

REDUCED AND EXTENDED WEAK COUPLING LIMIT

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Abstract. The main aim of our lectures is to give a pedagogical introduction to various mathematical formalisms used to describe open quantum systems: completely positive semigroups, dilations of semigroups, quantum Langevin dynamics and the so-called Pauli-Fierz Hamiltonians.

We explain two kinds of the weak coupling limit. Both of them show that Hamiltonian dynamics of a small quantum system interacting with a large reservoir can be approximated by simpler dynamics. The better known reduced weak coupling limit leads to completely positive dynamics. The main topic of our lecture notes, the extended weak coupling limit, also known as the stochastic limit, leads to quantum Langevin dynamics.

Our lecture notes are based partly on the results of our recent articles [DD1, DD2].

1. Introduction. Physicists often describe quantum systems by *completely positive* (c.p.) semigroups [Haa, AL, Al2]. It is generally believed that this approach is only a phenomenological approximation to a more fundamental description. One usually assumes that on the fundamental level the dynamics of quantum systems is unitary, more precisely, is of the form $t \mapsto e^{itH} \cdot e^{-itH}$ for some self-adjoint H .

One of justifications for the use of c.p. semigroups in quantum physics is based on the so-called weak coupling limit for the reduced dynamics [VH, Da1], which we will call the *reduced weak coupling limit*. One assumes that a *small system* is coupled to a *large reservoir* and the dynamics of the full system is unitary. The interaction between the small system and the reservoir is multiplied by a small coupling constant λ . Often the reservoir is described by a *free Bose gas*.

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The basic steps of the reduced weak coupling limit are:

- Reduce the dynamics to the small system.
- Rescale time as t/λ^2 .
- Subtract the dynamics of the small system.
- Consider the weak coupling $\lambda \rightarrow 0$.

In the limit one obtains a dynamics given by a c.p. Markov semigroup.

Another possible justification of c.p. dynamics goes as follows. One considers the tensor product of the small system and an appropriate bosonic reservoir. On this enlarged space one constructs a certain unitary dynamics whose reduction to the small system is a c.p. semigroup. We will call it a *quantum Langevin dynamics*. Another name used in this context in the literature is a *quantum stochastic dynamics*. Its construction has a long history, let us mention [AFLe, HP, Fr, Maa].

Thus one can obtain a Markov c.p. semigroup by reducing a *single* unitary dynamics, without invoking a family of dynamics and taking its limit. However, the generator of a quantum Langevin dynamics equals $i[Z, \cdot]$ where Z is a self-adjoint operator that does not look like a physically realistic Hamiltonian. In particular, it is unbounded from both below and above. Thus one can question the physical relevance of this construction.

It turns out, however, that one can extend the weak coupling limit in such a way, that it involves not only the small system, but also the reservoir. As a result of this approach one can obtain a quantum Langevin dynamics. One can argue that this approach gives a physical justification of quantum Langevin dynamics.

The above idea was first implemented in [AFL] by Accardi, Frigerio and Lu under the name of the *stochastic limit* (see also [ALV]). Recently we presented our version of this approach, under the name of the *extended weak coupling limit* [DD1, DD2], which we believe is simpler and more natural than that of [AFL]. The basic steps of the extended weak coupling limit are:

- Introduce the so-called *asymptotic space*—the tensor product of the space of the small system and of the *asymptotic reservoir*.
- Introduce an *identification operator* that maps the asymptotic reservoir into the physical reservoir and rescales its energy by λ^2 around the Bohr frequencies.
- Rescale time as t/λ^2 .
- Subtract the “fast degrees of freedom”.
- Consider the weak coupling $\lambda \rightarrow 0$.

In the limit one obtains a quantum Langevin dynamics on the asymptotic space. Note that the asymptotic reservoir is given by a bosonic Fock space (just as the physical reservoir). Its states are however different—they correspond only to those physical bosons whose energies differ from the *Bohr frequencies* by at most $O(\lambda^2)$. Only such bosons survive the weak coupling limit.

Let us mention yet another scheme of deriving quantum Langevin equations that has received attention in the literature, namely the ‘repeated interaction models’ where the reservoir is continuously refreshed, see [AtP, AtJ].

In this article we review various aspects of the weak coupling limit, reduced and, especially, extended, mostly following our papers [DD1, DD2]. We also describe some background material, especially related to completely positive semigroups, quantum Langevin dynamics and the Detailed Balance Condition.

The plan of our article is as follows. In Section 2 we describe both kinds of the weak coupling limit on a class of toy-examples—the so-called *Friedrichs Hamiltonians* and their dilations. They are less relevant physically than the main model treated in our article—the one based on Pauli-Fierz operators. Nevertheless, they illustrate some of the main ideas of this limit in a simple and mathematically instructive context. This section is based on [DD1].

In Sections 3 we recall some facts about completely positive maps and semigroups, sketching proofs of the *Stinespring dilation* theorem [St] and of the so-called *Lindblad form* of the generator of a c.p. semigroup [Li, GKS]. In particular, we discuss the freedom of choosing various terms in the Lindblad form. This question, which we have not seen discussed in the literature, is relevant for the construction of quantum Langevin dynamics and the weak coupling limit.

C.p. semigroups that arise in the weak coupling limit have an additional property—they commute with the unitary dynamics generated by the Hamiltonian K of the small system—for brevity we say that they are *K-invariant*. If in addition the reservoir is thermal, they satisfy another special property—the so-called *Detailed Balance Condition (DBC)* [DF1, Ag, FKGV, Al1]. We devote a large part of Sect. 3 to an analysis of the K -invariance and the DBC. We show that the generator of a c.p. semigroup with these properties has some features that curiously resemble the *Tomita-Takesaki theory* and the *KMS condition*. Let us note that in our article the DBC is considered jointly with the K -invariance, because c.p. semigroups obtained in the weak coupling limit always have the latter property.

In Section 4 we describe the terminology and notation that we use to describe second-quantized bosonic reservoirs interacting with a small system. In particular, we introduce *Pauli-Fierz operators* [DJ1]—used often (also under other names) in the physics literature to describe physically realistic systems. In Subsect. 4.3 we discuss thermal reservoirs. In our definition of a thermal reservoir at inverse temperature β one needs to check a simple condition for the interaction without explicitly invoking the concept of a KMS state on an operator algebra, or of a thermal Araki-Woods representation of the CCR [DF1, DJ1]. Of course, this condition is closely related to the KMS property.

In Subsection 5 we describe a construction of quantum Langevin dynamics. We include a discussion of the so-called quadratic noises, even though they are still not used in our version of the extended weak coupling limit. (See however [Go] for some partial results in the context of the formalism of [AFL]).

