics. Suppose that

$$\int_0^\infty \|A_{01} U_t A_{10}\| dt < \infty. \tag{40}$$

Then for every  $\bar{\tau} > 0$  and  $0 < \xi < 2$  we have

$$\lim_{\lambda \rightarrow 0} \left\{ \sup_{0 \leq t \leq \lambda^{-2} \bar{\tau}} \|\tilde{W}_t^\lambda - \hat{W}_t^\lambda\| \right\} = 0. \tag{41}$$

As with our previous theorem, we defer the proof to Appendix B for the mathematically inclined reader. The physical argument that lets us understand why we must suppose the asymptotics  $0 < \xi < 2$  refers to some difficulty already encountered: here we are saying that *not only* the subsystem time-rescaled interaction picture evolution moves slowly with respect to the  $r$  variable in Eq. (20), but *it also moves slowly with respect to our observation time*  $T(\lambda)$ . This obviously fixes the scale  $\xi < 2$ . The remaining inequality  $0 < \xi$  has already been discussed when we underlined the need to make  $T$  go to infinity in the weak coupling.

As promised, we can now make some physical guess on the observation time  $T$ : we know that it must scale with  $|\lambda|^{-\xi}$

with  $0 < \xi < 2$  strictly. The most natural case  $\xi = 1$  seems appropriate. Now, the meaning of  $T$  is that of the time needed to observe the subsystem: we could argue that we must observe it for a long time, if the interaction  $A$  is small. So we may tentatively propose

$$T(\lambda) = \frac{1}{|\lambda| \|A\|} \tag{42}$$

In fact, this is to us the only ‘‘physical’’ time that can be constructed to satisfy the stated properties, starting from known features belonging to the original global system dynamics: in fact, it is clear that  $T$  must be ascribed to some relaxation process, which, in our theory, are brought by the perturbation  $A$ —the energy brought by  $Z$ , instead, just makes the system (and the subsystem) rotate with unitarities. Here the norm of the perturbation  $A$  has a simple meaning: it is the greatest eigenvalue of  $A$ . This is indeed finite, as we are supposing  $A$  to be bounded, and represents the greatest internal energy transition, brought by the perturbation, that leaves some density matrix invariant. Then, the highest is such a transition, the smaller the amount of time we need to observe a subsystem relaxation. This explains the name ‘‘completed collision time,’’ according to Eq. (42), the more energy is brought by our perturbation, the less is the time required to observe the subsystem relaxation. This is precisely what happens with our radio: the time we need to reach some fixed tuning precision depends on how high the frequency is that we look for.

We have shown that the exact dynamics is well described up to arbitrary long times  $\lambda^{-2} \bar{\tau} > 0$  by the (Markovian) semigroup  $\hat{W}_t^\lambda$  in the weak coupling limit. Such dynamics has been shown to be always well defined, irrespective of the subsystem spectral properties.

## V. POSITIVITY

We have already shown that in the (physically interesting and fairly general) case  $Z\rho = -i[H_0, \rho]$  for a self-adjoint  $H_0$  on a Hilbert space  $\mathcal{H}$  and  $A\rho = -i[H', \rho]$  ( $H'$  self-adjoint), then the dynamics generated by  $Z + \lambda^2 \tilde{K}_T$  is completely positive for any given  $T > 0$ , as the generator itself has been written in Lindblad form

$$\tilde{K}_T \rho = -i[H_T^{(2)}, \rho] - [\mathcal{L}_T, [\mathcal{L}_T, \rho]]. \tag{43}$$

This generator is physically completely meaningless if not projected, as it neither describes the global, Hamiltonian, dynamics, nor describes the subsystem projected dynamics: we shall make use of it only for convenience in some intermediate step, always remembering that the final results only come from its projected version  $K_T$ .

We now proceed to a simple analysis to determine some fairly general conditions on the projection  $P_0$  under which the superoperator  $\mathbb{L}_{\lambda T} = Z_0 + \lambda^2 K_T$  can also be put in Lindblad form, and thus generate a (completely positive) QDS. In what follows, we shall make use of the dual  $\tilde{P}_0$  of  $P_0$ , written in Heisenberg picture: the two objects will thus be linked by the duality  $\text{Tr}[P_0(\rho)X] = \text{Tr}[\rho \tilde{P}_0(X)]$ .



*Theorem V.1.* Suppose  $\tilde{P}_0$  is a completely positive projection on the observable space  $B(\mathcal{H})$ , so that it has Krauss decomposition

$$\tilde{P}_0 X = \sum_{\alpha \in \mathcal{I}} V_\alpha^\dagger X V_\alpha \quad (44)$$

for some operators  $V_\alpha$  on  $\mathcal{H}$ , and (possibly uncountably infinite) indexing set  $\mathcal{I}$ .

Suppose that  $\tilde{P}_0$  maps the observable space  $B(\mathcal{H})$  onto the subalgebra of observables  $\mathcal{X}$  defined as follows:  $X \in \mathcal{X}$  if and only if for every  $\alpha$

$$[X, V_\alpha] = [X, V_\alpha^\dagger] = 0. \quad (45)$$

Suppose also that  $\tilde{P}_0(1)=1$ , and that  $\tilde{P}_0$  is dual to the (completely positive projection)  $P_0$  on the state space of trace-class operators  $\mathcal{T}(\mathcal{H})$ .

Then for all real  $\lambda$  and  $T > 0$ , the operator  $L_{\lambda T} = Z_0 + \lambda^2 K_T$  generates a (completely positive and trace preserving) quantum dynamical semigroup.

*Proof.* We consider

$$L_{\lambda T} = P_0(Z + \lambda^2 \tilde{K}_T)P_0, \quad (46)$$

and note that  $Z + \lambda^2 \tilde{K}_T$  is dual to a generator

$$\tilde{L}_{\lambda T} X = i[\tilde{H}_{\lambda T}, X] - \frac{\lambda^2}{2} \{ \mathcal{L}_T \mathcal{L}_T, X \} + \lambda^2 \mathcal{L}_T X \mathcal{L}_T \quad (47)$$

of a completely positive QDS on  $B(\mathcal{H})$ , for the self-adjoint

$$\tilde{H}_{\lambda T} = H_0 + \lambda^2 H_T^{(2)} \quad (48)$$

[see Eqs. (35) and (36) for explicit expressions]. Then for  $X \in \mathcal{X}$  and  $\rho \in \mathcal{B}_0$  we have

$$\text{Tr}[L_{\lambda T}(\rho)X] = \text{Tr}[\rho \tilde{P}_0\{(Z + \lambda^2 \tilde{K}_T)X\}] = \text{Tr}[\rho \tilde{L}_{\lambda T}(X)], \quad (49)$$

for the superoperator

$$\tilde{L}_{\lambda T} = \tilde{P}_0(Z + \lambda^2 \tilde{K}_T) \quad (50)$$

on  $\mathcal{X}$ . Using the fact that every  $X \in \mathcal{X}$  commutes with  $V_\beta^{(\dagger)}$  we compute

$$\begin{aligned} \tilde{L}_{\lambda T} X &= i \left[ \sum_{\beta} V_{\beta}^{\dagger} \tilde{H}_{\lambda T} V_{\beta}, X \right] - \frac{\lambda^2}{2} \sum_{\beta} \{ V_{\beta}^{\dagger} \mathcal{L}_T \mathcal{L}_T V_{\beta}, X \} \\ &\quad + \lambda^2 \sum_{\beta} V_{\beta}^{\dagger} \mathcal{L}_T X \mathcal{L}_T V_{\beta}. \end{aligned} \quad (51)$$

