## QUASI-CLASSICAL SPIN BOSON MODELS

#### MICHELE CORREGGI, MARCO FALCONI, AND MARCO MERKLI

ABSTRACT. In this short note we study Spin-Boson Models from the Quasi-Classical standpoint. In the Quasi-Classical limit, the field becomes macroscopic while the particles it interacts with, they remain quantum. As a result, the field becomes a classical environment that drives the particle system with an explicit effective dynamics.

#### 1. Introduction and Main Result

The spin-boson model describes the interaction between a bosonic scalar field, playing the role of environment or reservoir, and a 'small' quantum system, whose spin degrees of freedom are the only relevant ones. It has been widely studied in the mathematical physics and physics literature, from various standpoints. The spin-boson model is one of *the* paradigmatic examples of an open quantum system. It is used to investigate general open system phenomena such as decoherence, entanglement, thermalization, to test the validity of markovian approximations and to analyze non-markovian behavior. We cannot attempt to give an exhaustive list of references of the model. We point the mathematically interested reader to the following inconclusive list of works, [ALN16, AJN17, ALN17, Ara90, Ara91, AH97, HH11], as well as to references therein contained.

On the more physical side, the spin-boson model is used to describe atom-radiation interaction in quantum optics, qubit-noise coupling in quantum information and computation, environment induced transport phenomena and chemical processes in quantum chemistry. Some of these aspects can be found in the references [LCD<sup>+</sup>87, PSE96, KMS15, XS94, KM16, moh14, Mer20, Mer22a, Mer22b, JMS20, MBS<sup>+</sup>16, MBS13, MBBG11, MSB07].

For the purpose of this paper, in which we focus on mathematical aspects, we assume that the reader is familiar with the basic mathematical tools of free quantum fields, namely Fock spaces, second quantization, creation/annihilation operators, etc.; if not, they may refer, e.g., to [Coo51, DG13]. Let us denote by  $\mathcal{H}$  the Hilbert space of the spin system, and by  $\mathfrak{h}$  the Hilbert space of a single bosonic excitation. We denote by  $\mathcal{G}_{\varepsilon}$  the second quantization functor<sup>1</sup>,

$$[a_{\varepsilon}(f), a_{\varepsilon}^*(g)] = \varepsilon \langle f, g \rangle_{\mathfrak{h}}.$$

The second quantization of an operator A on  $\mathfrak h$  is written thus as

$$d\mathcal{G}_{\varepsilon}(A) = \sum_{i,i=0}^{\infty} A_{ij} a_{\varepsilon,i}^* a_{\varepsilon,j} ,$$

with  $A_{ij} = \langle e_i, Ae_j \rangle_{\mathfrak{h}}$ , and  $a_{\varepsilon,k}^{\sharp} = a_{\varepsilon}^{\sharp}(e_k)$ , with  $\{e_k\}_{k \in \mathbb{N}}$  an O.N.B. of  $\mathfrak{h}$ . The quasi-classical parameter  $\varepsilon$  clearly plays the role of a semiclassical parameter for the (Segal) field  $\varphi_{\varepsilon}(f) = a_{\varepsilon}^{*}(f) + a_{\varepsilon}(f)$ : as  $\varepsilon \to 0$ , the field becomes a classical commutative observable [see CFO22b, for a gentler and more detailed introduction to the quasi-classical scaling], and [CCFO21, CF18, CFO19, CFO22a] for other recent papers concerning the quasi-classical regime.

<sup>&</sup>lt;sup>1</sup>We use a somewhat unorthodox notation for the second quantization functor. We denote by  $\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h}) = \bigoplus_{n \in \mathbb{N}} \mathfrak{h}_{n}$  the symmetric Fock space over  $\mathfrak{h}$  in which the canonical creation and annihilation operators have ε-dependent commutation relations:

where  $0 < \varepsilon \ll 1$  is a scale parameter. The spin-boson Hamiltonian has the general form

$$H_{\varepsilon} = \mathfrak{S} \otimes 1 + \nu(\varepsilon) \, 1 \otimes \mathrm{d} \mathcal{G}_{\varepsilon}(\omega) + \mathfrak{s} \otimes \varphi_{\varepsilon}(g) \,\,,$$

as an operator on  $\mathscr{H}\otimes\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})$ . Here,  $\mathfrak{S},\mathfrak{s}\in\mathscr{B}(\mathscr{H})$  are self-adjoint,  $\nu(\varepsilon)$  is either  $\nu(\varepsilon)=1$  or  $\nu(\varepsilon)=\frac{1}{\varepsilon}$ ,  $\omega$  is a positive – with possibly unbounded inverse – operator on  $\mathfrak{h}$ , and  $g\in\mathfrak{h}$ . The bipartition of the total Hilbert space  $\mathscr{H}\otimes G_{\varepsilon}^{s}(\mathfrak{h})$  reflects the separation of the total physical system into two subsystems. Commonly, especially in the physics literature, the Hilbert space  $\mathscr{H}$  is finite-dimensional. For instance,  $\mathscr{H}$  has dimension  $2^N$  in the case of N spins 1/2, or N qubits. One of the most studied cases is N=2, hence the name "spin-boson" model. A further characteristic of the spin-boson model is that the interaction operator is of the simple product form  $\mathfrak{s}\otimes\varphi_{\varepsilon}(g)$ , or a finite sum of such terms. This simplifies the (rigorous) analysis of the model. Nevertheless, other models in which the interaction term is more complicated, are also of interest. For instance, in the Nelson, the Pauli-Fierz or the polaron model, the interaction operator is of the form  $\int_{\mathbb{R}^3} \mathfrak{s}(k) \otimes \varphi_{\varepsilon}(k) \mathrm{d}^3k$ . While these models are also treatable with the methods explained here (see [CFO22b]), we focus in the present manuscript, for ease of presentation, on the simple form of the interaction as in  $H_{\varepsilon}$  above.

We shall consider a more general setup though. The guiding principle is that we want to describe two qualitatively unequal interacting parts. The 'spin' part which is 'small' and the boson part (or field, reservoir, environment) which is 'large'. A quantification of what small versus large means can be implemented in different ways, depending on the physical reality being modeled. For instance, finite dimensional ( $\mathscr{H}$ ) versus infinite dimensional ( $\mathscr{G}_{\varepsilon}^{s}(\mathfrak{h})$ ) Hilbert spaces, or Hamiltonians with discrete spectrum ( $\mathfrak{S}$ ) versus Hamiltonians with continuous spectrum ( $d\mathscr{G}_{\varepsilon}(\omega)$ ). In the quasi-classical setup we are discussing here, the field is large in the sense that it is in a state which contains many more particles (or excitations) than the spin system does. This is formalized by saying that the (average) number of particles of the spin system is fixed, while that number in the field state is  $\propto 1/\varepsilon \gg 1$  – constituting the quasi-classical limit.

We will soon explain how the choice of  $\nu(\varepsilon)$  affects the quasi-classical limit  $\varepsilon \to 0$ . There are further possible generalizations of the model, namely by taking  $\mathfrak{s}$  and g to be vector-valued, or by taking  $\mathfrak{S}$  to be only bounded from below, or by taking  $g \notin \mathfrak{h}$ . Self-adjointness for the latter case has been recently studied in [Lon22]. For our purposes, these generalizations do not present serious obstacles as long as  $H_{\varepsilon}$  can be defined as a self-adjoint operator, however for the sake of clarity we keep the setting as described above.

## **Proposition 1.1** (Self-adjointness of $H_{\varepsilon}$ ).

For all  $g \in \mathfrak{h}$ ,  $H_{\varepsilon}$  is essentially self-adjoint on  $D(d\mathcal{G}_{\varepsilon}(\omega)) \cap \mathcal{C}_{0}^{\infty}(d\mathcal{G}_{\varepsilon}(1))$ . In addition, if both  $g \in \mathfrak{h}$  and  $\omega^{-1/2}g \in \mathfrak{h}$ , then  $H_{\varepsilon}$  is self-adjoint on  $D(d\mathcal{G}_{\varepsilon}(\omega))$  and bounded from below.

*Proof.* The essential self-adjointness is proved in [Fal15], for a general class of operators describing the interaction between matter and radiation; self-adjointness and boundedness from below with the additional assumption  $\omega^{-1/2}g \in \mathfrak{h}$  is an easy consequence of the Kato-Rellich theorem on relatively bounded perturbations of self-adjoint operators.