In Section 6 we describe the two kinds of the weak coupling limit for Pauli-Fierz operators: reduced and extended. Most of this section is based on [DD2].

2. Toy model of the weak coupling limit. This section is somewhat independent of the remaining part of the article. It explains the (reduced and extended) weak coupling

limit in the setting of contractive semigroups on a Hilbert space and their unitary dilations. It gives us an opportunity to explain some of the main ideas of the weak coupling limit in a relatively simple setting. It is based on [DD1].

It is possible to construct physically interesting models based on the material of this section (e.g. by considering quadratic Hamiltonians obtained by second quantization). We will not discuss this possibility further, since in the remaining part of the article we will analyze more interesting and more realistic models.

2.1. Dilations of contractive semigroups. First let us recall the well known concept of a unitary dilation of a contractive semigroup. Let \mathcal{K} be a Hilbert space and $e^{-it\Upsilon}$ a strongly continuous contractive semigroup on \mathcal{K} . This implies that $-i\Upsilon$ is dissipative: $-i\Upsilon + i\Upsilon^* \leq 0$.

Let \mathcal{Z} be a Hilbert space containing \mathcal{K} , $I_{\mathcal{K}}$ the embedding of \mathcal{K} in \mathcal{Z} and U_t a unitary group on \mathcal{Z} . We say that $(\mathcal{Z}, I_{\mathcal{K}}, U_t)$ is a dilation of $e^{-it\Upsilon}$ iff

$$I_{\mathcal{K}}^* U_t I_{\mathcal{K}} = e^{-it\Upsilon}, \quad t \geq 0.$$

It is well known that every weakly continuous contractive semigroup possesses a unitary dilation (which is unique up to unitary equivalence if we additionally demand its minimality). The original and well known construction of a unitary dilation is due to Foias and Nagy and can be found in [NF] (see also [EL]). Below we present another construction, which looks different from that of Foias-Nagy. Its main idea is to view the generator of a unitary dilation as a kind of a *singular Friedrichs operator*. (See the next section, where Friedrichs operators are introduced). Such a definition is well adapted to the extended weak coupling limit. The construction that we present seems to be less known in the mathematics literature than that of Foias-Nagy. Nevertheless, similar constructions are scattered in the literature, especially in physics papers.

Let \mathfrak{h} be an auxiliary space and $\nu \in B(\mathcal{K}, \mathfrak{h})$ satisfy

$$\frac{1}{i}(\Upsilon - \Upsilon^*) = -\nu^* \nu. \quad (2.1)$$

Note that such \mathfrak{h} and ν always exist. One of possible choices is to take $\mathfrak{h} := \mathcal{K}$ and $\nu := \sqrt{i(\Upsilon - \Upsilon^*)}$.

If ϕ is a vector, then $|\phi\rangle$ will denote the operator $\mathbb{C} \ni \lambda \mapsto |\phi\rangle\lambda := \lambda\phi$. Similarly, $\langle\phi|$ will denote its adjoint: $f \mapsto \langle\phi|f := (\phi|f) \in \mathbb{C}$.

We will use a similar notation also for unbounded functionals. For instance, $(1|$ will denote the (unbounded) linear functional on $L^2(\mathbb{R})$ given by

$$(1|f = \int f(x)dx \quad (2.2)$$

with the domain $L^2(\mathbb{R}) \cap L^1(\mathbb{R})$. $|1\rangle$ will denote the hermitian conjugate of $(1|$ in the sense of sesquilinear forms: if $f \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$, then

$$(f|1) := \int \bar{f}(x)dx.$$

Let $Z_{\mathbb{R}}$ be the operator of multiplication on $L^2(\mathbb{R})$ by the variable x .

Introduce the Hilbert spaces $\mathcal{Z}_R := \mathfrak{h} \otimes L^2(\mathbb{R})$ and $\mathcal{Z} := \mathcal{K} \oplus \mathcal{Z}_R$. Clearly, \mathcal{K} is contained in \mathcal{Z} , so we have the obvious embedding $I_{\mathcal{K}} : \mathcal{K} \rightarrow \mathcal{Z}$. We also have the embedding $I_R : \mathcal{Z}_R \rightarrow \mathcal{Z}$.

For $t \geq 0$, consider the following sesquilinear form on $\mathcal{K} \oplus (\mathfrak{h} \otimes (\mathcal{L}^\infty(\mathbb{R}) \cap \mathcal{L}^\infty(\mathbb{R})))$:

$$\begin{aligned} U_t = & I_R e^{-itZ_R} I_R^* + I_{\mathcal{K}} e^{-it\Upsilon} I_{\mathcal{K}}^* - i(2\pi)^{-\frac{1}{2}} I_{\mathcal{K}} \int_0^t du e^{-i(t-u)\Upsilon} \nu^* \otimes (1|e^{-iuZ_R} I_R^* \\ & - i(2\pi)^{-\frac{1}{2}} I_R \int_0^t du e^{-i(t-u)Z_R} \nu \otimes |1\rangle e^{-iu\Upsilon} I_{\mathcal{K}}^* \\ & - (2\pi)^{-1} I_R \int_{0 \leq u_1, u_2, u_1+u_2 \leq t} du_1 du_2 e^{-iu_2 Z_R} \nu \otimes |1\rangle e^{-i(t-u_2-u_1)\Upsilon} \nu^* \otimes (1|e^{-iu_1 Z_R} I_R^*. \end{aligned} \quad (2.3)$$

By a straightforward computation we obtain [DD1]

THEOREM 2.1. *The form U_t extends to a strongly continuous unitary group and*

$$I_{\mathcal{K}}^* U_t I_{\mathcal{K}} = e^{-it\Upsilon}, \quad t \geq 0.$$

Thus $(\mathcal{Z}, I_{\mathcal{K}}, U_t)$ is a dilation of $e^{-it\Upsilon}$.

Let $-iZ$ denote the generator of U_t , so that $U_t = e^{-itZ}$. Z is a self-adjoint operator with a number of interesting properties. It is not easy to describe it with a well-defined formula. Formally it is given by the sesquilinear form

$$\begin{bmatrix} \frac{1}{2}(\Upsilon + \Upsilon^*) & (2\pi)^{-\frac{1}{2}} \nu^* \otimes (1| \\ (2\pi)^{-\frac{1}{2}} \nu \otimes |1\rangle & Z_R \end{bmatrix}. \quad (2.4)$$

Note that (2.4) looks like a special case of a Friedrichs operator (see Subsection 2.3 and [DF2]). As it stands, however, (2.4) does not define a unique self-adjoint operator. Nevertheless, we will sometimes use the expression (2.4) when referring to Z .