Inserting the completeness relation  $\sum_{\alpha} V_{\alpha}^{\dagger} V_{\alpha} = 1$ , which follows from  $\tilde{P}_0(1)=1$ , we obtain the Lindblad form

$$\begin{aligned} \tilde{L}_{\lambda T} X &= i \left[ \sum_{\beta} V_{\beta}^{\dagger} \tilde{H}_{\lambda T} V_{\beta}, X \right] - \frac{\lambda^2}{2} \sum_{\alpha, \beta} \{ (V_{\beta}^{\dagger} \mathcal{L}_T V_{\alpha}^{\dagger})(V_{\alpha} \mathcal{L}_T V_{\beta}), X \} \\ &\quad + \lambda^2 \sum_{\alpha, \beta} (V_{\beta}^{\dagger} \mathcal{L}_T V_{\alpha}^{\dagger}) X (V_{\alpha} \mathcal{L}_T V_{\beta}) \\ &= i[\tilde{P}_0(H_0), X] + \lambda^2 \left( i[\tilde{P}_0(H_T^{(2)}), X] \right. \end{aligned}$$

$$\left. - \frac{1}{2} \sum_{\alpha\beta} \{ D_{\alpha\beta}^T \dagger D_{\alpha\beta}^T, X \} + \sum_{\alpha\beta} D_{\alpha\beta}^T \dagger X D_{\alpha\beta}^T \right) \quad (52)$$

for scattering operators

$$D_{\alpha\beta}^T = V_{\alpha} \mathcal{L}_T V_{\beta} \quad (53)$$

defined on  $\mathcal{X}$ . This shows that  $L_{\lambda T} = Z_0 + \lambda^2 K_T$  generates a completely positive QDS on  $\mathcal{B}_0$  through its dual  $\tilde{L}_{\lambda T}$  on  $\mathcal{X}$ : this is so indeed, precisely because

$$\text{Tr}[e^{L_{\lambda T} t}(\rho)X] = \text{Tr}[\rho e^{\tilde{L}_{\lambda T} t}(X)]. \quad (54)$$

This completes the proof.  $\blacksquare$

As we see, the proof is fully constructive and gives an explicit form for our Lindblad generator, starting directly from fundamental objects that define the model, either algebraically through the projection, or dynamically through the global system Hamiltonian.

Before making some examples to show the flexibility of this whole theory, let us comment here on what we believe to be a widely spread misunderstanding: the projected superoperator  $Z + \lambda^2 \tilde{K}_T$ , for example, in Eq. (46), cannot be chosen at will. In other words, to take a general Lindblad operator  $L$  and project it with some given  $P_0$ , for studying the positivity of the dynamics  $e^{P_0 L t}$ , is not meaningful. We have shown that it is meaningful when  $L$  comes from some Markovian approximation that already involves the projection  $P_0$ , through the condition that no subsystems first-order energy renormalization is present ( $A_{00} = P_0 A P_0 = 0$ ). It could be argued that this last condition is not at all necessary, and only comes from simplicity in the proofs involved. This is true indeed, but it does not gauge the problem away: in the general case  $A_{00} \neq 0$ , the Nakajima, Prigogine, Resibois, and Zwanzig master equation (12) tells us that, whatever the Markovian approximation may be, it should have a projection  $P_0$  to the right as well as to the left, and an unavoidable  $P_1 = 1 - P_0$  in the middle. So once again, this rich and intrinsic dependence between the dynamics and the projection cannot be causally factored: no one comes first. Said in other words, the (highly nontrivial) dynamics of interest  $P_0 e^{L t} P_0$ , is simply *different* from  $e^{P_0 L P_0 t}$ , at least in general. We restate that, if  $A_{00} = 0$  and  $[Z, P_0] = 0$ , we have proven that

$$P_0 e^{(Z + \lambda A)t} P_0 \sim e^{(Z_0 + \lambda^2 K_{T(\lambda)})t}, \quad \lambda \sim 0 \quad (55)$$

up to  $\lambda^{-2}$ -rescaled times (we refer to our Theorem IV.1 for a more precise formulation), and the right-hand side is a positive map at any time if  $P_0$  fulfills the hypotheses of our Theorem V.1.

We can make a trivial counterexample along these lines: if one is given a global Hamiltonian dynamics  $L\rho = -i[H_0 + \lambda H', \rho]$ , and  $\rho$  is in the image of  $P_0$ , then  $P_0 L \rho = -i[P_0(H), \rho]$  not only does not give any dissipative effect, but also (we have now abundantly shown that) *it does not catch up with the exact projected dynamics*  $P_0 e^{L t} P_0$  (that we have been studying all throughout), not even in the case of the weak-coupling limit when  $H = H_0 + \lambda^2 H'$  and  $\lambda$  is small, and not even in case  $[Z, P_0] = 0$ .

This shows that the different projection techniques, that have been studied so far by various groups, all suffered from

the *dynamical* restrictions present in Davies' theory [1]. That is, one was forced to require (a global Hamiltonian dynamics and) that the subsystem Hamiltonian has discrete spectrum. Our work here has thus been devoted to free oneself from this restriction. This allows one to study projections (i.e., subsystems) in a much more general context, and we shall give an important example of this, straight away. We have to say that our analysis still suffers from the restriction  $A_{00}=0$ . But so did Davies's analysis in [1], and moreover we are currently obtaining already very encouraging results in the more general case  $A_{00} \neq 0$ .