## Remark 1.2 (Form factors).

There are form factors  $g \in \mathfrak{h}$  with  $\omega^{-1/2}g \notin \mathfrak{h}$  such that  $H_{\varepsilon}$  is unbounded from below (even

<sup>&</sup>lt;sup>2</sup>We denote by  $C_0^{\infty}(d\mathcal{G}_{\varepsilon}(1))$  the Fock space vectors with a finite number of particles (*i.e.*, for which the *k*-particle components are all zero for  $k > \underline{k}$ , for some  $\underline{k} \in \mathbb{N}$ ).

though it is still self-adjoint). This is analogous to what happens for the van Hove model, and it is caused by some infrared singularity: in physical models,  $\omega^{-1/2}$  is unbounded (and thus it could happen that  $\omega^{-1/2}g \notin \mathfrak{h}$ ) only if the field is massless [see Der03, for further details]. For our purposes, uniqueness of the quantum dynamics (*i.e.* essential self-adjointness of  $H_{\varepsilon}$ ) is enough.

1.1. **Main Result.** Our goal is to characterize explicitly the dynamics of quantum states, in the limit  $\varepsilon \to 0$ . In order to do that, let us define quantum states as density matrices

$$\Gamma_{\varepsilon} \in \mathfrak{L}^{1}_{+,1}(\mathscr{H} \otimes \mathcal{G}^{s}_{\varepsilon}(\mathfrak{h}))$$
,

where  $\mathfrak{L}^1$  is the trace ideal, and  $\mathfrak{L}^1_{+,1}$  stands for elements in the positive cone, with trace one. A time-evolved state is then given by

$$\Gamma_{\varepsilon}(t) = e^{-itH_{\varepsilon}} \Gamma_{\varepsilon} e^{itH_{\varepsilon}}$$
.

To be more precise, the question we will answer in this note is the following:

Knowing the behavior of the initial state  $\Gamma_{\varepsilon}$  as  $\varepsilon \to 0$ , what is the behavior of  $\Gamma_{\varepsilon}(t)$  as  $\varepsilon \to 0$ , for any time  $t \in \mathbb{R}$ ?

To answer the question, we shall first clarify what the general behavior is of a quantum state  $\Gamma_{\varepsilon}$ , as  $\varepsilon \to 0$ . The intuition is that as the boson degrees of freedom become classical, the state – restricted to the boson subsystem – becomes classical as well (in the statistical mechanics sense, *i.e.* a probability measure); on the other hand, the spin subsystem retains its quantum nature, and thus its description shall still be given by a density matrix.

This picture is satisfactorily described mathematically in terms of a so-called *state-valued* measure, introduced in [CFO22b, Fal18]. A state-valued measure is a couple  $\mathfrak{m}=(\mu,\gamma)$  consisting of a (Borel Radon) measure  $\mu$  on the classical configuration space  $\mathfrak{h}$  for the Boson subsystem, and a  $\mu$ -almost-everywhere defined function  $\mathfrak{h}\ni z\mapsto \gamma(z)\in\mathfrak{L}^1_{+,1}(\mathscr{H})$  with values in the density matrices of the Spin subsystem. The function  $\gamma(z)$  acts as a vector-valued Radon-Nikodým derivative (it is in fact one), and thus the measure element  $d\mathfrak{m}(z)$  can be written as

$$d\mathfrak{m}(z) = \gamma(z)d\mu(z) .$$

Integrating a scalar measurable bounded function F with respect to  $\mathfrak{m}$  gives an element in  $\mathfrak{L}^1(\mathcal{H})$ , that we denote by

$$\int_{\mathfrak{h}} F(z) d\mathfrak{m}(z) = \int_{\mathfrak{h}} F(z) \gamma(z) d\mu(z) .$$

It is also possible to integrate suitable functions  $\mathfrak{F}$  with values in the bounded operators on  $\mathscr{H}$ , however in this case the relative order between the function and the measure matters: in general,

$$\int_{\mathfrak{h}} \mathfrak{F}(z) \mathrm{d}\mathfrak{m}(z) = \int_{\mathfrak{h}} \mathfrak{F}(z) \gamma(z) \mathrm{d}\mu(z) \neq \int_{\mathfrak{h}} \gamma(z) \mathfrak{F}(z) \mathrm{d}\mu(z) = \int_{\mathfrak{h}} \mathrm{d}\mathfrak{m}(z) \mathfrak{F}(z) \;.$$

A detailed study of state-valued measures and their properties is given in the aforementioned references [CFO22b, CFO22a, Fal18]; we will make extensive use of the results proved in those papers, so the interested reader shall refer to them.

The last concept needed to understand the main results is that of the (non-commutative) Fourier transform of a quantum state, and of the Fourier transform of a state-valued measure.

These tools allow to put quantum states and state-valued measures on the same grounds, to set up the quasi-classical convergence of the former to the latter. The Fourier transform of a quantum state  $\Gamma_{\varepsilon}$  is the function  $\hat{\Gamma}_{\varepsilon}: \mathfrak{h} \to \mathfrak{L}^{1}(\mathscr{H})$  given by

$$\hat{\Gamma}_{\varepsilon}(\eta) = \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} (\Gamma_{\varepsilon}(W_{\varepsilon}(\eta))) ,$$

with  $W_{\varepsilon}(\eta)$  being the bosonic Weyl operator

$$W_{\varepsilon}(\eta) = e^{i\varphi_{\varepsilon}(\eta)} = e^{i\left(a_{\varepsilon}^*(\eta) + a_{\varepsilon}(\eta)\right)}$$

and  $\operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})}$  denoting the partial trace w.r.t. the bosonic degrees of freedom. The Fourier transform of a state-valued measure  $\mathfrak{m}$  is the function  $\hat{\mathfrak{m}}: \mathfrak{h} \to \mathfrak{L}^{1}(\mathscr{H})$  given by

$$\hat{\mathfrak{m}}(\eta) = \int_{\mathfrak{h}} e^{2i\operatorname{Re}\langle \eta, z\rangle_{\mathfrak{h}}} d\mathfrak{m}(z) = \int_{\mathfrak{h}} e^{2i\operatorname{Re}\langle \eta, z\rangle_{\mathfrak{h}}} \gamma(z) d\mu(z) .$$

We say that a state  $\Gamma_{\varepsilon}$  converges quasi-classically to a state-valued measure  $\mathfrak{m}$ , denoted by  $\Gamma_{\varepsilon} \underset{\varepsilon \to 0}{\longrightarrow} \mathfrak{m}$ , if and only if for all  $\eta \in \mathfrak{h}$ ,

$$w^*-\lim_{\varepsilon\to 0} \hat{\Gamma}_{\varepsilon}(\eta) = \hat{\mathfrak{m}}(\eta) ,$$

where w\*-lim stands for the limit in the weak-\* topology of  $\mathfrak{L}^1(\mathcal{H})$ , *i.e.* when tested with compact operators  $\mathfrak{k} \in \mathfrak{L}^{\infty}(\mathcal{H})$ :

$$\Gamma_{\varepsilon} \xrightarrow{\longrightarrow} \mathfrak{m} \quad \stackrel{\text{def}}{\Longleftrightarrow} \quad \operatorname{tr}_{\mathscr{H}} (\hat{\Gamma}_{\varepsilon}(\eta) \mathfrak{k}) \xrightarrow{\varepsilon \to 0} \operatorname{tr}_{\mathscr{H}} (\hat{\mathfrak{m}}(\eta) \mathfrak{k}), \quad \forall \eta \in \mathfrak{h}, \mathfrak{k} \in \mathfrak{L}^{\infty}(\mathscr{H}).$$

Proposition 1.3 (Quasi-classical convergence [CFO22b, Prop. 2.3]).

Let  $\Gamma_{\varepsilon}$  be a state such that there exist  $\delta, C > 0$  with

$$\operatorname{tr}\left((\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1)^{\delta}\Gamma_{\varepsilon}\right)\leqslant C$$
. (1.1)

Then there exists a sequence  $\varepsilon_n \xrightarrow[n \to \infty]{} 0$ , and a state-valued measure  $\mathfrak{m}$  (in general depending on the sequence) such that

$$\Gamma_{\varepsilon_n} \xrightarrow[n \to \infty]{} \mathfrak{m}$$
.

*Proof (sketch)*. The proof of this proposition adapts to the quasi-classical setting the semi-classical analysis for quantum fields developed by Ammari and Nier in [AN08, AN09, AN11, AN15], with some crucial differences. A complete proof is given in [CFO22b], however the key ideas could be summarized as follows.

The Fourier transform of a quantum state enjoys some special properties [see Seg59, Seg61], namely:

- $\operatorname{tr}_{\mathscr{H}}(\hat{\Gamma}_{\varepsilon}(0)) = 1;$
- $\hat{\Gamma}_{\varepsilon}$  is weak-\* continuous when restricted to any finite-dimensional subspace of  $\mathfrak{h}$ ;
- $\hat{\Gamma}_{\varepsilon}$  is "quantum-" completely positive definite: for any finite collection  $\{\eta_j\}_{j=1}^J \subset \mathfrak{h}$ , and  $\{\mathfrak{t}_j\}_{j=1}^J \subset \mathcal{B}(\mathcal{H})$ ,

$$\sum_{j,k=1}^{J} \mathfrak{t}_{j} \hat{\Gamma}_{\varepsilon} (\eta_{j} - \eta_{k}) \mathfrak{t}_{k}^{*} e^{i\varepsilon \operatorname{Im}\langle \eta_{j}, \eta_{k} \rangle} \geqslant 0$$

as an operator on  $\mathcal{H}$ .