Note that it is possible to give a compact formula for the resolvent of Z , (which is another possible method of defining Z). For $z \in \mathbb{C}_+$,

$$\begin{aligned} (z - Z)^{-1} := & I_R (z - Z_R)^{-1} I_R^* + I_{\mathcal{K}} (z - \Upsilon)^{-1} I_{\mathcal{K}}^* \\ & + (2\pi)^{-\frac{1}{2}} I_{\mathcal{K}} (z - \Upsilon)^{-1} \nu^* \otimes (1|(z - Z_R)^{-1} I_R^* \\ & + (2\pi)^{-\frac{1}{2}} I_R (z - Z_R)^{-1} \nu \otimes |1\rangle (z - \Upsilon)^{-1} I_{\mathcal{K}}^* \\ & + (2\pi)^{-1} I_R (z - Z_R)^{-1} \nu \otimes |1\rangle (z - \Upsilon)^{-1} \nu^* \otimes (1|(z - Z_R)^{-1} I_R^*. \end{aligned}$$

Yet another approach that allows to define Z involves a ‘‘cut-off procedure’’. In fact, Z is the norm resolvent limit for $r \rightarrow \infty$ of the following regularized operators:

$$Z_r := \begin{bmatrix} \frac{1}{2}(\Upsilon + \Upsilon^*) & (2\pi)^{-\frac{1}{2}} \nu^* \otimes (1|1_{[-r,r]}(Z_R) \\ (2\pi)^{-\frac{1}{2}} \nu \otimes 1_{[-r,r]}(Z_R)|1\rangle & 1_{[-r,r]}(Z_R) Z_R \end{bmatrix}.$$

Note that it is important to remove the cut-off in a symmetric way. If we replace $[-r, r]$ with $[-r, ar]$ we usually obtain a different operator. The convergence of Z_r to Z is the reason why we can treat (2.4) as the formal expression for Z .

Next, let us mention a certain invariance property of Z . For $\lambda \in \mathbb{R}$, introduce the following unitary operator on \mathcal{Z}

$$j_\lambda u = u, \quad u \in \mathcal{K}; \quad j_\lambda g(y) := \lambda^{-1} g(\lambda^{-2} y), \quad g \in \mathcal{Z}_\mathbb{R}.$$

Note that

$$j_\lambda^* Z_\mathbb{R} j_\lambda = \lambda^2 Z_\mathbb{R}, \quad j_\lambda^* |1\rangle = \lambda |1\rangle.$$

Therefore, the operator Z is invariant with respect to the following scaling:

$$Z = \lambda^{-2} j_\lambda^* \begin{bmatrix} \lambda^2 \frac{1}{2} (\Upsilon + \Upsilon^*) & \lambda (2\pi)^{-\frac{1}{2}} \nu^* \otimes |1\rangle \\ \lambda (2\pi)^{-\frac{1}{2}} \nu \otimes |1\rangle & Z_\mathbb{R} \end{bmatrix} j_\lambda. \quad (2.5)$$

(2.5) will play an important role in the extended weak coupling limit.

Note that in the weak coupling limit it is convenient to use the representation of $Z_\mathbb{R}$ as a multiplication operator. Another natural possibility is to represent it as the differentiation operator. Let us describe this alternative version of the dilation.

The (unitary) Fourier transformation on $\mathfrak{h} \otimes L^2(\mathbb{R})$ will be denoted as follows:

$$\mathcal{F}f(\tau) := (2\pi)^{-1/2} \int f(x) e^{-i\tau x} dx. \quad (2.6)$$

We will use τ as the generic variable after the application of \mathcal{F} . The operator Z transformed by $1_\mathcal{K} \oplus \mathcal{F}$ will be denoted

$$\hat{Z} := (1_\mathcal{K} \oplus \mathcal{F}) Z (1_\mathcal{K} \oplus \mathcal{F}^*). \quad (2.7)$$

Introduce

$$D_\tau := \frac{1}{i} \partial_\tau. \quad (2.8)$$

Let $(\delta_0|$ have the meaning of an (unbounded) linear functional on $L^2(\mathbb{R})$ with the domain, say, the first Sobolev space $H^1(\mathbb{R})$, such that

$$(\delta_0|f) := f(0). \quad (2.9)$$

Similarly, let $|\delta_0)$ be its hermitian adjoint in the sense of forms. By applying the Fourier transform to (2.4), we can write

$$\hat{Z} = \begin{bmatrix} \frac{1}{2} (\Upsilon + \Upsilon^*) \nu^* \otimes (\delta_0| \\ \nu \otimes |\delta_0) & D_\tau \end{bmatrix}. \quad (2.10)$$

Clearly, $e^{-it\hat{Z}}$ is also a dilation of $e^{-it\Upsilon}$.

The operator \hat{Z} (or Z) and the unitary group it generates has a number of curious and confusing properties. Let us describe one of them. Consider the space $\mathcal{D} := \mathcal{K} \oplus (\mathfrak{h} \otimes H^1(\mathbb{R}))$. Clearly, it is a dense subspace of \mathcal{Z} . Let us define the following quadratic form on \mathcal{D} :

$$\hat{Z}^+ := \begin{bmatrix} \Upsilon & \nu^* \otimes (\delta_0| \\ \nu \otimes |\delta_0) & D_\tau \end{bmatrix}. \quad (2.11)$$

Then, for $\psi, \psi' \in \mathcal{D}$,

$$\lim_{t \downarrow 0} \frac{1}{t} (\psi | (e^{-it\hat{Z}} - 1) \psi') = -i (\psi | \hat{Z}^+ \psi'). \quad (2.12)$$

One could think that $\hat{Z}^+ = \hat{Z}$. But \hat{Z}^+ is in general non-self-adjoint, which is incompatible with the fact that $e^{-it\hat{Z}}$ is a unitary group.

To explain this paradox we notice that $(\psi|e^{-it\hat{Z}}\psi')$ is in general not differentiable at zero: its right and left derivatives exist but are different. Hence \mathcal{D} is not contained in the domain of the generator of \hat{Z} . We will call \hat{Z}^+ the *false form of the generator of $e^{it\hat{Z}}$* .

In order to make an even closer contact with the usual form of the quantum Langevin equation [HP, At, Fa, Bar, Me], define the cocycle unitary

$$\hat{W}(t) := e^{itD_\tau} e^{-it\hat{Z}}. \quad (2.13)$$

Then for $t > 0$, or for $t = 0$ and the right derivative, we have the “toy Langevin (stochastic) equation” which holds in the sense of quadratic forms on \mathcal{D} ,

$$i \frac{d}{dt} \hat{W}(t) = (\Upsilon + \nu \otimes |\delta_t\rangle) \hat{W}(t) + \nu^* \otimes \langle \delta_t|. \quad (2.14)$$

2.2. “Toy quadratic noises”. The formula for \hat{Z} or for \hat{Z}^+ has one interesting feature: it involves a perturbation that is localized just at $\tau = 0$. One can ask whether one can consider other dilations with more general perturbations localized at $\tau = 0$. In this subsection we will describe such dilations. This construction will not be needed in the present version of the weak coupling limit. We believe it is an interesting “toy version” of “quadratic noises”, which we will discuss in Subsect 5.2. We also expect to extend the results of [DD1] to “toy quadratic noises”.