### A. Quantum Fermi's "golden rule"

As a first important example, suppose  $V_\alpha = V_\alpha^\dagger$  are mutually orthogonal projections on the Hilbert space  $\mathcal{H}$ , and call the "quantum populations"

$$\rho_\alpha = V_\alpha \rho V_\alpha \tag{56}$$

for a given  $\rho \in \mathcal{B}_0$ . Suppose also that  $[P_0, Z]=0$ , with  $Z\rho = -i[H_0, \rho]$ , so that  $H_0 = \sum_\alpha H_\alpha$  with

$$V_\beta H_\alpha V_{\beta'} = \delta_{\alpha\beta} \delta_{\alpha\beta'} H_\alpha, \tag{57}$$

and put  $A\rho = -i[H', \rho]$ . Then the operators  $D_{\alpha\beta}^T$  in Eq. (53) can be interpreted as "quantum transition rates" among the "quantum populations"  $\{\rho_\alpha\}$ , and one obtains an evolution

$$\begin{aligned} \partial\rho_\alpha = & -i[H_\alpha, \rho_\alpha] + \lambda^2 \left( -i[H_{T,\alpha}^{(2)}, \rho_\alpha] - \frac{1}{2} \sum_\beta \{D_{\beta\alpha}^T D_{\beta\alpha}^T \rho_\alpha\} \right. \\ & \left. + \sum_\beta D_{\alpha\beta}^T \rho_\beta D_{\alpha\beta}^T \right) \end{aligned} \tag{58}$$

(with  $H_{T,\alpha}^{(2)} = V_\alpha H_T^{(2)} V_\alpha$ ) that in fact couples the different "quantum populations" and/or density matrices and guarantees positivity of each  $\rho_\alpha$ , as one can easily see. Since the projections are mutually orthogonal ( $V_\alpha V_\beta = \delta_{\alpha\beta} V_\beta$ ), the sum over the index  $\beta$  in the last equation can be restricted on all values such that  $\beta \neq \alpha$ , as the condition  $A_{00}=0$  amounts to  $D_{\alpha\alpha}^T = 0$ , as can easily be seen.

The generator in Eq. (58) for  $P_0\rho$ , or alternatively this coupled linear system for density matrices  $\rho_\alpha$ , is of special interest, as it is a clear generalization of the classical Fokker-Planck equation, and on the other hand it is peculiar to the case  $\mathcal{B}_0$  is not finite dimensional and  $Z_0$  has continuous spectrum. In fact, only in these conditions one can hope to show that

$$\int_0^\infty \|A_{01} U_t A_{10}\| dt < \infty, \tag{59}$$

which is a necessary requirement for all the theorems on the weak limit that have been proven by us here and by Davies in [1,2]. Again, as said before, one could say that only when the free Hamiltonian spectrum is continuous, the "polarizations"  $V_\alpha \rho V_\beta$  ( $\alpha \neq \beta$ ) contain enough degrees of freedom to allow an exponentially decaying solution instead of Bloch oscillations. Current work on the possibility of applying these ideas to the theory of quantum transport are being addressed by us. As it is, Eq. (58) could thus be addressed as a

quantum Fermi's "golden rule," as the "quantum populations"  $\rho_\alpha$  are in fact (positive definite) density matrices rather than (positive) real numbers.

Note also that Eq. (58) is a linear homogeneous system of (dissipative) master equations that guarantees conservation of a "global trace," i.e.,  $\text{Tr}(\sum_\alpha \rho_\alpha) = \text{const}$ , and positivity at all times for each quantum population  $\rho_\alpha$ . This presents striking formal similarities with a very recent work [9], where the author discusses a most interesting "entangling" projection on bipartite systems that could be thought of as a generalization of the usual partial trace projection. There, as here, the author arrives to a linear homogeneous system of (dissipative) master equations describing (in his case) the dissipative and/or decoherent interplay among the different entangled sectors that make up the subsystem density matrix. Now, from one side, we will show in a moment that this entangling projection can be easily incorporated in our theory, as it is a particular (but maybe not so much) case of the projections we consider in Theorem V.1. From another side, our example here is different in that *it does not refer to a bipartite system*: our subsystem is, so to say, closed, with no environment whatsoever, and with none of its subsectors  $\rho_\alpha$  decohering to any given thermal state. This could implement the idea of many systems interacting together, and finally decohering to a steady state just because information continuously (and irreversibly) flows from them to their quantum polarization space. This we feel is much closer to the original idea that led Fermi to his celebrated Fermi's "golden rule" [14], as contrary to what has been done in recent years (see, for example, [7]), he did *not* consider bipartite systems, nor the idea that information irreversibly flew from a system to an environment. Rather, information was lost in the system polarizations for some unperturbed Hamiltonian basis, and this is exactly what we do here, extending his Fokker-Planck dynamics [19] among (positive) populations to a quantum Fokker-Planck dynamics among (positive definite) density matrices.

It could be argued that our generator is unphysical, or unsubstantial, as it completely disappears (it goes to zero) in the limit  $T \rightarrow 0$ . We hope to have here reported enough physical (and mathematical) evidence that such a procedure *should not* be undertaken [this is clear, for example, by looking at Eq. (42)]. Rather, one could, for example, study the steady states  $\rho = \rho(T)$  as a function of the collision time  $T$ , and *only at that point* perform the limit  $\rho_{\text{steady}} = \lim_{T \rightarrow \infty} \rho(T)$ . This limit will of course give a nontrivial result. The situation here is very similar to that of the weak coupling limit, at variance with the thermodynamical limit: the two limits simply *do not commute*, and the order to be taken depends upon one's interest, as justified on physical grounds. Our argument for the completed collision limit  $T \rightarrow \infty$  is, again, that the semigroup approximation holds only for intermediate times  $T$ , between the subsystem relaxation times and the global Poincaré recurrences (see, for example, [14], or the brilliant exposition in [15]). Thus, it must be finite every step of the way, and be brought to infinity only in a second step. There is one notable exception to this: precisely when the free Hamiltonian spectrum is discrete, there will be a finite  $T$  (as said before) over which we will clearly distinguish among all the different frequencies. If we used a higher  $T' > T$ , the

physics will then be left unchanged, exactly because we already reached infinite precision with  $T$ . This explains, physically and mathematically, the reason why one could free himself of  $T$  in the discrete case, by letting it go to infinity.

So we understand why we all had to study the FGR in the (rather cumbersome) case of a free Hamiltonian with mixed spectrum [15]: on one side, one needs a continuous spectrum to hope to see dissipation, but on the other side, the diagonal part of the scattering operator is well defined only in the discrete case. The only way out seems to force the interacting Hamiltonian communicate between the discrete and the continuous part of the free one. Here what we do is essentially to relax the condition that the relevant degrees of freedom are the free Hamiltonian eigenvalues, and rather take them as diagonal boxes. Our model is thus fully preserving the quantum features within each sector.