Intuitively, by taking the ( $\mathfrak{h}$ -pointwise) weak-\* limit (using a compactness argument), one tries to prove that there exists a sequence  $\varepsilon_n \to 0$  such that  $\hat{\Gamma}_0 = \lim_{n \to \infty} \hat{\Gamma}_{\varepsilon_n}$  satisfies

- $\operatorname{tr}_{\mathscr{H}}(\hat{\Gamma}_0(0)) = 1;$
- $\hat{\Gamma}_0$  is weak-\* continuous when restricted to any finite-dimensional subspace of  $\mathfrak{h}$ ;
- $\hat{\Gamma}_0$  is completely positive definite: for any finite collection  $\{\eta_j\}_{j=1}^J \subset \mathfrak{h}$ , and  $\{\mathfrak{t}_j\}_{j=1}^J \subset \mathfrak{B}(\mathcal{H})$ ,

$$\sum_{j,k=1}^{J} \mathfrak{t}_{j} \hat{\Gamma}_{0}(\eta_{j} - \eta_{k}) \mathfrak{t}_{k}^{*} \geqslant 0.$$

It turns out that, under the assumption (1.1) above, the second and third properties are indeed satisfied, thus by the infinite dimensional version of Bochner's theorem [Fal18],  $\hat{\Gamma}_0$  identifies uniquely a cylindrical state-valued measure<sup>3</sup>  $\mathfrak{m}$ . In addition, (1.1) also implies that  $\mathfrak{m}$  is tight, and thus a Borel Radon measure. The first property, namely that the mass is preserved in the limit, does not hold in general in the quasi-classical case, contrarily to the semiclassical case where it is again ensured by (1.1). This is due to the fact that some mass may be lost "at infinity" if the spin subsystem has infinitely many degrees of freedom, see § 1.2 for a detailed discussion.

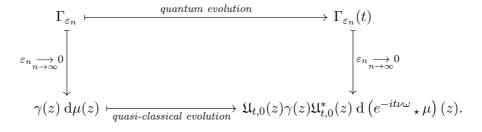
We are now in a position to state the main result of this note, in an informal but intuitive manner.

Theorem 1.4 (Quasi-classical dynamics).

Let  $\Gamma_{\varepsilon} \in \mathfrak{L}^1_{+,1}(\mathscr{H} \otimes \mathcal{G}^s_{\varepsilon}(\mathfrak{h}))$  be such that there exists  $\delta, C > 0$  such that, uniformly w.r.t.  $\varepsilon \in (0,1)$ ,

$$\operatorname{tr}\left(\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{\delta}\Gamma_{\varepsilon}\right)\leqslant C.$$

Then there is a sequence  $\varepsilon_n \to 0$  such that, with  $\nu := \lim_{\varepsilon \to 0} \varepsilon \nu(\varepsilon)$ , the following diagram is commutative, for any  $t \in \mathbb{R}$ :



In the above theorem, the symbol  $(\cdot)_{\star}(\cdot)$  stands for the pushforward of the measure on the right by means of the map on the left, and  $\mathfrak{U}_{t,s}(z)$  is the two-parameter unitary group on  $\mathscr{H}$  generated by the self-adjoint, generally time-dependent effective Hamiltonian<sup>4</sup>

$$\mathfrak{H}(z) = \mathfrak{S} + 2 \operatorname{Re} \langle e^{-it\nu\omega} z, g \rangle_{\mathfrak{h}} \mathfrak{s} .$$

The operator  $\mathfrak{H}(z)$  is a time-dependent generator if  $\nu=1$ , and it is time-independent if  $\nu=0^5$ . More precisely, for  $\nu=1$  the classical bosonic field described by  $e^{-it\omega}_{\star}\mu$  evolves freely, while for  $\nu=0$  it does not evolve at all and is described by  $\mu$  at all times; in both cases it drives

<sup>&</sup>lt;sup>3</sup>A cylindrical measure is a finitely additive measure that is  $\sigma$ -additive on any subalgebra of cylinders generated by a finite number of vectors.

 $<sup>{}^4\</sup>mathfrak{U}_{t,s}(z)$  is the unique solution of  $i\partial_t\mathfrak{U}_{t,s}(z)=\mathfrak{H}(z)\mathfrak{U}_{t,s}(z)$  and  $\mathfrak{U}_{t,t}(z)=1$ .

<sup>&</sup>lt;sup>5</sup>We restrict our attention only to the limits  $\nu=1$  and  $\nu=0$ , since they encode all different and well-defined outcomes that one could obtain for the effective dynamics. In fact, every choice of  $\nu(\varepsilon)$  such that  $\lim_{\varepsilon\to 0} \varepsilon \nu(\varepsilon) = \lambda > 0$  would amount in a rescaling of the field dispersion relation, while any choice such that either  $\lim_{\varepsilon\to 0} \varepsilon \nu(\varepsilon) = \lambda = \infty$  or such that the limit does not exist would prevent an explicit definition of the effective dynamics in the limit  $\varepsilon\to 0$ 

the spin state through  $\mathfrak{U}_{t,0}(z)$ , mediated over all possible configurations z in the support of  $\mu$ . Let us also remark that  $\mathfrak{U}_{t,0}(z)\gamma(z)\mathfrak{U}_{t,0}^*(z)$  shall be seen as a Radon-Nikodým derivative, and as such the pushforward does not act on it.

Theorem 1.4 therefore explains how the semiclassical bosonic subsystem becomes an environment driving the spin system, unaffected by the latter, if the quasi-classical parameter  $\varepsilon$  is small enough. This also motivates the terminology used so far, *i.e.*, the identification of the spin component as the 'small' system, while the bosonic field is the 'large' environment or reservoir. In addition, the effective dynamics of the spin system can be characterized explicitly, being unitary and described by  $\mathfrak{U}_{t,0}(z)$  for any fixed configuration z of the classical field, but not unitary (and not even Markovian<sup>6</sup>) in general, due to the integration over all configurations reached by the classical bosonic state  $e^{-it\nu\omega}_{\phantom{a}\star}\mu$ . Both a stationary and a freely evolving bosonic environment can be obtained, tuning the microscopic initial state accordingly in a way that makes  $\nu(\varepsilon)$  either 1 (stationary) or  $\frac{1}{\varepsilon}$  (freely evolving). Let us stress that even if  $\nu(\varepsilon)$  appears in the Hamiltonian, it should be thought as a feature of the chosen initial state, fixing the scale of energy for the bosonic subsystem.

1.2. Loss of mass in the quasi-classical limit. An interesting feature of quasi-classical systems is that some mass can be lost in the limit  $\varepsilon \to 0$ , due to the entanglement between the two subsystems, when the spin part is infinite dimensional. By loss of mass we mean that the measure in the quasi-classical limit satisfies  $\mu(\mathfrak{h}) < 1$ . There are many well-known examples of loss of mass (also called loss of compactness) in semiclassical analysis, both in finite and infinite dimensions [see, e.g., AN08, LP93]. In those cases, however, conditions like (1.1) are enough to guarantee that no mass is lost.

Here, on the contrary, mass can be lost "through the spin system", provided the systems are entangled, and the spin system components could escape to infinity. In fact, if the microscopic state is unentangled (in a natural quasi-classical way), *i.e.* it is of the form

$$\begin{split} \Gamma_\varepsilon &= \gamma_0 \otimes \xi_\varepsilon \;, \\ \text{with } \gamma_0 &\in \mathfrak{L}^1_{+,1}\big(\mathscr{H}\big) \;, \; \xi_\varepsilon \in \mathfrak{L}^1_{+,1}\big(\mathcal{G}^s_\varepsilon(\mathfrak{h})\big) \;, \end{split}$$

the quasi-classical convergence in Proposition 1.3 "decouples" and no mass can be lost: for this class of states (1.1) implies  $\mathfrak{m}=(\mu,\gamma_0)$ , with  $\mu(\mathfrak{h})=1$ . Similarly, if the spin subsystem is finite dimensional or its particles are confined, again no mass can be lost. More precisely, if either  $\dim(\mathscr{H})<+\infty$  or there exists an operator  $\mathfrak{A}>0$  on  $\mathscr{H}$  with compact resolvent such that there exists C>0 with

$$\operatorname{tr}(\Gamma_{\varepsilon}(\mathfrak{A}\otimes 1)) \leqslant C, \tag{1.2}$$

then the measure  $\mathfrak{m} = (\mu, \gamma)$  in Proposition 1.3 is such that  $\mu(\mathfrak{h}) = 1$ .