Clearly, for any unitary operator U on $\mathfrak{h} \otimes L^2(\mathbb{R})$, $(1_{\mathcal{K}} \oplus U)e^{itZ}(1_{\mathcal{K}} \oplus U^*)$ is a dilation of $e^{-it\Upsilon}$. Let us choose a special U , which will lead to a perturbation localized at $\tau = 0$.

Let S be a unitary operator on \mathfrak{h} . For $\psi \in \mathfrak{h} \otimes L^2(\mathbb{R}) \simeq L^2(\mathbb{R}, \mathfrak{h})$ we set

$$\gamma(S)\psi(\tau) := \begin{cases} S\psi(\tau), & \tau > 0, \\ \psi(\tau), & \tau \leq 0. \end{cases} \quad (2.15)$$

Then $\gamma(S)$ is a unitary operator on $\mathfrak{h} \otimes L^2(\mathbb{R})$. Set

$$\hat{Z}_S := (1_{\mathcal{K}} \oplus \gamma(S)^*) \hat{Z} (1_{\mathcal{K}} \oplus \gamma(S)).$$

Clearly, $e^{it\hat{Z}_S}$ is a dilation of $e^{-it\Upsilon}$. It is awkward to write down a formula for \hat{Z}_S in the matrix form, even just formally. It is more natural to write down the “false form of Z_S ”:

$$\hat{Z}_S^+ := (1_{\mathcal{K}} \oplus \gamma(S)^*) \hat{Z}^+ (1_{\mathcal{K}} \oplus \gamma(S)) = \begin{bmatrix} \Upsilon & \nu^* S \otimes \langle \delta_0| \\ \nu \otimes |\delta_0\rangle & D_\tau + i(1 - S) \otimes |\delta_0\rangle \langle \delta_0| \end{bmatrix}.$$

For $\psi, \psi' \in \mathcal{D}$ we have

$$\lim_{t \downarrow 0} \frac{1}{t} (\psi | (e^{-it\hat{Z}_S} - 1) \psi') = -i (\psi | \hat{Z}_S^+ \psi'), \quad (2.16)$$

Again, as in (2.14), one can extend this formula to derivatives at $t > 0$. Let

$$\hat{W}_S(t) := e^{itD_\tau} e^{-it\hat{Z}_S}, \quad (2.17)$$

then, in the sense of quadratic forms on \mathcal{D} ,

$$i \frac{d}{dt} \hat{W}_S(t) = (\Upsilon + \nu \otimes |\delta_t\rangle) \hat{W}_S(t) + \nu^* S \otimes \langle \delta_t| + i(1 - S) \otimes |\delta_t\rangle \langle \delta_t|. \quad (2.18)$$

2.3. Weak coupling limit for Friedrichs operators. Let $\mathcal{H} := \mathcal{K} \oplus \mathcal{H}_R$ be a Hilbert space, where \mathcal{K} is finite dimensional. Let $I_{\mathcal{K}}$ be the embedding of \mathcal{K} in \mathcal{H} . Let K be a self-adjoint operator on \mathcal{K} and H_R be a self-adjoint operator on \mathcal{H}_R . Let V be a linear operator from \mathcal{K} to H_R . The following class of operators will be called *Friedrichs operators*:

$$H_{\lambda} := \begin{bmatrix} K & \lambda V^* \\ \lambda V & H_R \end{bmatrix}.$$

Assume that $\int \|V^* e^{-itH_R} V\| dt < \infty$. Then we can define the following operator, sometimes called the *Level Shift Operator*, since it describes the shift of eigenvalues of H_{λ} in perturbation theory at the 2nd order in λ :

$$\Upsilon := \sum_{k \in \text{sp}K} \int_0^{\infty} 1_k(K) V^* e^{-it(H_R - k)} V 1_k(K) dt, \quad (2.19)$$

where $1_k(K)$ denotes the spectral projection of K onto the eigenvalue k ; $\text{sp}K$ denotes the spectrum of K . Note that $\Upsilon K = K \Upsilon$.

The following theorem is a special case of a result of Davies [Da1, Da2, Da3], see also [DD1]:

THEOREM 2.2 (Reduced weak coupling limit for Friedrichs operators).

$$\lim_{\lambda \rightarrow 0} e^{itK/\lambda^2} I_{\mathcal{K}}^* e^{-itH_{\lambda}/\lambda^2} I_{\mathcal{K}} = e^{-it\Upsilon}.$$

In order to study the extended weak coupling limit for Friedrichs operators we need to make additional assumptions. They are perhaps a little complicated to state, but they are satisfied in many concrete situations.

ASSUMPTION 2.3. *We suppose that for any $k \in \text{sp}K$ there exists an open $I_k \subset \mathbb{R}$ and a Hilbert space \mathfrak{h}_k such that $k \in I_k$,*

$$\text{Ran} 1_{I_k}(H_R) \simeq \mathfrak{h}_k \otimes L^2(I_k, dx),$$

$1_{I_k}(H_R)H_R$ is the multiplication operator by the variable $x \in I_k$ and

$$1_{I_k}(H_R)V \simeq \int_{I_k}^{\oplus} v(x) dx.$$

We assume that I_k are disjoint for distinct k and the measurable function $I_k \ni x \mapsto v(x) \in B(\mathcal{K}, \mathfrak{h}_k)$ is continuous at k .

In other words, we assume that the reservoir Hamiltonian H_R and the interaction V are “nice” around the spectrum of K . In fact, in the extended weak coupling limit only a vicinity of $\text{sp}K$ matters.

We set $\mathfrak{h} := \oplus_k \mathfrak{h}_k$, $\mathcal{Z}_R := \mathfrak{h} \otimes L^2(\mathbb{R})$ and $\mathcal{Z} := \mathcal{K} \oplus \mathcal{Z}_R$. \mathcal{Z}_R and \mathcal{Z} are the so-called *asymptotic spaces*, which are in general different from the *physical spaces* \mathcal{H}_R and \mathcal{H} .

Next, let us describe the *asymptotic dynamics*. Let $\nu : \mathcal{K} \rightarrow \mathfrak{h}$ be defined as

$$\nu := (2\pi)^{\frac{1}{2}} \oplus_k v(k) 1_k(K).$$

Note that it satisfies (2.1) with Υ defined by (2.19). This follows by extending the integration in (2.19) to \mathbb{R} and using the inverse Fourier transform. As before, we set \mathcal{Z}_R to

be the multiplication by x on $L^2(\mathbb{R})$ and we define e^{-itZ} by (2.3), so that $(\mathcal{Z}, I_{\mathcal{K}}, e^{-itZ})$ is a dilation of $e^{-it\Upsilon}$.