### B. Entangling projection

As promised, we shall now make contact with the work in [9] and show how the projections there considered can be implemented in our formalism. We just here anticipate that this is going to be a generalization of the standard trace projection over the bath. Let  $\mathcal{H}=\mathcal{H}_A \otimes \mathcal{H}_B$  be the tensor product of two Hilbert spaces, representing a coupled system-environment pair. Let  $\mathcal{B}=\mathcal{T}(\mathcal{H})$  be the space of trace-class operators on  $\mathcal{H}$ , and  $B(\mathcal{H})$  the observable algebra of bounded operators on  $\mathcal{H}$  (the same goes for  $\mathcal{H}_A$  and  $\mathcal{H}_B$ ).

Take a finite number  $C_n$  and  $D_n$  ( $n=1, \dots, N$ ), of operators in  $B(\mathcal{H}_B)$ , such that

$$D_n^\dagger D_{n'} = \delta_{nn'} B_n \quad (60)$$

for (positive definite) trace-class  $B_n=D_n^\dagger D_n$  in  $\mathcal{T}(\mathcal{H}_B)$ . Name the (positive definite) operators

$$A_n = C_n^\dagger C_n \quad (61)$$

in  $B(\mathcal{H}_B)$  and suppose

$$\sum_{n=1}^N A_n = 1, \quad (62)$$

$$A_n A_{n'} = \delta_{nn'} A_n, \quad (63)$$

and

$$\text{Tr}(A_n B_{n'}) = \delta_{nn'}. \quad (64)$$

Take a basis  $\{|\alpha\rangle\}$  of  $\mathcal{H}_B$ , and define the operators

$$V_{\alpha\alpha'} = 1_A \otimes \sum_{n=1}^N D_n^\dagger |\alpha\rangle \langle \alpha'| C_n \quad (65)$$

on  $\mathcal{H}$ . With these operators define the completely positive map  $\tilde{P}_0$  on  $B(\mathcal{H})$  by

$$\tilde{P}_0 X = \sum_{\alpha\alpha'} V_{\alpha\alpha'}^\dagger X V_{\alpha\alpha'}. \quad (66)$$

This map can be checked to be a projection thanks to the hypotheses (60) and (64). The completeness hypothesis (62)

guarantees that  $\tilde{P}_0(1)=1$ , and hypothesis (63) guarantees that  $\mathcal{X}=\tilde{P}_0(B(\mathcal{H}))$  is a subalgebra of the global observable algebra  $B(\mathcal{H})$ . So  $\tilde{P}_0$  fulfills the hypotheses of our Theorem V.1. In particular, one can see that the projected subalgebra is

$$\mathcal{X} = \left\{ X \in B(\mathcal{H}) \mid X = \sum_{n=1}^N X_n \otimes A_n, X_n \in B(\mathcal{H}_A) \right\}. \quad (67)$$

Using our hypotheses we then compute

$$P_0 \rho = \sum_{\alpha\alpha'} V_{\alpha\alpha'} \rho V_{\alpha\alpha'}^\dagger = \sum_n \text{Tr}_B[\rho(1 \otimes A_n)] \otimes B_n, \quad (68)$$

which is precisely Eq. (12) in [9]. Then it is possible to check that  $P_0$  is also a (completely positive) projection, precisely because of hypothesis (64). Our procedure used to obtain it is however different from [9], and it would be surely worth the effort to compare the two approaches further. For example, the only common hypothesis to obtain such an entangling projection is our equation (64), which in [9] is Eq. (6), while it seems to us that all other hypotheses differ in the two approaches.

But the most fundamental difference is that here we have to satisfy, as amply discussed before, a dynamical compatibility hypothesis, that intrinsically links  $P_0$  with the form of the Lindblad operator that one wants to project. We have shown that if one starts from a free Hamiltonian dynamics,  $Z\rho=-i[H_0, \rho]$  and perturbs with  $\lambda A\rho=-i\lambda[H', \rho]$ , then one arrives to a Lindblad generator for the projected subsystem if  $[Z, P_0]=0$ , or alternatively if  $[U_t, P_0]=0$  for all times. For example, if, as normally assumed, the unperturbed Hamiltonian is of the form  $H_0=H_A \otimes 1 + 1 \otimes H_B$ , this *dynamical commutation condition for the subsystem* can be checked to be fulfilled *if and only if* for every  $n=1 \dots N$  we have

$$[H_B, A_n] = [H_B, B_n] = 0. \quad (69)$$

Then we have proven that *if*  $A_{00}=0$  our dynamics correctly describes the exact projected dynamics in the weak limit, and is a (completely positive Markovian) quantum dynamical semigroup. If then one would like to take  $A$  as a Lindblad generator (instead of a safe self-adjoint derivation) things would become much more complex, as in any case one should always prove that  $X_t^\lambda = e^{(Z_0 + \lambda A_{00})t}$  is a group of isometries (see [2]), which gives nontrivial conditions on  $A_{00}$ , when the latter is switched on (again a condition that links the choice of  $P_0$  to the dynamics). This leaves the possibility that  $A - A_{00}$  is dissipative while  $A_{00}$  is a self-adjoint derivation (i.e., it comes from a Hamiltonian): again, we are currently working on this interesting and important path. But we have to remember that the perturbation must have a “ $\lambda$ ” attached to it, and the (dissipative) subsystem will describe the projected (phenomenological and dissipative) global dynamics, only up to second order in  $\lambda$ , when  $\lambda \sim 0$ .

### VI. REMARKS AND CONCLUSION

Although all our results suffer from being restricted to Hilbert spaces, we feel very confident in saying that they can be extended to more general (and natural) Banach spaces,

and we are currently working on that promising direction.

Another severe restriction is our hypothesis  $A_{00}=0$  of absence of first-order subsystem energy renormalizations. Just as before, we currently obtaining very promising results in effort to free the theory from this restriction.

Apart from these key remarks, we have shown that, under the only consistency with the weak-coupling limit, the Markovian approximation of the memory terms in the quantum mechanical master equation is far from unique. We found a generator for a quantum dynamical semigroup that generalizes more standard approaches, and contrary to them guarantees both consistency in the weak limit and complete positivity, irrespective of the spectral properties of the system. We have thus been able to propose a quantum generalization of the celebrated Fermi's "golden rule," giving an unprecedented linear homogeneous system of (dissipative) master equations *for a closed subsystem* that guarantees positivity at all times for each of the subsystem sectors. It is worth noting that our model requires a continuous spectrum for the free Hamiltonian, and thus is peculiar to our general theory. We have also shown that our theory dynamically incorporates some recently proposed models for entangled bipartite subsystems, and compared to them. All this opens up the way to an entirely new formalism for modeling nowadays mesoscopic-scale electronic and optoelectronic devices, as well as to investigations on the fundamental, and everlasting, problem irreversibility in more abstract quantum theories.