In general however, part or all of the mass can be lost in the limit  $\varepsilon \to 0$  of a generic quantum state  $\Gamma_{\varepsilon}$ . Theorem 1.4 is also interesting if (some) mass is lost. In fact, the mass is preserved by the quasi-classical dynamics: this means that the same amount of mass is lost at any time, and therefore that one should check if any mass is lost only at the initial time.

 $<sup>^6</sup>$ We plan to investigate the non-Markovian character of the quasi-classical effective dynamics in an upcoming paper.

<sup>&</sup>lt;sup>7</sup>If  $\mathfrak{S}$  has compact resolvent (and it is bounded from below),  $\mathfrak{A} = \mathfrak{S} + |\inf \sigma(\mathfrak{S})| + 1$  would be a natural choice, and the associated condition (1.2) would mean that mass is not lost if one restricts to states with  $\varepsilon$ -uniformly-bounded Spin kinetic energy.

We think that this loss of mass phenomenon peculiar to the quasi-classical entanglement is worth pointing out, and could be explored further in concrete applications.

## 2. Heuristic Derivation

If the initial state is quasi-classically unentangled, i.e.

$$\Gamma_{\varepsilon} = \gamma_0 \otimes \xi_{\varepsilon}$$

(see § 1.2 above), it is possible to use the factorized nature of the spin-boson interaction to formally obtain a result akin to Theorem 1.4 in a very intuitive way, that hopefully helps to illustrate the main ideas behind the general proof.

In order to discuss the strategy, let us set some useful notation. Define the free Hamiltonian

$$H_{\varepsilon}^{\mathrm{f}} := H_{\varepsilon}|_{g=0} = \mathfrak{S} \otimes 1 + \nu(\varepsilon) \, 1 \otimes \mathrm{d}\mathcal{G}_{\varepsilon}(\omega) =: H^{\mathrm{fs}} + H_{\varepsilon}^{\mathrm{fb}} ,$$

and define the interaction

$$H_{\varepsilon}^{\rm i} = H_{\varepsilon} - H_{\varepsilon}^{\rm f}$$
.

The Dyson expansion for the evolution in the interaction picture is

$$e^{itH_{\varepsilon}^{f}}e^{-itH_{\varepsilon}} = 1 + \sum_{n \in \mathbb{N}_{+}} (-i)^{n} \int_{0}^{t} ds_{1} \int_{0}^{s_{1}} ds_{2} \cdots \int_{0}^{s_{n-1}} ds_{n} \, \mathfrak{s}_{s_{1}} \cdots \mathfrak{s}_{s_{n}} \otimes \varphi_{\varepsilon, s_{1}} \cdots \varphi_{\varepsilon, s_{n}} ,$$

where

$$\begin{split} \mathfrak{s}_s &= e^{isH^{\mathrm{fs}}} \mathfrak{s} e^{-isH^{\mathrm{fs}}} \;, \\ \varphi_{\varepsilon,s} &= e^{isH^{\mathrm{fb}}_{\varepsilon}} \varphi_{\varepsilon}(g) e^{-isH^{\mathrm{fb}}_{\varepsilon}} = \varphi_{\varepsilon}(e^{i\nu(\varepsilon)s\omega}g) \;; \end{split}$$

and in addition

$$e^{itH_{\varepsilon}}e^{-itH_{\varepsilon}^{f}} = 1 + \sum_{m \in \mathbb{N}_{*}} i^{m} \int_{0}^{t} du_{1} \int_{0}^{u_{1}} du_{2} \cdots \int_{0}^{u_{m-1}} du_{m} \,\mathfrak{s}_{u_{m}} \cdots \mathfrak{s}_{u_{1}} \otimes \varphi_{\varepsilon, u_{m}} \cdots \varphi_{\varepsilon, u_{1}}.$$

It follows that

$$\begin{split} \tilde{\gamma}_{\varepsilon}(t) &:= \mathrm{tr}_{\mathcal{G}_{\varepsilon}^{\mathrm{s}}(\mathfrak{h})} \Big( e^{itH^{\mathrm{fs}}} e^{-itH_{\varepsilon}} (\gamma_{0} \otimes \xi_{\varepsilon}) e^{itH_{\varepsilon}} e^{-itH^{\mathrm{fs}}} \Big) \\ &= \sum_{m,n \in \mathbb{N}} i^{m-n} \int_{0}^{t} \mathrm{d}s_{1} \cdots \int_{0}^{s_{n-1}} \mathrm{d}s_{n} \int_{0}^{t} \mathrm{d}u_{1} \cdots \int_{0}^{u_{m-1}} \mathrm{d}u_{m} \; \mathfrak{s}_{s_{1}} \cdots \mathfrak{s}_{s_{n}} \; \gamma_{0} \, \mathfrak{s}_{u_{m}} \cdots \mathfrak{s}_{u_{1}} \\ &\qquad \qquad \qquad \mathrm{tr}_{\mathcal{G}_{\varepsilon}^{\mathrm{s}}(\mathfrak{h})} \Big( \xi_{\varepsilon} \varphi_{\varepsilon,u_{m}} \cdots \varphi_{\varepsilon,u_{1}} \varphi_{\varepsilon,s_{1}} \cdots \varphi_{\varepsilon,s_{n}} \Big) \; . \end{split}$$

Now, in order to take the limit  $\varepsilon \to 0$ , one should focus on the expectation with respect to  $\xi_{\varepsilon}$ :

$$\langle \varphi_{\varepsilon,u_m} \cdots \varphi_{\varepsilon,u_1} \varphi_{\varepsilon,s_1} \cdots \varphi_{\varepsilon,s_n} \rangle_{\xi_{\varepsilon}} := \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} \Big( \xi_{\varepsilon} \varphi_{\varepsilon,u_m} \cdots \varphi_{\varepsilon,u_1} \varphi_{\varepsilon,s_1} \cdots \varphi_{\varepsilon,s_n} \Big) .$$

It is possible to write such an expectation as follows, where  $f_1, \ldots, f_k \in \mathfrak{h}$ ,

$$\langle \varphi_{\varepsilon}(f_{1}) \cdots \varphi_{\varepsilon}(f_{k}) \rangle_{\xi_{\varepsilon}} = (-i)^{k} \partial_{\lambda_{1}} \cdots \partial_{\lambda_{k}} \left( \langle W_{\varepsilon}(\lambda_{1} f_{1}) \cdots W_{\varepsilon}(\lambda_{k} f_{k}) \rangle_{\xi_{\varepsilon}} \right) \Big|_{\lambda_{1} = \cdots = \lambda_{k} = 0}$$
$$=: D_{k} \langle W_{\varepsilon}(\lambda_{1} f_{1}) \cdots W_{\varepsilon}(\lambda_{k} f_{k}) \rangle_{\xi_{\varepsilon}} \Big|_{\lambda = 0}.$$

It then follows from the Weyl CCR

$$W_{\varepsilon}(\lambda_1 f_1) W_{\varepsilon}(\lambda_2 f_2) = e^{-i\varepsilon \operatorname{Im}\langle \lambda_1 f_1, \lambda_2 f_2 \rangle} W_{\varepsilon}(\lambda_1 f_1 + \lambda_2 f_2)$$

that

$$\lim_{\varepsilon \to 0} D_k \langle W_{\varepsilon}(\lambda_1 f_1) \cdots W_{\varepsilon}(\lambda_k f_k) \rangle_{\xi_{\varepsilon}} \bigg|_{\lambda = 0} = \lim_{\varepsilon \to 0} D_k \langle W_{\varepsilon}(\lambda_1 f_1 + \cdots + \lambda_k f_k) \rangle_{\xi_{\varepsilon}} \bigg|_{\lambda = 0}.$$