Finally, we need an identification operator that maps the asymptotic space into the physical space. This is the least canonical part of the construction. In fact, there is some arbitrariness in its definition for the frequencies away from $\text{sp}K$. For $\lambda > 0$, we define the family of partial isometries $J_{\lambda,k} : L^2(\mathbb{R}, \mathfrak{h}_k) \rightarrow L^2(I_k, \mathfrak{h}_k) \subset \mathcal{H}$:

$$(J_{\lambda,k}g_k)(y) = \begin{cases} \frac{1}{\lambda}g_k\left(\frac{y-k}{\lambda^2}\right), & \text{if } y \in I_k; \\ 0, & \text{if } y \in \mathbb{R} \setminus I_k. \end{cases}$$

We set $J_\lambda : \mathcal{Z} \rightarrow \mathcal{H}$, defined for $g = (g_k) \in \mathcal{Z}_{\mathbb{R}}$ by

$$J_\lambda g := \sum_k J_{\lambda,k}g_k,$$

and on \mathcal{K} equal to the identity. Note that J_λ are partial isometries and

$$\text{s-}\lim_{\lambda \searrow 0} J_\lambda^* J_\lambda = 1.$$

The following result is proven in [DD1]:

THEOREM 2.4 (Extended weak coupling limit for Friedrichs operators).

$$\text{s}^* \text{-}\lim_{\lambda \searrow 0} J_\lambda^* e^{i\lambda^{-2}tH_0} e^{\lambda^{-2}(t-t_0)H_\lambda} e^{i\lambda^{-2}t_0H_0} J_\lambda = e^{itZ_{\mathbb{R}}} e^{-i(t-t_0)Z} e^{it_0Z_{\mathbb{R}}}.$$

Here we used the strong* limit: $\text{s}^* \text{-}\lim_{\lambda \searrow 0} A_\lambda = A$ means that for any vector ψ we have $\lim_{\lambda \searrow 0} A_\lambda \psi = A\psi$, $\lim_{\lambda \searrow 0} A_\lambda^* \psi = A^* \psi$.

Note that in the extended weak coupling limit for Friedrichs operators the asymptotic space is a direct sum of parts belonging to various eigenvalues of K that “do not talk to one another”—they have independent asymptotic dynamics.

3. Completely positive maps and semigroups. This section presents basic material about completely positive maps and semigroups. In particular, we describe a construction of the Stinespring dilation [St] and of the so-called Lindblad form of the generator of a c.p. semigroup [Li, GKS]. These beautiful classic results are described in many places in the literature. Nevertheless, some of their aspects, mostly concerning the freedom of choice of various terms in the Lindblad form, are difficult to find in the literature. Therefore, we describe this material at length, including sketches of proofs.

In Subsect. 3.3 we recall the usual concept of a (classical) Markov semigroups (on a finite state space). When discussing c.p. (quantum) Markov semigroups, it is useful to compare it to their classical analogs, which are usually much simpler.

In Subsect 3.4 we discuss c.p. semigroups invariant with respect to a certain unitary dynamics. Such c.p. semigroups arise in the weak coupling limit—therefore, one can argue that they are “more physical than others”.

Finally, in Subsect. 3.5 we analyze the Detailed Balance Condition, which singles out c.p. dynamics obtained from a thermal reservoir.

3.1. Completely positive maps. Let $\mathcal{K}_1, \mathcal{K}_2$ be Hilbert spaces. We say that a map $\Xi : B(\mathcal{K}_1) \rightarrow B(\mathcal{K}_2)$ is positive iff $A \geq 0$ implies $\Xi(A) \geq 0$. We say that Ξ is Markov iff

$\Xi(1) = 1$. We say that a map Ξ is n -positive iff

$$\Xi \otimes \text{id} : B(\mathcal{K}_1 \otimes \mathbb{C}^n) \rightarrow B(\mathcal{K}_2 \otimes \mathbb{C}^n)$$

is positive. (id denotes the identity). We say that Ξ is completely positive, or c.p. for short, iff it is n -positive for any n .

It is easy to see that if \mathfrak{h} be a Hilbert space and $\nu \in B(\mathcal{K}_2, \mathcal{K}_1 \otimes \mathfrak{h})$. Then

$$\Xi(A) := \nu^* A \otimes 1 \nu \quad (3.1)$$

is c.p. The following theorem says that the above representation of a c.p. map is universal. 2) means that this representation is unique up to unitary isomorphism.

THEOREM 3.1 (Stinespring). *Assume that $\mathcal{K}_1, \mathcal{K}_2$ are finite dimensional.*

- 1) *If Ξ is c.p. from $B(\mathcal{K}_1)$ to $B(\mathcal{K}_2)$, then there exist a Hilbert space \mathfrak{h} and $\nu \in B(\mathcal{K}_2, \mathcal{K}_1 \otimes \mathfrak{h})$ such that (3.1) is true and*

$$\{(\phi \otimes 1_{\mathfrak{h}} \nu \psi : \phi \in \mathcal{K}_1, \psi \in \mathcal{K}_2)\} = \mathfrak{h}. \quad (3.2)$$

- 2) *If in addition to the \mathfrak{h}' and ν' also satisfy the above properties, then there exists a unique unitary operator U from \mathfrak{h} to \mathfrak{h}' such that $\nu' = 1_{\mathcal{K}_1} \otimes U \nu$.*

The right hand side of (3.1) is called a *Stinespring dilation* of a c.p. map Ξ . If the condition (3.2) holds, then it is called a *minimal*.

REMARK 3.2. If we choose a basis in \mathfrak{h} , so that we identify \mathfrak{h} with \mathbb{C}^n , then we can identify ν with $\nu_1, \dots, \nu_n \in B(\mathcal{K}_2, \mathcal{K}_1)$. Then we can rewrite (3.1) as

$$\Xi(A) = \sum_{j=1}^n \nu_j^* A \nu_j. \quad (3.3)$$

In the literature, (3.3) is called a *Kraus decomposition*, even though the work of Stinespring is much earlier than that of Kraus.

Note that physically the space \mathfrak{h} can be interpreted as a part of the reservoir that directly interacts with the small system.