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#### APPENDIX A: PROOF OF THEOREM (IV.1)

*Proof.* Let  $\mathcal{V}$  be the Banach space of norm continuous  $\mathcal{B}_0$ -valued functions on  $[0, \bar{\tau}]$ , and let  $b \in \mathcal{B}_0$ . Define the "interaction picture" time rescaled solution

$$\bar{f}_\lambda(\tau) = U_{-\lambda-2\tau} \bar{W}_{\lambda-2\tau}^\lambda b. \quad (\text{A1})$$

Then  $\bar{f}_\lambda$  is a solution to the integral equation

$$\bar{f}_\lambda = b + \bar{\mathcal{H}}_\lambda \bar{f}_\lambda, \quad (\text{A2})$$

where the integral operator  $\bar{\mathcal{H}}_\lambda$  is defined by

$$(\bar{\mathcal{H}}_\lambda g)(\tau) = \int_0^\tau ds U_{-\lambda-2s} K_D U_{\lambda-2s} g(s). \quad (\text{A3})$$

Now  $\bar{\mathcal{H}}_\lambda$  is a Volterra operator, so

$$\|\bar{\mathcal{H}}_\lambda^n\| \leq c^n \bar{\tau}^n / n!, \quad (\text{A4})$$

where  $c$  does not depend upon  $\lambda$ , and we have convergence of the associated Neumann series expansion

$$\bar{f}_\lambda = b + \bar{\mathcal{H}}_\lambda b + \bar{\mathcal{H}}_\lambda^2 b + \dots \quad (\text{A5})$$

So far everything can be restated for  $\bar{f}_\lambda \leftrightarrow \bar{W}^\lambda$  in exactly the same way, leading to the corresponding definition of  $\bar{\mathcal{H}}_\lambda$ .

Subtracting the similar expansions for  $\bar{f}_\lambda$  and  $\tilde{f}_\lambda$  we obtain

$$\sup_{0 \leq t \leq \lambda^{-2\bar{\tau}}} \|\bar{W}_t^\lambda b - \tilde{W}_t^\lambda b\| = \|\bar{f}_\lambda - \tilde{f}_\lambda\|_\infty \leq \sum_{n=0}^{\infty} \|\bar{\mathcal{H}}_\lambda^n b - \tilde{\mathcal{H}}_\lambda^n b\|_\infty \quad (\text{A6})$$

It is easy to see that this series is dominated uniformly with respect to  $\lambda$ , so it only remains to show that

$$\lim_{\lambda \rightarrow 0} \|\bar{\mathcal{H}}_\lambda - \tilde{\mathcal{H}}_\lambda\| = 0. \quad (\text{A7})$$

This means that for every  $\epsilon > 0$  there is a  $\bar{\lambda} > 0$  such that  $|\lambda| < \bar{\lambda}$  implies that for every  $g \in \mathcal{V}$

$$\left\| \int_0^\tau ds U_{-\lambda-2s} \Delta K U_{\lambda-2s} g(s) \right\| < \frac{\epsilon}{2^2}. \quad (\text{A8})$$

Before proceeding we have to keep divergences under control: the time variable inside the integrals that define  $K_D$  and  $K_R$  goes from 0 to  $\infty$ : we show that it can be stopped at a finite value. To do this, we write explicitly the definition of the operators involved in the last inequality:

$$\begin{aligned} & \int_0^\tau ds U_{-\lambda-2s} \Delta K U_{\lambda-2s} g(s) \\ &= \int_0^\infty dx \int_0^\tau ds [U_{-x/2}, U_{-\lambda-2s-x/2} B_x U_{\lambda-2s-x/2}] g(s), \end{aligned} \quad (\text{A9})$$

where we have put  $B_x = A_{01} U_x A_{10}$ . Now the integral over the  $x$  variable on  $[0, \infty]$  can be split into  $[0, \bar{x}] \cup [\bar{x}, \infty]$ , which gives

$$\left\| \int_0^\tau ds U_{-\lambda-2s} \Delta K U_{\lambda-2s} g(s) \right\| \leq \left\| \int_0^{\bar{x}} \dots \right\| + 2\|g\|_\infty \bar{\tau} \int_{\bar{x}}^\infty \|B_x\| dx. \quad (\text{A10})$$

According to our hypothesis (24) on  $B_x$  we can choose a suitable  $\bar{x}$  such that the last term is smaller than  $\epsilon/2^3$ , independently of  $\lambda$ :

$$2\|g\|_\infty \bar{\tau} \int_{\bar{x}}^\infty \|B_x\| dx < \frac{\epsilon}{2^3}. \quad (\text{A11})$$

Once we fix such an  $\bar{x}$ , our problem becomes to find a  $0 < \bar{\lambda}_2 \leq \lambda_1$  such that if  $|\lambda| < \bar{\lambda}_2$ , then for every  $0 \leq \tau \leq \bar{\tau}$ .

$$\left\| \int_0^{\bar{x}} dx \int_0^\tau ds [U_{-x/2}, U_{-\lambda-2s-x/2} B_x U_{\lambda-2s-x/2}] g(s) \right\| < \frac{\epsilon}{2^4}. \quad (\text{A12})$$

We now make use of the spectral theorem: if

$$Z = \int_{-\infty}^{\infty} i\omega dE_{\omega} \quad (\text{A13})$$

is the spectral decomposition of  $Z$  for its spectral family  $E_{\omega}$  (if  $Z\rho = -i[H, \rho]$ ) then the  $\omega$ 's have meaning of energy differences, or characteristic frequencies of the global system), then

$$U_t = \int_{-\infty}^{\infty} e^{i\omega t} dE_{\omega}. \quad (\text{A14})$$

As for the time variable  $x$ , we split the frequency range into  $(-\infty, -\bar{\omega}) \cup [-\bar{\omega}, \bar{\omega}] \cup (\bar{\omega}, \infty)$  and define

$$U_t^{(\bar{\omega})} = \int_{-\bar{\omega}}^{\bar{\omega}} e^{i\omega t} dE_{\omega}. \quad (\text{A15})$$

Adding and subtracting  $U_{-\lambda^{-2}s-x}^{(\bar{\omega})}$  and  $U_{-\lambda^{-2}s-x/2}^{(\bar{\omega})}$  we are led to consider the quantities

$$\int_0^{\bar{x}} dx \int_0^{\tau} ds \|(U_{-\lambda^{-2}s-x} - U_{-\lambda^{-2}s-x}^{(\bar{\omega})})B_x U_{-\lambda^{-2}s} g(s)\| \quad (\text{A16})$$

and

$$\int_0^{\bar{x}} dx \int_0^{\tau} ds \|(U_{-\lambda^{-2}s-x/2} - U_{-\lambda^{-2}s-x/2}^{(\bar{\omega})})B_x U_{-\lambda^{-2}s-x/2} g(s)\|. \quad (\text{A17})$$