Now, in this formal reasoning we feel free to exchange  $\lim_{\varepsilon\to 0}$  with  $D_k$ ; thus we obtain, provided that  $\xi_{\varepsilon} \xrightarrow[\varepsilon\to 0]{} \mu$ ,

$$D_k \lim_{\varepsilon \to 0} \langle W_{\varepsilon}(\lambda_1 f_1 + \dots + \lambda_k f_k) \rangle_{\xi_{\varepsilon}} \bigg|_{\underline{\lambda} = 0} = D_k \hat{\mu}(\lambda_1 f_1 + \dots + \lambda_k f_k) \bigg|_{\underline{\lambda} = 0} = \int_{\mathfrak{h}} \alpha_{f_1}(z) \cdots \alpha_{f_k}(z) d\mu(z) ;$$

where

$$\alpha_f(z) := 2 \operatorname{Re}\langle z, f \rangle_{\mathfrak{h}} .$$

Applying these results to  $\lim_{\varepsilon \to 0} \tilde{\gamma}_{\varepsilon}(t)$  yields:

$$\lim_{\varepsilon \to 0} \tilde{\gamma}_{\varepsilon}(t) = \sum_{m,n \in \mathbb{N}} i^{m-n} \int_0^t \mathrm{d}s_1 \cdots \int_0^{s_{n-1}} \mathrm{d}s_n \int_0^t \mathrm{d}u_1 \cdots \int_0^{u_{m-1}} \mathrm{d}u_m \, \mathfrak{s}_{s_1} \cdots \mathfrak{s}_{s_n} \, \gamma \, \mathfrak{s}_{u_m} \cdots \mathfrak{s}_{u_1} \\ \int_{\mathfrak{h}} \alpha_{s_1}(z) \cdots \alpha_{s_n}(z) \alpha_{u_1}(z) \cdots \alpha_{u_m}(z) \mathrm{d}\mu(z) \; ,$$

with

$$\alpha_s(z) = 2\text{Re}\langle z, e^{i\nu s\omega}g\rangle_{\mathfrak{h}} .$$
 (2.1)

We have thus

$$\gamma(t) := \lim_{\varepsilon \to 0} \gamma_{\varepsilon}(t) := \lim_{\varepsilon \to 0} \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} \left( e^{-itH_{\varepsilon}} (\gamma_{0} \otimes \xi_{\varepsilon}) e^{itH_{\varepsilon}} \right) \\
= \int_{\mathfrak{h}} \mathfrak{U}_{t,0}(z) \gamma(z) \mathfrak{U}_{t,0}^{*}(z) \mathrm{d} \left( e^{-it\nu\omega} \star \mu \right) (z) , \quad (2.2)$$

where  $\mathfrak{U}_{t,0}(z)$  is defined in Theorem 1.4, that can also formally be seen as

$$\mathfrak{U}_{t,0}(z) = e^{-itH^{\mathrm{fs}}} \sum_{n \in \mathbb{N}} (-i)^n \int_0^t \mathrm{d}s_1 \cdots \int_0^{s_{n-1}} \mathrm{d}s_n \, \mathfrak{s}_{s_1} \alpha_{s_1}(z) \cdots \mathfrak{s}_{s_n} \alpha_{s_n}(z) .$$

One can see last equality in (2.2) as a 'resummation of the Dyson series'.

#### 3. Proof of Theorem 1.4

As we have seen in § 2, the factorized structure of the spin-boson interaction can be used to simplify the study of the quasi-classical limit, compared to, say, the Nelson, polaron, or Pauli-Fierz models, where such a factorization is not present [see CFO22b, CFO22a, for their quasi-classical analysis]. The proof of Theorem 1.4 reflects this as well, as illustrated below. Since the proof follows closely [CFO22b] – and directly utilizes some of its results – we will mostly focus on highlighting the features specific to the spin-boson model.

The proof is organized in a few steps, namely:

- write a Duhamel-type formula for the Fourier transform of evolved quantum states in the interaction representation;
- extract a subsequence  $\varepsilon_{n_k}$  of common quasi-classical convergence for regular enough evolved states at any given time;

<sup>&</sup>lt;sup>8</sup>The scalar convergence  $\xi_{\varepsilon} \xrightarrow[\varepsilon \to 0]{} \mu$  is perfectly analogous to the quasi-classical one, and could be seen as a particular case of it where the additional degrees of freedom are trivial. Let us remark again that for the scalar case – and thus also for the unentangled quasi-classical states considered here – (1.1) is sufficient to guarantee that  $\mu(\mathfrak{h}) = 1$ .

- take the limit  $\varepsilon_{n_k} \to 0$  along the aforementioned subsequence of the Duhamel formula;
- study the resulting transport equation to identify the evolved measure, and uniqueness of the limit;
- relax the regularity assumption needed at step two to the assumption in the theorem. We will review these steps below separately.
- 3.1. The Duhamel Formula. For technical reasons, related mostly to the possible unboundedness of  $\omega$ , it is convenient to pass to the so-called interaction representation. Let us define the evolution in the interaction representation as

$$\Upsilon_{\varepsilon}(t) := e^{itH_{\varepsilon}^{\mathrm{f}}} \Gamma_{\varepsilon}(t) e^{-itH_{\varepsilon}^{\mathrm{f}}}$$
.

The Schrödinger differential equation of quantum evolution requires too much regularity for its solutions; it is more convenient to use its integral (or Duhamel) form. To write it, it is sufficient to suppose that for all  $t \in \mathbb{R}$ ,  $\operatorname{tr}\left(\Upsilon_{\varepsilon}(t)(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1)^{1/2}\right) < +\infty$ . Under this assumption the Fourier transform  $\hat{\Upsilon}_{\varepsilon}(t)$  satisfies the following integral equation, weakly on  $\mathfrak{L}^1(\mathscr{H})$ , for any  $t,s \in \mathbb{R}$  and  $\eta \in \mathfrak{h}$ :

$$[\hat{\Upsilon}_{\varepsilon}(t)](\eta) - [\hat{\Upsilon}_{\varepsilon}(s)](\eta) = -i \int_{s}^{t} \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} \left( \left[ \mathfrak{s}(\tau) \otimes \varphi_{\varepsilon}(\tau), \Upsilon_{\varepsilon}(\tau) \right] W_{\varepsilon}(\eta) \right) d\tau$$

$$= i \int_{s}^{t} \left( \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} \left( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \right) \mathfrak{s}(\tau) - \mathfrak{s}(\tau) \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})} \left( \varphi_{\varepsilon}(\tau) \Upsilon_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \right) \right) d\tau . \quad (3.1)$$

Here, we write

$$\mathfrak{s}(\tau) = e^{i\tau H^{\mathrm{fs}}} \mathfrak{s} e^{-i\tau H^{\mathrm{fs}}}$$
 and  $\varphi_{\varepsilon}(\tau) = e^{i\tau H_{\varepsilon}^{\mathrm{fb}}} \varphi_{\varepsilon}(g) e^{-i\tau H_{\varepsilon}^{\mathrm{fb}}}$ .

Once the required regularity is taken care of, this equation follows directly from the algebraic properties of the quantum evolution (in interaction representation)  $e^{itH_{\varepsilon}^{f}}e^{-itH_{\varepsilon}}$ , as already outlined in § 2. The Duhamel formula is the starting point for our study of the dynamical quasi-classical limit.

The regularity bound concerning the average of the number operator at all times that we used above – especially in its form that is uniform w.r.t.  $\varepsilon \in (0,1)$  – will be crucial also in what follows, so let us formulate it as an auxiliary "black box" result. Such propagation results are typically heavily dependent on the model under consideration; for the Spin-Boson system one could adapt very easily the results available for the Nelson model with ultraviolet cutoff [Fal13, Proposition 4.2], obtaining the lemma below.

**Lemma 3.1.** For any  $\delta, C > 0$  and for all  $t \in \mathbb{R}$ , there exists  $K(\delta, C, t) > 0$  such that

$$\operatorname{tr}\left(\Gamma_{\varepsilon}\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{\delta}\right)\leqslant C\implies \left(\operatorname{tr}\left(\Gamma_{\varepsilon}(t)\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{\delta}\right)\leqslant K(\delta,C,t)\right.$$
 
$$\wedge \operatorname{tr}\left(\Upsilon_{\varepsilon}(t)\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{\delta}\right)\leqslant K(\delta,C,t)\right).$$

3.2. Common subsequence extraction at all times. Thanks to the propagation lemma, Lemma 3.1, it is possible to prove that  $t \mapsto \hat{\Upsilon}_{\varepsilon}(t)$  is uniformly equicontinuous w.r.t.  $\varepsilon \in (0,1)$ . This in turn implies, by a diagonal extraction argument, that starting from any sequence  $\varepsilon_n \to 0$ , it is possible to extract a subsequence  $\varepsilon_{n_k} \to 0$  that guarantees convergence of  $\Upsilon_{\varepsilon_{n_k}}(\tau)$  to some state-valued measure  $\mathfrak{n}_{\tau}$  for any  $\tau$  in a given compact interval [s,t] (actually for any given time). This is the crucial ingredient allowing to study the limit  $\varepsilon \to 0$  of the

Duhamel formula (3.1), for the latter involves the integral over all evolved states between s and t. The result reads as follows, and it has been proved in [CFO22b, Propositions 4.2 and 4.3], with a general argument that does not depend on the nature of  $\mathcal{H}$  or on the Hamiltonian (one only requires that a form of Lemma 3.1 is available).