Proof of Theorem 3.1. Let us prove 1). We equip the algebraic tensor product $\mathcal{H}_0 := B(\mathcal{K}_1) \otimes \mathcal{K}_2$ with the following scalar product: for

$$\tilde{v} = \sum_i X_i \otimes v_i, \quad \tilde{w} = \sum_i Y_i \otimes w_i \in \mathcal{H}_0$$

we set

$$(\tilde{v} | \tilde{w}) = \sum_{i,j} (v_i | \Xi(X_i^* Y_j) w_j).$$

By the complete positivity, it is positive definite.

Next we note that there exists a unique linear map $\pi_0 : B(\mathcal{K}_1) \rightarrow B(\mathcal{H}_0)$ satisfying

$$\pi_0(A) \tilde{v} := \sum_i A X_i \otimes v_i.$$

We check that

$$(\pi_0(A) \tilde{v} | \pi_0(A) \tilde{v}) \leq \|A\|^2 (\tilde{v} | \tilde{v}), \quad \pi_0(AB) = \pi_0(A) \pi_0(B), \quad \pi_0(A^*) = \pi_0(A)^*.$$

Let \mathcal{N} be the set of $\tilde{v} \in \mathcal{H}_0$ with $(\tilde{v}|\tilde{v}) = 0$. Then the completion of $\mathcal{H} := \mathcal{H}_0/\mathcal{N}$ is a Hilbert space. There exists a nondegenerate $*$ -representation π of $B(\mathcal{K}_1)$ in $B(\mathcal{H})$ such that

$$\pi(A)(\tilde{v} + \mathcal{N}) = \pi_0(A)\tilde{v}.$$

Using the fact that all our spaces are finite dimensional we see that for some Hilbert space \mathfrak{h} we can identify \mathcal{H} with $\mathcal{K}_1 \otimes \mathfrak{h}$ and $\pi(A) = A \otimes 1$.

We set

$$\nu v := 1 \otimes v + \mathcal{N}.$$

We check that

$$\Xi(A) = \nu^* A \otimes 1 \nu.$$

This ends the proof of the existence of the Stinespring dilation.

Let us now prove 2). If \mathfrak{h}', ν' is another pair that gives a Stinespring dilation, we check that

$$\left\| \sum_i X_i \otimes 1_{\mathfrak{h}} \nu v_i \right\| = \left\| \sum_i X_i \otimes 1_{\mathfrak{h}'} \nu' v_i \right\|.$$

Therefore, there exists a unitary $U_0 : \mathcal{K}_2 \otimes \mathfrak{h} \rightarrow \mathcal{K}_2 \otimes \mathfrak{h}'$ such that $U_0 \nu = \nu'$. We check that $U_0 A \otimes 1_{\mathfrak{h}} = A \otimes 1_{\mathfrak{h}'} U_0$. Therefore, there exists a unitary $U : \mathfrak{h} \rightarrow \mathfrak{h}'$ such that $U_0 = 1 \otimes U$. ■

We will need the following inequality for c.p. maps:

THEOREM 3.3 (Kadison-Schwarz inequality for c.p. maps). *If Ξ is 2-positive and $\Xi(1)$ is invertible, then*

$$\Xi(A)^* \Xi(1)^{-1} \Xi(A) \leq \Xi(A^* A). \quad (3.4)$$

Proof. Let $z \in \mathbb{C}$. $\begin{bmatrix} A^* A & z A^* \\ \bar{z} A & |z|^2 \end{bmatrix} \geq 0$ implies $\begin{bmatrix} \Xi(A^* A) & z \Xi(A^*) \\ \bar{z} \Xi(A) & |z|^2 \Xi(1) \end{bmatrix} \geq 0$. Hence, for $\phi, \psi \in \mathcal{K}$,

$$(\phi | \Xi(A^* A) \phi) + 2 \operatorname{Re} \bar{z} (\psi | \Xi(1)^{-1/2} \Xi(A) \phi) + |z|^2 (\psi | \psi) \geq 0. \quad (3.5)$$

Therefore,

$$(\phi | \Xi(A^* A) \phi) (\psi | \psi) \geq |(\psi | \Xi(1)^{-1/2} \Xi(A) \phi)|^2, \quad (3.6)$$

which implies (3.4). ■

3.2. Completely positive semigroups. Let \mathcal{K} be a finite dimensional Hilbert space. Let us consider a c.p. semigroup on $B(\mathcal{K})$. We will always assume the semigroup to be continuous, so that it can be written as e^{tM} for a bounded operator M on $B(\mathcal{K})$. We will call e^{tM} Markov if it preserves the identity.

C.p. Markov semigroups appear in the literature under various names. Among them let us mention *quantum Markov semigroups* and *quantum dynamical semigroups*.

If M_1, M_2 are the generators of (Markov) c.p. semigroups and $c_1, c_2 \geq 0$, then $c_1 M_1 + c_2 M_2$ is the generator of a (Markov) c.p. semigroup. This follows by the Trotter formula.

Here are two classes of examples of c.p. semigroups:

1) Let $\Upsilon = \Theta + i\Delta$ be an operator on \mathcal{K} , with Θ, Δ self-adjoint. Then

$$M(A) := i\Upsilon A - iA\Upsilon^* = i[\Theta, A] - [\Delta, A]_+$$

is the generator of a c.p. semigroup and

$$e^{tM}(A) = e^{it\Upsilon} A e^{-it\Upsilon^*}.$$

2) Let Ξ be a c.p. map on $B(\mathcal{K})$. Then it is the generator of a c.p. semigroup and

$$e^{t\Xi}(A) = \sum_{j=0}^{\infty} \frac{t^j}{j!} \Xi^j(A).$$

Let Θ, Δ be self-adjoint operators on \mathcal{K} . Let \mathfrak{h} be an auxiliary Hilbert space and $\nu \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$. Then it follows from what we wrote above that

$$M(S) = i[\Theta, A] - [\Delta, A]_+ + \nu^* A \otimes 1 \nu, \quad A \in B(\mathcal{K}), \quad (3.7)$$

is the generator of a c.p. semigroup. e^{tM} is Markov iff $2\Delta = \nu^* \nu$.

The following theorem gives a complete characterization of generators of c.p. semigroups on a finite dimensional space [Li, GKS].

THEOREM 3.4 (Lindblad, Gorini-Kossakowski-Sudarshan).

1) Let e^{tM} be a c.p. semigroup on $B(\mathcal{K})$ for a finite dimensional Hilbert space \mathcal{K} . Then there exist self-adjoint operators Θ, Δ on \mathcal{K} , an auxiliary Hilbert space \mathfrak{h} and an operator $\nu \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$ such that M can be written in the form (3.7) and

$$\{(\phi | \otimes 1 \nu \psi : \phi, \psi \in \mathcal{K})\} = \mathfrak{h}. \quad (3.8)$$

2) We can always choose Θ and ν so that

$$\text{Tr } \Theta = 0, \quad \text{Tr } \nu = 0.$$

(Above, we take the trace of ν on the space \mathcal{K} obtaining a vector in \mathfrak{h}). If this is the case, then Θ and Δ are determined uniquely, and ν is determined uniquely up to the unitary equivalence.