The first is dominated by (for compactness of the involved intervals,  $\sup = \max$ )

$$\begin{aligned} & \bar{x}\bar{\tau} \max\{\|(U_{-\lambda^{-2}s-x} - U_{-\lambda^{-2}s-x}^{(\bar{\omega})})B_x U_{-\lambda^{-2}s} g(s)\|, \\ & 0 \leq s \leq \bar{\tau}, 0 \leq x \leq \bar{x}\} \\ & \leq \bar{x}\bar{\tau} \left\| \left( \int_{-\infty}^{-\bar{\omega}} + \int_{-\bar{\omega}}^{\infty} \right) e^{i(\lambda^{-2}s+x)\omega} dE_{\omega} B_{\bar{x}} U_{-\lambda^{-2}s} g(s) \right\| \\ & \leq \bar{x}\bar{\tau} \left( \int_{-\infty}^{-\bar{\omega}} + \int_{-\bar{\omega}}^{\infty} \right) \|dE_{\omega} B_{\bar{x}} U_{-\lambda^{-2}s} g(s)\|. \end{aligned} \quad (\text{A18})$$

But since the  $E_{\omega}$ 's are orthogonal projections

$$\int_{-\infty}^{\infty} \|dE_{\omega} B_{\bar{x}} U_{-\lambda^{-2}s} g(s)\| = \|B_{\bar{x}} U_{-\lambda^{-2}s} g(s)\| \leq \|B_{\bar{x}}\| \|g(s)\| \quad (\text{A19})$$

is bounded independently of  $\lambda$ , so we can choose  $\bar{\omega}$  such that the quantity in the last line in Eq. (A18) is dominated by  $\frac{\epsilon}{2^5}$  independently of  $\lambda$  (it can however depend on  $g$ , as a consequence of the estimation above, but this will not bother us),

$$\bar{x}\bar{\tau} \left( \int_{-\infty}^{-\bar{\omega}} + \int_{-\bar{\omega}}^{\infty} \right) \|dE_{\omega} B_{\bar{x}} U_{-\lambda^{-2}s} g(s)\| < \frac{\epsilon}{2^5} \quad (\text{A20})$$

Following the same reasoning, we can choose  $\bar{\omega}$  such that also the difference in Eq. (A17) is controlled by  $\frac{\epsilon}{2^6}$ . In fact, again with the same reasoning, by adding and subtracting

$U_{\lambda^{-2}s}^{(\bar{\omega})}$  and  $U_{\lambda^{-2}s-x/2}^{(\bar{\omega})}$  we easily see that we can fix an  $\bar{\omega}$  such that

$$\int_0^{\bar{x}} dx \int_0^{\tau} ds \|U_{-\lambda^{-2}s-x}^{(\bar{\omega})} B_x (U_{\lambda^{-2}s} - U_{\lambda^{-2}s}^{(\bar{\omega})}) g(s)\| < \frac{\epsilon}{2^7} \quad (\text{A21})$$

and

$$\int_0^{\bar{x}} dx \int_0^{\tau} ds \|U_{-\lambda^{-2}s-x/2}^{(\bar{\omega})} B_x (U_{\lambda^{-2}s-x/2} - U_{\lambda^{-2}s-x/2}^{(\bar{\omega})}) g(s)\| < \frac{\epsilon}{2^8} \quad (\text{A22})$$

independently of  $\lambda$ . So we now have to prove that, when we fix  $\bar{x}$  and  $\bar{\omega}$  as done before, we can find a  $0 < \bar{\lambda}_2 \leq \lambda_1$  such that when  $|\lambda| < \bar{\lambda}_2$ , for every  $0 \leq \tau \leq \bar{\tau}$ .

$$\left\| \int_0^{\bar{x}} dx \int_0^{\tau} ds [U_{-x/2}^{(\bar{\omega})}, U_{-\lambda^{-2}s-x/2}^{(\bar{\omega})} B_x U_{\lambda^{-2}s-x/2}^{(\bar{\omega})}] g(s) \right\| < \frac{\epsilon}{2^9}. \quad (\text{A23})$$

We proceed by plugging in the definition of Stiltjes integral involved in the spectral decompositions of the unitarities  $U_t$  (see, for example, [20]). If  $\Sigma(-\bar{\omega}, \bar{\omega})$  is the set of subdivisions of the interval  $[-\bar{\omega}, \bar{\omega}]$ , and  $\sigma \in \Sigma(-\bar{\omega}, \bar{\omega})$  has points  $-\bar{\omega} = \omega_0 < \omega_1 < \dots < \omega_{N_{\sigma}} = \bar{\omega}$ , we put

$$d(\sigma) = \max_{k=1, \dots, N_{\sigma}} |\omega_k - \omega_{k-1}|. \quad (\text{A24})$$

Then the limit

$$\int_{-\bar{\omega}}^{\bar{\omega}} e^{i\omega t} dE_{\omega} f = \lim_{d(\sigma) \rightarrow 0} \sum_{k=0}^{N_{\sigma}-1} e^{i\bar{\omega}_k t} (E_{\omega_{k+1}} - E_{\omega_k}) f, \quad (\text{A25})$$

where  $\bar{\omega}_k \in [\omega_k, \omega_{k+1}[$ , exists and defines the left-hand side. Then Eq. (A23) becomes

$$\begin{aligned} & \left\| \lim_{d(\sigma_1), d(\sigma_2) \rightarrow 0} \int_0^{\bar{x}} dx \int_0^{\tau} ds \sum_{k_1=0}^{N_{\sigma_1}-1} \sum_{k_2=0}^{N_{\sigma_2}-1} \{e^{i\bar{\omega}_{k_1}^{(1)}(-\lambda^{-2}s-x) + i\bar{\omega}_{k_2}^{(2)}\lambda^{-2}s} \right. \\ & \quad \left. - e^{i\bar{\omega}_{k_1}^{(1)}(-\lambda^{-2}s-x/2) + i\bar{\omega}_{k_2}^{(2)}(\lambda^{-2}s-x/2)}\} (E_{\omega_{k_1+1}^{(1)}} - E_{\omega_{k_1}^{(1)}}) \right. \\ & \quad \left. \times B_x (E_{\omega_{k_2+1}^{(2)}} - E_{\omega_{k_2}^{(2)}}) g(s) \right\| \end{aligned} \quad (\text{A26})$$

with obvious notations. But clearly it suffices to consider only one subdivision instead of two, and prove that there exist a  $\bar{\lambda}_2 > 0$  and a subdivision  $\bar{\sigma}$  such that if  $|\lambda| < \bar{\lambda}_2$  and  $d(\sigma) < d(\bar{\sigma})$  then