**Proposition 3.2.** Let  $\Gamma_{\varepsilon}$  be such that

$$\operatorname{tr}\left(\Gamma_{\varepsilon}\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{1/2}\right)\leqslant C$$
.

Then  $\mathbb{R} \times \mathfrak{h} \ni (t, \eta) \mapsto [\hat{\Upsilon}_{\varepsilon}(t)](\eta) \in \mathfrak{L}^{1}(\mathscr{H})$  is uniformly equicontinuous w.r.t.  $\varepsilon \in (0, 1)$  on bounded subsets of  $\mathbb{R} \times \mathfrak{h}$ , having endowed  $\mathfrak{L}^{1}(\mathscr{H})$  with the weak-\* topology.

In addition, for any sequence  $\varepsilon_n \to 0$ , there exists a subsequence  $\varepsilon_{n_k} \to 0$  and a family  $\{\mathfrak{n}_t\}_{t\in\mathbb{R}}$  of state-valued measures such that for all  $t\in\mathbb{R}$ ,

$$\Upsilon_{\varepsilon_{n_k}}(t) \xrightarrow[k \to \infty]{} \mathfrak{n}_t$$
.

As a byproduct (again this is a general result concerning unitary evolutions generated by operators of the type  $\nu(\varepsilon)d\mathcal{G}_{\varepsilon}(\cdot)$ ), we also get the following information on the limit of the "true" evolution  $\Gamma_{\varepsilon}(t)$ . Remember that we defined  $\nu = \lim_{\varepsilon \to 0} \varepsilon \nu(\varepsilon)$ .

**Corollary 3.3.** Under the same assumptions as in Proposition 3.2, and given the subsequence  $\varepsilon_{n_k} \to 0$  and measures  $\{\mathfrak{n}_t\}_{t\in\mathbb{R}}$ , we have that for any  $t\in\mathbb{R}$ ,

$$\Gamma_{\varepsilon_{n_k}}(t) \underset{k \to \infty}{\longrightarrow} \mathfrak{m}_t = e^{-itH^{\mathrm{fs}}} (e^{-it\nu\omega} \star \mathfrak{n}_t) e^{itH^{\mathrm{fs}}}.$$

In other words, we are able to relate the quasi-classical evolution in the interaction picture to the one not in interaction picture "as it should be", *i.e.* by acting with the expected free evolution on both the Spin and classical Boson subsystems. It follows that once we have characterized the map  $t \to \mathfrak{n}_t$ , we have also a characterization for the map  $t \to \mathfrak{m}_t$ .

3.3. The limit of the Duhamel formula. We are now in a position to take the limit  $\varepsilon \to 0$  of the Duhamel formula (3.1). In taking this step, the factorized nature of the spin-boson interaction helps greatly, essentially allowing to transform the problem from quasi-classical to semiclassical, allowing us to avoid completely the use the heavy machinery of quasi-classical calculus developed in [CFO22b, §2] (that is however necessary whenever the interaction is not factorized as for the spin boson). Let  $\mathfrak{k} \in \mathfrak{L}^{\infty}(\mathscr{H})$  be a compact operator on the Spin subsystem, then Duhamel's formula (3.1) becomes

$$\operatorname{tr}_{\mathscr{H}}\left(\left[\hat{\Upsilon}_{\varepsilon}(t)\right](\eta)\mathfrak{k}\right) - \operatorname{tr}_{\mathscr{H}}\left(\left[\hat{\Upsilon}_{\varepsilon}(s)\right](\eta)\mathfrak{k}\right) \\
= i \int_{s}^{t} \left(\operatorname{tr}\left(\Upsilon_{\varepsilon}(\tau)\varphi_{\varepsilon}(\tau)W_{\varepsilon}(\eta)\mathfrak{s}(\tau)\mathfrak{k}\right) - \operatorname{tr}\left(\mathfrak{k}\mathfrak{s}(\tau)\varphi_{\varepsilon}(\tau)\Upsilon_{\varepsilon}(\tau)W_{\varepsilon}(\eta)\right)\right) d\tau .$$

It is possible to exchange the trace w.r.t.  $\mathscr{H}$  and the integral by dominated convergence, using the bound for  $\Gamma_{\varepsilon}$  assumed in Proposition 3.2, and its time propagation given by Lemma 3.1. By Proposition 3.2, and the definition of quasi-classical convergence, it follows immediately that, along the common subsequence  $\varepsilon_{n_k} \to 0$ ,

$$\begin{split} &\lim_{k\to\infty} \mathrm{tr}_{\mathscr{H}}\Big([\hat{\Upsilon}_{\varepsilon_{n_k}}(t)](\eta)\mathfrak{k}\Big) = \mathrm{tr}_{\mathscr{H}}\Big(\hat{\mathfrak{n}}_t(\eta)\mathfrak{k}\Big)\;,\\ &\lim_{k\to\infty} \mathrm{tr}_{\mathscr{H}}\Big([\hat{\Upsilon}_{\varepsilon_{n_k}}(s)](\eta)\mathfrak{k}\Big) = \mathrm{tr}_{\mathscr{H}}\Big(\hat{\mathfrak{n}}_s(\eta)\mathfrak{k}\Big)\;. \end{split}$$

Let us now focus on the interaction term, and in particular on the expression

$$\operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s}(\tau) \mathfrak{k} \Big) ,$$

the other one being analogous. Let us now decompose the operator  $\mathfrak{s}(\tau)\mathfrak{k}$  in its real positive, negative, and imaginary positive, negative parts:

$$\mathfrak{s}(\tau)\mathfrak{k} = \mathfrak{s}\mathfrak{k}_{r+} - \mathfrak{s}\mathfrak{k}_{r-} + i(\mathfrak{s}\mathfrak{k}_{i+} - \mathfrak{s}\mathfrak{k}_{i-})$$

with  $\mathfrak{st}_{r+},\mathfrak{st}_{r-},\mathfrak{st}_{i+},\mathfrak{st}_{i-}\geqslant 0$ . Therefore, we have that

$$\begin{split} \operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s}(\tau) \mathfrak{k} \Big) &= \operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s} \mathfrak{k}_{r+} \Big) - \operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s} \mathfrak{k}_{r-} \Big) \\ &+ i \bigg( \operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s} \mathfrak{k}_{i+} \Big) - \operatorname{tr} \Big( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{s} \mathfrak{k}_{i-} \Big) \bigg) \;. \end{split}$$

Now, we would like to treat all these terms in the same fashion, so let us focus on the first one. We can split the total trace in the two partial traces, but we do it *in reverse order w.r.t.* before:

$$\operatorname{tr}\Big(\Upsilon_{\varepsilon}(\tau)\varphi_{\varepsilon}(\tau)W_{\varepsilon}(\eta)\mathfrak{sk}_{r+}\Big) = \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{s}(\mathfrak{h})}\bigg(\operatorname{tr}_{\mathscr{H}}\Big(\Upsilon_{\varepsilon}(\tau)\mathfrak{sk}_{r+}\Big)\varphi_{\varepsilon}(\tau)W_{\varepsilon}(\eta)\bigg)\;.$$

The partial trace w.r.t. to  $\mathcal{H}$  is the expectation over a state of a positive operator, so

$$\zeta_{arepsilon}( au,\mathfrak{st}_{r+}) := \mathrm{tr}_{\mathscr{H}}\Big(\Upsilon_{arepsilon}( au)\mathfrak{st}_{r+}\Big) \in \mathfrak{L}^1_+(\mathfrak{h}) \;,$$

and we finally obtain

$$\operatorname{tr} \Bigl( \Upsilon_{\varepsilon}(\tau) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \mathfrak{sk}_{r+} \Bigr) = \operatorname{tr}_{\mathcal{G}_{\varepsilon}^{\mathbf{s}}(\mathfrak{h})} \Biggl( \zeta_{\varepsilon}(\tau, \mathfrak{sk}_{r+}) \varphi_{\varepsilon}(\tau) W_{\varepsilon}(\eta) \Biggr) \; .$$

The state  $\zeta_{\varepsilon}(\tau, \mathfrak{st}_{r+})$  is a semiclassical (scalar) state, living on the Fock space. On one hand, by Proposition 3.2 and the definition of quasi-classical convergence<sup>9</sup> we know that

$$\zeta_{\varepsilon_{n_k}}(\tau, \mathfrak{st}_{r+}) \underset{k \to \infty}{\longrightarrow} \mathrm{d}\mu_{\tau, \mathfrak{st}_{r+}}(z) = \mathrm{tr}_{\mathscr{H}}(\mathrm{d}\mathfrak{n}_{\tau}(z)\mathfrak{st}_{r+}).$$

On the other hand, by semiclassical calculus in infinite dimensions [see AN08], we also know that

$$\lim_{k\to\infty} \mathrm{tr}_{\mathcal{G}^{\mathtt{s}}_{\varepsilon n_k}(\mathfrak{h})} \bigg( \zeta_{\varepsilon_{n_k}}(\tau, \mathfrak{st}_{r+}) \varphi_{\varepsilon_{n_k}}(\tau) W_{\varepsilon_{n_k}}(\eta) \bigg) = \int_{\mathfrak{h}} \alpha_{\tau}(z) e^{2i \mathrm{Re} \langle \eta, z \rangle_{\mathfrak{h}}} \mathrm{d} \mu_{\tau, \mathfrak{st}_{r+}}(z) \;,$$

where the shorthand  $\alpha_{\tau}(z)$  has been defined in (2.1). Combining the two things, and repeating the same reasoning for all the other remaining terms, we end up obtaining the following integral equation for the map  $t \to \mathfrak{n}_t$  (another dominated convergence argument allows to pass the limit  $\varepsilon_{n_k} \to 0$  inside the time integral, this time exploiting the uniformity w.r.t.  $\varepsilon \in (0,1)$  of the number operator bounds at any time).