We will say that a c.p. semigroup is *purely dissipative* if $\Theta = 0$. We will call (3.7) a *Lindblad form* of M . We will say that it is *minimal* iff (3.8) holds.

REMARK 3.5. If we identify \mathfrak{h} with \mathbb{C}^n , then we can write

$$\nu^* A \otimes 1 \nu = \sum_{j=1}^n \nu_j^* A \nu_j.$$

Then $\text{Tr } \nu = 0$ means $\text{Tr } \nu_j = 0, j = 1, \dots, n$.

Proof of Theorem 3.4. Let us prove 1). The unitary group on \mathcal{K} , denoted $U(\mathcal{K})$, is compact. Therefore, there exists the Haar measure on $U(\mathcal{K})$, which we denote dU . Note that

$$\int U X U^* dU = \text{Tr } X.$$

Define

$$i\Theta - \Delta_0 := \int M(U^*) U dU,$$

where Θ and Δ_0 are self-adjoint.

Let us show that

$$\int M(XU^*)UdU = (i\Theta - \Delta_0)X. \quad (3.9)$$

First check this identity for unitary X , which follows by the invariance of the measure dU . But every operator is a linear combination of unitaries. So (3.9) follows in general.

We can apply the Kadison-Schwarz inequality to the semigroup e^{tM} :

$$e^{tM}(X)^* e^{tM}(1)^{-1} e^{tM}(X) \leq e^{tM}(X^*X). \quad (3.10)$$

Differentiating (3.10) at $t = 0$ yields

$$M(X^*X) + X^*M(1)X - M(X^*)X - X^*M(X) \geq 0. \quad (3.11)$$

Replacing X with UX , where U is unitary, we obtain

$$M(X^*X) + X^*U^*M(1)UX - M(X^*U^*)UX - X^*U^*M(UX) \geq 0. \quad (3.12)$$

Integrating (3.12) over $U(\mathcal{K})$ we get

$$M(X^*X) + X^*X \operatorname{Tr} M(1) - (i\Theta - \Delta_0)X^*X - X^*X(-i\Theta - \Delta_0)^* \geq 0. \quad (3.13)$$

Define

$$\Delta_1 := \Delta_0 + \frac{1}{2} \operatorname{Tr} M(1), \quad \Xi(A) := M(A) - (i\Theta - \Delta_1)A - A(-i\Theta - \Delta_1).$$

Using (3.13) we see that Ξ is positive. A straightforward extension of the above argument shows that Ξ is also completely positive. Hence, by Theorem 3.1 1), it can be written as

$$\Xi(A) = \nu_1^* A \otimes 1 \nu_1,$$

for some auxiliary Hilbert space \mathfrak{h} and a map $\nu_1 : \mathcal{K} \rightarrow \mathcal{K} \otimes \mathfrak{h}$.

Finally, let us prove 2). The operator Θ has trace zero, because

$$\begin{aligned} i \operatorname{Tr} \Theta - \operatorname{Tr} \Delta_0 &= \int U_1 M(U^*) U U_1^* dU dU_1 = \int U_2 U M(U^*) U_2^* dU dU_2 \\ &= -i \operatorname{Tr} \Theta - \operatorname{Tr} \Delta_0. \end{aligned}$$

Let w be an arbitrary vector in \mathfrak{h} and

$$\Delta := \Delta_1 + \nu^* 1 \otimes |w\rangle + \frac{1}{2} (w|w), \quad \nu := \nu_1 + 1 \otimes |w\rangle.$$

Then the same generator of a c.p. semigroup can be written in two Lindblad forms:

$$(i\Theta - \Delta_1)A + A(-i\Theta - \Delta_1) + \nu_1^* A \nu_1, = (i\Theta - \Delta)A + A(-i\Theta - \Delta) + \nu^* A \nu.$$

In particular, choosing $w := -\operatorname{Tr} \nu_1$, we can make sure that $\operatorname{Tr} \nu = 0$. ■

3.3. Classical Markov semigroups. It is instructive to compare c.p. Markov semigroups with usual (classical) Markov semigroups.

Consider the space \mathbb{C}^n . For $u = (u_1, \dots, u_n) \in \mathbb{C}^n$ we will write $u \geq 0$ iff $u_1, \dots, u_n \geq 0$. We define $\mathbf{1} := (1, \dots, 1)$. We say that a linear map T is *pointwise positive* iff $u \geq 0$ implies $Tu \geq 0$. We say that it is *Markov* iff $T\mathbf{1} = \mathbf{1}$.

A one-parameter semigroup $\mathbb{R}_t \mapsto T_t \in B(\mathbb{C}^n)$ will be called a (*classical*) *Markov semigroup* iff T_t is pointwise positive and Markov for any $t \geq 0$.

Every continuous one-parameter semigroup on \mathbb{C}^n is of the form $\mathbb{R}_+ \ni t \mapsto e^{tm}$ for some $n \times n$ matrix m . Clearly, the transformations e^{tm} are pointwise positive for any $t \geq 0$ iff $m_{ij} \geq 0$, $i \neq j$. They are Markov for any $t \geq 0$ iff in addition $\sum_j m_{ij} = 0$.

Markov c.p. semigroups often lead to classical Markov semigroups, as described in the following easy fact:

THEOREM 3.6. *Let $P_1, \dots, P_n \in B(\mathcal{K})$ satisfy $P_j^* = P_j$ and $P_j P_k = \delta_{jk} P_j$. Let \mathcal{P} be the (commutative) $*$ -algebra generated by P_1, \dots, P_n . Clearly, \mathcal{P} is naturally isomorphic to \mathbb{C}^n . Let e^{tM} be a Markov c.p. semigroup on $B(\mathcal{K})$ that preserves the algebra \mathcal{P} . Then $e^{tM}|_{\mathcal{P}}$ is a classical Markov semigroup.*

Conversely, from a classical Markov semigroup one can construct c.p. Markov semigroups:

THEOREM 3.7. *Let e^{tm} be a classical Markov semigroup on \mathbb{C}^n . Let e_1, \dots, e_n denote the canonical basis of \mathbb{C}^n and $E_{ij} := |e_i\rangle\langle e_j|$. Let $\theta_1, \dots, \theta_n$ be real numbers and set $\Theta := \theta_1 E_{11} + \dots + \theta_n E_{nn}$. For $A \in B(\mathbb{C}^n)$ define*

$$M(A) := i[\Theta, A] - \frac{1}{2} \sum_j m_{jj} [E_{jj}, A]_+ + \sum_{i \neq j} m_{ij} E_{ij} A E_{ji}. \quad (3.14)$$

Then M is the generator of a Markov c.p. semigroup on $B(\mathbb{C}^n)$. The algebra \mathcal{P} generated by E_{11}, \dots, E_{nn} is preserved by e^{tM} and naturally isomorphic to \mathbb{C}^n . Under this identification, $M|_{\mathcal{P}}$ equals m .