$$\left\| \int_0^{\bar{x}} dx \int_0^\tau ds \sum_{k_1, k_2=0}^{N_\sigma-1} \{ e^{i\bar{\omega}_{k_1}(-\lambda^{-2}s-x)+i\bar{\omega}_{k_2}\lambda^{-2}s} - e^{i\bar{\omega}_{k_1}(-\lambda^{-2}s-x/2)+i\bar{\omega}_{k_2}(\lambda^{-2}s-x/2)} \} (E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) \times B_x(E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) g(s) \right\| < \frac{\epsilon}{2^9}, \quad (\text{A27})$$

that is, rearranging terms,

$$\left\| \sum_{k_1, k_2=0}^{N_\sigma-1} \int_0^{\bar{x}} dx e^{-ix/2\bar{\omega}_{k_1}} \{ e^{-ix/2\bar{\omega}_{k_1}} - e^{-ix/2\bar{\omega}_{k_2}} \} (E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) \times B_x(E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1}-\bar{\omega}_{k_2})} g(s) \right\| < \frac{\epsilon}{2^9}. \quad (\text{A28})$$

But the left-hand side is dominated by

$$\sum_{k_1, k_2=0}^{N_\sigma-1} \int_0^{\bar{x}} dx |e^{-ix/2\bar{\omega}_{k_1}} - e^{-ix/2\bar{\omega}_{k_2}}| \left\| (E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) \times B_x(E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1}-\bar{\omega}_{k_2})} g(s) \right\| \quad (\text{A29})$$

and we can safely control the slowly varying phase oscillations by

$$|e^{-ix/2\bar{\omega}_{k_1}} - e^{-ix/2\bar{\omega}_{k_2}}| \leq |\bar{\omega}_{k_1} - \bar{\omega}_{k_2}| \frac{\bar{x}}{2} \quad (\text{A30})$$

(this explains the splitting in the time variable  $x$ ). In passing, we note that we can discard the contribution with equal frequencies  $k_1=k_2$  in the sum for the subdivision  $\sigma$ .

As the rapidly oscillating integral is concerned, we take a  $\lambda$ -smoothed version of the Dirac  $\delta$  functional: for a suitable real number  $\zeta > 0$  we define

$$\delta_\lambda(x) = \frac{1}{\pi} \frac{\sin\left(\frac{x}{|\lambda|^\zeta \bar{\tau}}\right)}{x} = \frac{1}{2\pi} \int_{-\Omega_\lambda}^{\Omega_\lambda} d\Omega e^{i\Omega x}, \quad (\text{A31})$$

with  $\Omega_\lambda = |\lambda|^{-\zeta}/\bar{\tau}$ , and consider the approximation

$$\begin{aligned} & \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1}-\bar{\omega}_{k_2})} g(s) \\ & \sim \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1}-\bar{\omega}_{k_2})} \int_0^\tau dr g(r) \delta_\lambda(s-r) \\ & = \frac{1}{2\pi} \int_{-\Omega_\lambda}^{\Omega_\lambda} d\Omega \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1}-\bar{\omega}_{k_2})-i\Omega s} \\ & \quad \times \int_0^\tau dr e^{i\Omega r} g(r) \end{aligned} \quad (\text{A32})$$

valid for  $\lambda \sim 0$ . Then the term in Eq. (A29) is bounded by

$$\begin{aligned} & \sum_{k_1, k_2=0}^{N_\sigma-1} \int_0^{\bar{x}} dx |\bar{\omega}_{k_1} - \bar{\omega}_{k_2}| \frac{\bar{x}}{2} \frac{1}{\pi} \\ & \quad \times \int_{-\Omega_\lambda}^{\Omega_\lambda} d\Omega \frac{1}{|\lambda^{-2}(\bar{\omega}_{k_1} - \bar{\omega}_{k_2}) + \Omega|} \\ & \quad \times \int_0^\tau dr \|(E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) B_x(E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) g(r)\|. \end{aligned} \quad (\text{A33})$$

Now the integral in  $d\Omega$  can be computed easily if, for sufficiently small values for  $\lambda$ , the integrand is never singular. This is the case provided that  $\zeta < 2$ , as we shall assume. Then the integrand is either always positive or always negative, so

$$\int_{-\Omega_\lambda}^{\Omega_\lambda} d\Omega \frac{1}{|\lambda^{-2}(\bar{\omega}_{k_1} - \bar{\omega}_{k_2}) + \Omega|} \sim \frac{\lambda^{2-\zeta}}{|\bar{\omega}_{k_1} - \bar{\omega}_{k_2}| \bar{\tau}}. \quad (\text{A34})$$

Putting things together, we estimate Eq. (A29) by

$$\begin{aligned} & \sum_{k_1, k_2=0}^{N_\sigma-1} |\bar{\omega}_{k_1} - \bar{\omega}_{k_2}| \frac{\bar{x}}{2} \frac{1}{\pi} \frac{\lambda^{2-\zeta}}{(\bar{\omega}_{k_1} - \bar{\omega}_{k_2}) \bar{\tau}} \\ & \quad \times \int_0^{\bar{x}} dx \int_0^\tau dr \|(E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) B_x(E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) g(r)\| \\ & = \frac{\bar{x}}{2} \frac{1}{\pi} \frac{\lambda^{2-\zeta}}{\bar{\tau}} \int_0^{\bar{x}} dx \int_0^\tau dr \|B_x g(r)\| \\ & \leq \frac{\lambda^{2-\zeta} \bar{x}}{2\pi} \|g\|_\infty \int_0^\infty dx \|B_x\| \end{aligned} \quad (\text{A35})$$

(the second line follows because the  $E_\omega$ 's are orthogonal projections). Now this goes to zero as  $\lambda \rightarrow 0$ , thus completing the proof. ■

## APPENDIX B: PROOF OF THEOREM (IV.1)

*Proof.* (Throughout when there is no possible misunderstanding we should use the notation  $K_T$  instead of the complete  $K_{T(\lambda)}$ ). With a completely analogous notation, we follow the very same steps in the proof of theorem III.1: we then have to show that

$$\lim_{\lambda \rightarrow 0} \|\tilde{\mathcal{H}}_\lambda - \hat{\mathcal{H}}_\lambda\| = 0, \quad (\text{B1})$$

where both  $\tilde{\mathcal{H}}_\lambda$  and  $\hat{\mathcal{H}}_\lambda$  are defined analogously to Eq. (A3),

respectively, for  $K_R$  and  $K_{T(\lambda)}$ . Now defining  $\hat{\mathcal{H}}_\lambda$  by

$$\begin{aligned} & \hat{\mathcal{H}}_\lambda g(\tau) = \int_0^\tau ds U_{-\lambda^{-2}s} \\ & \quad \times \left\{ \frac{1}{\sqrt{\pi T}} \int_{-\infty}^\infty dq e^{-q^2/T^2} U_{-q} K_R U_q \right\} U_{\lambda^{-2}s} g(s), \end{aligned} \quad (\text{B2})$$

where  $g \in \mathcal{V}$ , leads to the estimation

$$\|\tilde{\mathcal{H}}_\lambda - \hat{\mathcal{H}}_\lambda\| \leq \|\tilde{\mathcal{H}}_\lambda - \overset{\Delta}{\mathcal{H}}_\lambda\| + \|\overset{\Delta}{\mathcal{H}}_\lambda - \hat{\mathcal{H}}_\lambda\|. \quad (\text{B3})$$