**Proposition 3.4.** The family of state-valued measures  $\{\mathfrak{n}_t\}_{t\in\mathbb{R}}$  of Proposition 3.2 satisfies the following transport equation for the Fourier transform, in the weak sense on  $\mathfrak{L}^1(\mathcal{H})$ :

$$\hat{\mathfrak{n}}_t(\eta) - \hat{\mathfrak{n}}_s(\eta) = i \int_0^t \int_{\mathfrak{h}} [\gamma_{\mathfrak{n}_\tau}(z), \mathfrak{s}(\tau)] \alpha_\tau(z) e^{2i\operatorname{Re}\langle \eta, z \rangle_{\mathfrak{h}}} d\mu_{\mathfrak{n}_\tau}(z) d\tau.$$

<sup>&</sup>lt;sup>9</sup>Quasi-classical convergence is the pointwise convergence of Fourier transforms in weak-\* topology, *i.e.* when tested with compact operators. Since  $\mathfrak{st}_{r+}$  is compact, we have pointwise convergence of  $\hat{\Upsilon}_{\varepsilon}(\tau)$  traced together with  $\mathfrak{st}_{r+}$ .

# 3.4. Uniqueness of the solution to the transport equation, uniqueness of the limit.

The transport equation for the Fourier transform of  $\mathfrak{n}_t$  can be easily translated in an equation for the measure:

$$\gamma_{\mathfrak{n}_t}(z)\mathrm{d}\mu_{\mathfrak{n}_t}(z) - \gamma_{\mathfrak{n}_s}(z)\mathrm{d}\mu_{\mathfrak{n}_s}(z) = i\int_s^t [\gamma_{\mathfrak{n}_\tau}(z),\mathfrak{s}(\tau)]\alpha_\tau(z)\mathrm{d}\mu_{\mathfrak{n}_\tau}(z)\mathrm{d}\tau \ .$$

Now, let us fix s = 0, and suppose that we have the quasi-classical convergence at initial time

$$\Gamma_{\varepsilon_n} \xrightarrow[n \to \infty]{} \mathfrak{m}$$
.

It then follows that

$$\mathfrak{n}_0 = \mathfrak{m}$$
,

and the transport equation reads

$$\gamma_{\mathfrak{n}_t}(z)\mathrm{d}\mu_{\mathfrak{n}_t}(z) - \gamma_{\mathfrak{m}}(z)\mathrm{d}\mu_{\mathfrak{m}}(z) = i\int_0^t [\gamma_{\mathfrak{n}_\tau}(z),\mathfrak{s}(\tau)]\alpha_{\tau}(z)\mathrm{d}\mu_{\mathfrak{n}_\tau}(z)\mathrm{d}\tau$$
.

The family of state-valued measures  $\{\mathfrak{n}_t\}_{t\in\mathbb{R}}$  given by

$$dn_t(z) = \tilde{\mathfrak{U}}_{t,0}(z)\gamma_{\mathfrak{m}}(z)\tilde{\mathfrak{U}}_{t,0}^*(z) ,$$

with  $\tilde{\mathfrak{U}}_{t,0}(z)$  the two-parameter unitary group on  $\mathscr{H}$  generated by

$$\alpha_{\tau}(z)\mathfrak{s}(\tau)$$

is easily checked to be a solution to the transport equation. Such solution is actually *unique*, as is proved in a general fashion in [CFO22b, Proposition 5.3]. Therefore, we have proved that given

$$\Gamma_{\varepsilon_n} \underset{n \to \infty}{\longrightarrow} \mathfrak{m} \quad \text{and} \quad \operatorname{tr} \left( \Gamma_{\varepsilon} \left( d \mathcal{G}_{\varepsilon}(1) + 1 \right)^{1/2} \right) \leqslant C ,$$

there exists a subsequence  $\varepsilon_{n_k}$  along which for any  $t \in \mathbb{R}$  we have the convergence

$$\Upsilon_{\varepsilon_{n_k}}(t) \xrightarrow[k \to \infty]{} \mathfrak{n}_t$$
,

with

$$dn_t(z) = \tilde{\mathfrak{U}}_{t,0}(z)\gamma_{\mathfrak{m}}(z)\tilde{\mathfrak{U}}_{t,0}^*(z) .$$

By Corollary 3.3, it also follows that for any  $t \in \mathbb{R}$ ,

$$\Gamma_{\varepsilon_{n_k}}(t) \xrightarrow[k\to\infty]{} \mathfrak{m}_t$$
,

with

$$d\mathfrak{m}_{t}(z) = \mathfrak{U}_{t,0}(z)\gamma(z)\mathfrak{U}_{t,0}^{*}(z) d\left(e^{-it\nu\omega} \star \mu\right)(z) ,$$

as stated in Theorem 1.4. However, a couple of steps are still missing to complete the proof of the latter.

First of all, one shall prove convergence along the original sequence of convergence at initial time  $\varepsilon_n \to 0$ , rather than on some existing subsequence  $\varepsilon_{n_k} \to 0$ . This is readily established exploiting once more the uniqueness of the solution to the transport equation. Suppose in fact that we have another subsequence  $\varepsilon_{n_j} \to 0$  of convergence for  $\Upsilon_{\varepsilon_{n_j}}(t)$  at all times  $t \in \mathbb{R}$ , with possibly different limit measure  $\{\mathfrak{n}_t'\}_{t\in\mathbb{R}}$ . Then, by the same argument as in § 3.3,  $\mathfrak{n}_t'$  would satisfy the very same transport equation given in Proposition 3.4 for  $\mathfrak{n}_t$ . Since the solution to that transport equation is unique, this would imply  $\mathfrak{n}_t' = \mathfrak{n}_t$ . In other words, there is a unique possible cluster point for the sequence  $\Upsilon_{\varepsilon_n}(t)$ , thus it converges itself to the very same limit

 $\mathfrak{n}_t$ . We can thus conclude that, that if

$$\Gamma_{\varepsilon_n} \underset{n \to \infty}{\longrightarrow} \mathfrak{m} \quad \text{and} \quad \operatorname{tr} \Big( \Gamma_{\varepsilon} \big( d \mathcal{G}_{\varepsilon}(1) + 1 \big)^{1/2} \Big) \leqslant C ,$$

then for any  $t \in \mathbb{R}$ ,

$$\Gamma_{\varepsilon_n}(t) \xrightarrow[k \to \infty]{} \mathfrak{m}_t ,$$

with

$$d\mathfrak{m}_{t}(z) = \mathfrak{U}_{t,0}(z)\gamma(z)\mathfrak{U}_{t,0}^{*}(z) d\left(e^{-it\nu\omega} \star \mu\right)(z) .$$

# 3.5. Relaxing the regularity assumption on the expectation of the number operator. The final step for the proof is to relax the initial time assumption

$$\operatorname{tr}\left(\Gamma_{\varepsilon}\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{1/2}\right)\leqslant C$$

used in the above, to

$$\operatorname{tr}\left(\Gamma_{\varepsilon}\left(\mathrm{d}\mathcal{G}_{\varepsilon}(1)+1\right)^{\delta}\right)\leqslant C$$

for some  $\delta > 0$ . This is done using standard approximation techniques and density arguments, as detailed in [AN11, §2]. This concludes the proof of Theorem 1.4.

#### References

- [AH97] A. Arai, M. Hirokawa. On the existence and uniqueness of ground states of a generalized spin-boson model. *J. Funct. Anal.* **151** (2), pp. 455–503 (1997).
- [AJN17] L. Amour, L. Jager, J. Nourrigat. Infinite dimensional semiclassical analysis and applications to a model in NMR. *ArXiv e-prints* arXiv:1705.07097 (2017). arXiv:1705.07097.
- [ALN16] L. Amour, R. Lascar, J. Nourrigat. Weyl calculus in Wiener spaces and in QED. ArXiv e-prints (2016). arXiv:1610.06379.
- [ALN17] L. Amour, R. Lascar, J. Nourrigat. Weyl calculus in QED I. The unitary group. J. Math. Phys. 58 (1), pp. 013,501, 24 (2017). arXiv:1510.05293.
- [AN08] Z. Ammari, F. Nier. Mean field limit for bosons and infinite dimensional phase-space analysis. *Ann. Henri Poincaré* **9** (8), pp. 1503–1574 (2008). arXiv:0711.4128.
- [AN09] Z. Ammari, F. Nier. Mean field limit for bosons and propagation of Wigner measures. J. Math. Phys. **50** (4), pp. 042,107, 16 (2009). arXiv:0807.3108.
- [AN11] Z. Ammari, F. Nier. Mean field propagation of Wigner measures and BBGKY hierarchies for general bosonic states. *J. Math. Pures Appl.* (9) **95** (6), pp. 585–626 (2011). arXiv:1003.2054.
- [AN15] Z. Ammari, F. Nier. Mean field propagation of infinite-dimensional Wigner measures with a singular two-body interaction potential. *Ann. Sc. Norm. Super. Pisa Cl. Sci.* (5) **XIV** (1), pp. 155–220 (2015). arXiv:1111.5918.
- [Ara90] A. Arai. An asymptotic analysis and its application to the nonrelativistic limit of the Pauli-Fierz and a spin-boson model. J. Math. Phys. 31 (11), pp. 2653–2663 (1990).
- [Ara91] A. Arai. A theorem on essential selfadjointness with application to Hamiltonians in non-relativistic quantum field theory. J. Math. Phys. 32 (8), pp. 2082–2088 (1991).
- [CCFO21] R. Carlone, M. Correggi, M. Falconi, M. Olivieri. Emergence of Time-Dependent Point Interactions in Polaron Models. SIAM J. Math. Anal. 53 (4), pp. 4657–4691 (2021). arXiv:1904.11012.
  - [CF18] M. Correggi, M. Falconi. Effective Potentials Generated by Field Interaction in the Quasi-Classical Limit. Ann. Henri Poincaré 19 (1), pp. 189–235 (2018). arXiv:1701.01317.

- [CFO19] M. Correggi, M. Falconi, M. Olivieri. Magnetic Schrödinger Operators as the Quasi-Classical Limit of Pauli-Fierz-type Models. J. Spectr. Theory 9 (4), pp. 1287–1325 (2019). arXiv:1711.07413.
- [CFO22a] M. Correggi, M. Falconi, M. Olivieri. Ground State Properties in the Quasi-Classical Regime. Anal. PDE (2022). In press, arXiv:2007.09442.
- [CFO22b] M. Correggi, M. Falconi, M. Olivieri. Quasi-Classical Dynamics. J. Eur. Math. Soc. (JEMS) (2022). Published online first, arXiv:1909.13313.
  - [Coo51] J. M. Cook. The mathematics of second quantization. Proc. Nat. Acad. Sci. U. S. A. 37, pp. 417–420 (1951).
  - [Der03] J. Dereziński. Van Hove Hamiltonians—exactly solvable models of the infrared and ultraviolet problem. *Ann. Henri Poincaré* 4 (4), pp. 713–738 (2003).
  - [DG13] J. Dereziński, C. Gérard. Mathematics of quantization and quantum fields. Cambridge Monographs on Mathematical Physics (Cambridge University Press, Cambridge, 2013). ISBN 978-1-107-01111-3, xii+674 pp.
  - [Fal13] M. Falconi. Classical limit of the Nelson model with cutoff. *J. Math. Phys.* **54** (1), pp. 012,303, 30 (2013). arXiv:1205.4367.
  - [Fal15] M. Falconi. Self-adjointness criterion for operators in Fock spaces. Math. Phys. Anal. Geom. 18 (1), pp. Art. 2, 18 (2015). arXiv:1405.6570.
  - [Fal18] M. Falconi. Cylindrical Wigner measures. Doc. Math. 23, pp. 1677–1756 (2018). arXiv:1605.04778.
  - [HH11] D. Hasler, I. Herbst. Ground states in the spin boson model. *Ann. Henri Poincaré* 12 (4), pp. 621–677 (2011).
  - [JMS20] A. Joye, M. Merkli, D. Spehner. Adiabatic transitions in a two-level system coupled to a free boson reservoir. *Ann. Henri Poincaré* **21** (10), pp. 3157–3199 (2020).
  - [KM16] M. Könenberg, M. Merkli. On the irreversible dynamics emerging from quantum resonances. J. Math. Phys. 57 (3), pp. 033,302, 26 (2016).
- [KMS15] M. Könenberg, M. Merkli, H. Song. Ergodicity of the spin-boson model for arbitrary coupling strength. Comm. Math. Phys. 336 (1), pp. 261–285 (2015).
- [LCD<sup>+</sup>87] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, W. Zwerger. Dynamics of the dissipative two-state system. *Rev. Mod. Phys.* 59, pp. 1–85 (1987). Erratum: Rev. Mod. Phys. 67(1), 725 (1995).
  - [Lon22] D. Lonigro. Generalized spin-boson models with non-normalizable form factors. *J. Math. Phys.* **63** (7), pp. Paper No. 072,105, 31 (2022).
  - [LP93] P.-L. Lions, T. Paul. Sur les mesures de Wigner. Rev. Mat. Iberoamericana 9 (3), pp. 553-618 (1993).
- [MBBG11] M. Merkli, G. P. Berman, F. Borgonovi, K. Gebresellasie. Evolution of entanglement of two qubits interacting through local and collective environments. *Quantum Inf. Comput.* 11 (5-6), pp. 390–419 (2011).
  - [MBS13] M. Merkli, G. P. Berman, R. Sayre. Electron transfer reactions: generalized spin-boson approach. J. Math. Chem. 51 (3), pp. 890–913 (2013).
- [MBS+16] M. Merkli, G. P. Berman, R. T. Sayre, S. Gnanakaran, M. Könenberg, A. I. Nesterov, H. Song. Dynamics of a chlorophyll dimer in collective and local thermal environments. J. Math. Chem. 54 (4), pp. 866–917 (2016).
  - [Mer20] M. Merkli. Quantum markovian master equations: Resonance theory shows validity for all time scales. *Annals of Physics* **412**, p. 167,996 (2020).
  - [Mer22a] M. Merkli. Dynamics of open quantum systems i, oscillation and decay. *Quantum* **6**, p. 615 (2022).

- [Mer22b] M. Merkli. Dynamics of open quantum systems ii, markovian approximation. *Quantum* 6, p. 616 (2022).
- [moh14] Quantum Effects in Biology (Cambridge University Press, 2014).
- [MSB07] M. Merkli, I. M. Sigal, G. P. Berman. Decoherence and thermalization. *Phys. Rev. Lett.* 98 (13), pp. 130,401, 4 (2007).
- [PSE96] G. M. Palma, K.-A. Suominen, A. K. Ekert. Quantum computers and dissipation. Proc. Roy. Soc. London Ser. A 452 (1946), pp. 567–584 (1996).
- [Seg59] I. E. Segal. Foundations of the theory of dynamical systems of infinitely many degrees of freedom. I. *Mat.-Fys. Medd. Danske Vid. Selsk.* **31** (12), p. 39 pp. (1959) (1959).
- [Seg61] I. E. Segal. Foundations of the theory of dyamical systems of infinitely many degrees of freedom. II. Canad. J. Math. 13, pp. 1–18 (1961).
- [XS94] D. Xu, K. Schulten. Coupling of protein motion to electron transfer in a photosynthetic reaction center: investigating the low temperature behavior in the framework of the spin—boson model. *Chem. Phys.* **182** (2), pp. 91–117 (1994).

DIPARTIMENTO DI MATEMATICA, POLITECNICO DI MILANO, PIAZZA LEONARDO DA VINCI 32, 20133, MILANO, ITALY.

Email address: michele.correggi@gmail.com

URL: https://sites.google.com/view/michele-correggi

DIPARTIMENTO DI MATEMATICA, POLITECNICO DI MILANO, PIAZZA LEONARDO DA VINCI 32, 20133, MILANO, ITALY.

Email address: marco.falconi@polimi.it

URL: https://www.mfmat.org/

DEPARTMENT OF MATHEMATICS AND STATISTICS, MEMORIAL UNIVERSITY OF NEWFOUNDLAND, St. JOHN'S, NL A1C 5S7, CANADA.

Email address: merkli@mun.ca

URL: https://www.math.mun.ca/~merkli/