The easiest part to estimate is the last term: one can see that

$$\begin{aligned} & \|(\mathcal{H}_\lambda g)(\tau) - (\hat{\mathcal{H}}_\lambda g)(\tau)\| \\ & \leq \bar{\tau} \|g\|_\infty \|K_R - K^{T(\lambda)}\| \\ & \leq \bar{\tau} \|g\|_\infty \int_0^\infty dx (1 - e^{-(x/2)^2/T^2(\lambda)}) \|A_{01} U_x A_{10}\|. \end{aligned} \quad (\text{B4})$$

Now for any given  $x \in [0, \infty)$  one has

$$\lim_{\lambda \rightarrow 0} (1 - e^{-(x/2)^2/T^2(\lambda)}) = 0 \quad (\text{B5})$$

because of the hypothesis  $T(\lambda) \sim |\lambda|^{-\xi} \bar{T}$  with  $\xi > 0$ . This together with the boundedness hypothesis

$$\int_0^\infty dx \|A_{01} U_x A_{10}\| < \infty \quad (\text{B6})$$

implies that the last term in Eq. (B4) goes to zero as  $\lambda \rightarrow 0$ .

It remains to show that

$$\|\tilde{\mathcal{H}}_\lambda - \overset{\Delta}{\mathcal{H}}_\lambda\| \rightarrow 0, \lambda \rightarrow 0, \quad (\text{B7})$$

or, more explicitly, we have to show convergence to zero, for any  $g \in \mathcal{V}$  and uniformly on  $\tau$ , of

$$\begin{aligned} & \left\| \int_0^\tau ds U_{-\lambda^{-2}s} \left\{ \frac{1}{\sqrt{\pi T}} \int_{-\infty}^\infty dq e^{q^2/T^2} U_{-q} K_R U_q - K_R \right\} \right. \\ & \left. \times U_{\lambda^{-2}s} g(s) \right\|. \end{aligned} \quad (\text{B8})$$

Now the very same arguments we used for theorem (III.1) apply here, so  $U_{\pm q}$  can be substituted with  $\tilde{U}_{\pm q}$ , for a suitable cutoff frequency  $\bar{\omega}$ : the difference with Eq. (B8) is shown to be arbitrarily small in exactly the same way as before. Again as before, we can evaluate the limit in the Stiltjes integral for the spectral decomposition over a single common spectral subdivision  $\sigma = \{-\bar{\omega} = \omega_0 < \dots < \omega_{N_\sigma} = \bar{\omega}\}$ . So proceeding as in theorem (III.1) we are now left with the problem of finding, for any given  $\epsilon > 0$ , a suitable  $\bar{\lambda} > 0$  and spectral subdivision  $\bar{\sigma}$  such that for any  $|\lambda| < \bar{\lambda}$  and  $d(\sigma) < d(\bar{\sigma})$  we have

$$\begin{aligned} & \left\| \sum_{k_1, k_2=0}^{N_\sigma-1} \left\{ \left( \frac{1}{\sqrt{\pi T}} \int_{-\infty}^\infty dq e^{-q^2/T^2} e^{iq(\bar{\omega}_{k_1} - \bar{\omega}_{k_2})} \right) - 1 \right\} \right. \\ & \quad \times (E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) K_R (E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) \\ & \quad \times \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1} - \bar{\omega}_{k_2})} g(s) \left. \right\| \\ & \leq \sum_{k_1, k_2=0}^{N_\sigma-1} |e^{-T^2(\bar{\omega}_{k_1} - \bar{\omega}_{k_2})^2} - 1| \\ & \quad \times \left\| (E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) K_R (E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) \right. \\ & \quad \times \int_0^\tau ds e^{-i\lambda^{-2}s(\bar{\omega}_{k_1} - \bar{\omega}_{k_2})} g(s) \left. \right\| < \epsilon. \end{aligned} \quad (\text{B9})$$

We multiply and divide by  $T|\bar{\omega}_{k_1} - \bar{\omega}_{k_2}|$  inside the sum and note that

$$\frac{1}{T|\bar{\omega}_{k_1} - \bar{\omega}_{k_2}|} |1 - e^{-T^2(\bar{\omega}_{k_1} - \bar{\omega}_{k_2})^2}| \leq C < \infty \quad (\text{B10})$$

is bounded uniformly on  $\omega_k$  and  $T$  by a constant  $C$ . This means that the divergences brought by the rapid  $\lambda^{-2}$  oscillations cancel with the slowly varying ‘‘spectral average’’ or ‘‘damping’’ oscillations, which we treat exactly as in the previous theorem [see Eq. (A29) and the following, also for the definition of the subsequent  $\zeta$ ] and the norm of the previous sum is controlled by

$$\begin{aligned} & \frac{\lambda^{2-\zeta} C}{T(\lambda) \pi \bar{\tau}} \int_0^\infty dr \sum_{k_1, k_2=0}^{N_\sigma-1} \|(E_{\omega_{k_1+1}} - E_{\omega_{k_1}}) K_R (E_{\omega_{k_2+1}} - E_{\omega_{k_2}}) g(r)\| \\ & \leq \frac{\lambda^{2-\zeta} C}{T(\lambda) \pi} \|g\|_\infty \|K_R\|. \end{aligned} \quad (\text{B11})$$

This shows the uniform boundedness of the last term with respect to  $\|g\|=1$  and  $0 \leq \tau \leq \bar{\tau}$ , so convergence to zero comes from the fact that

$$\frac{\lambda^{2-\zeta}}{T(\lambda)} \rightarrow 0, \quad \lambda \rightarrow 0, \quad (\text{B12})$$

as we have supposed  $T(\lambda) \sim |\lambda|^{-\xi} \bar{T}$  for  $\lambda \rightarrow 0$  and  $\xi < 2$ , and we can take  $0 < \zeta < 2$  such that  $2 + \zeta - \xi > 0$ . This finishes the proof. ■

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