3.4. Invariant c.p. semigroups. Let K be a self-adjoint operator on \mathcal{K} . Let M be the generator of a c.p. semigroup on \mathcal{K} . We say that M is K -invariant iff

$$M(A) = e^{-itK} M(e^{itK} A e^{-itK}) e^{itK}, \quad t \in \mathbb{R}. \quad (3.15)$$

We will see later on that c.p. semigroups obtained in the weak coupling limit are always K -invariant with respect to the Hamiltonian of the small system.

Note that M can be split in a canonical way into $M = i[\Theta, \cdot] + M_d$, where M_d is its purely dissipative part. M is K -invariant iff $[\Theta, K] = 0$ and M_d is K -invariant. Thus in what follows it is enough to restrict ourselves to the purely dissipative case.

The following two theorems extend Theorems 3.6 and 3.7.

THEOREM 3.8. *Consider the set-up of Theorem 3.6. Suppose in addition that K is a self-adjoint operator on \mathcal{K} with the eigenvalues k_1, \dots, k_n and $P_j = \mathbf{1}_{k_j}(K)$. Let M be K -invariant. Then the algebra \mathcal{P} is preserved by e^{tM} (and hence the conclusion of Theorem 3.6 holds).*

THEOREM 3.9. *Consider the set-up of Theorem 3.7. If k_1, \dots, k_n are real and $K := k_1 E_{11} + \dots + k_n E_{nn}$, then M is K -invariant.*

The following theorem describes the K -invariance on the level of a Lindblad form. We restrict ourselves to the Markov case.

THEOREM 3.10. *Let $\nu \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$ and let Y be a self-adjoint operator on \mathfrak{h} such that*

$$M(A) = -\frac{1}{2}[\nu^* \nu, A]_+ + \nu^* A \otimes 1 \nu, \quad (3.16)$$

$$\nu K = (K \otimes 1 + 1 \otimes Y) \nu. \quad (3.17)$$

Then M is the generator of a K -invariant purely dissipative Markov c.p. semigroup.

Proof. We check that $\nu^* \nu$ commutes with K . Then it is enough to verify that $A \mapsto \nu^* A \otimes 1 \nu$ is K -invariant. ■

There exists a partial converse of Theorem 3.10.

THEOREM 3.11. *Let M be the generator of a K -invariant purely dissipative Markov c.p. semigroup. Let \mathfrak{h}, ν realize its minimal Lindblad form (3.16). Then there exists a self-adjoint operator Y on \mathfrak{h} such that (3.17) is true.*

Proof. By the uniqueness part of Theorem 3.1 there exists a unique unitary operator U_t on \mathfrak{h} such that $e^{itK} \otimes U_t \nu e^{-itK} = \nu$. We easily check the U_t is a continuous 1-parameter unitary group so that U_t can be written as e^{itY} for some self-adjoint Y . ■

Note that Theorems 3.10 and 3.11 have a clear physical meaning. The operator ν is responsible for “quantum jumps”. The operator Y describes the energy of the reservoir (or actually of the part of the reservoir “directly seen” by the interaction). The equation (3.17) describes the energetic balance in each quantum jump.

3.5. Detailed Balance Condition. In the literature the name Detailed Balance Condition (DBC) is given to several related but non-equivalent concepts. In this subsection we discuss some of the versions of the DBC relevant in the weak coupling limit.

Some of the definitions of the DBC (both for classical and quantum systems) involve the time reversal [Ag, Ma, MaSt]. In the weak coupling limit one does not need to introduce the time reversal, hence we will only discuss versions of the DBC that do not involve this operation. (See however [DM] for a discussion of time-reversal in semigroups obtained in the weak coupling limit.)

Let us first recall the definition of the classical Detailed Balance Condition. Let $p = (p_1, \dots, p_n) \in \mathbb{C}^n$ be a vector with $p_1, \dots, p_n > 0$. Introduce the scalar product on \mathbb{C}^n :

$$(u|u')_p := \sum_j \bar{u}_j u'_j p_j. \quad (3.18)$$

Let e^{tm} be a classical Markov semigroup on \mathbb{C}^n . We say that m satisfies the Detailed Balance Condition for p iff m is self-adjoint for $(\cdot|\cdot)_p$.

Let us now consider the quantum case. Let ρ be a nondegenerate density matrix. As usual, we assume that \mathcal{K} is finite dimensional. On $B(\mathcal{K})$ we introduce the scalar product

$$(A|B)_\rho := \text{Tr} \rho^{1/2} A^* \rho^{1/2} B. \quad (3.19)$$

Let M be the generator of a c.p. semigroup on $B(\mathcal{K})$. Recall that it can be uniquely represented as

$$M = i[\Theta, \cdot] + M_d,$$

where M_d is its purely dissipative part and $i[\Theta, \cdot]$ its Hamiltonian part. We say that M satisfies the Detailed Balance Condition (or DBC) for ρ iff M_d is self-adjoint and $i[\Theta, \cdot]$ is anti-self-adjoint for $(\cdot)_\rho$.

Note that M satisfies the DBC for ρ iff $[\Theta, \rho] = 0$ and M_d satisfies the DBC for ρ . Therefore, in our further analysis we will often restrict ourselves to the purely dissipative case.

We believe that in the quantum finite dimensional case the above definition of the DBC is the most natural. It was used e.g. in [DF1] under the name of the *standard Detailed Balance Condition*.

A similar but different definition of the DBC can be found in [FKGV, A11]. The only difference is the replacement of the scalar product $(\cdot)_\rho$ given in (3.19) with

$$\text{Tr } \rho A^* B. \quad (3.20)$$

Note that if M is K -invariant and ρ is a function of K , then both definitions are equivalent.

The weak coupling limit applied to a small system with a Hamiltonian K interacting with a thermal reservoir at some fixed temperature β always yields a Markov c.p. semigroup that is K -invariant and satisfies the DBC for $\rho = e^{-\beta K} / \text{Tr } e^{\beta K}$; see e.g. [LeSp, DF1] and Subsect 4.3.

There exists a close relationship between the classical and quantum DBC.

THEOREM 3.12. *Consider the set-up of Theorem 3.6. Let ρ be a density matrix on \mathcal{K} with the eigenvalues p_1, \dots, p_n and let P_j equal the spectral projections of ρ for the eigenvalue p_j . If M satisfies the DBC for ρ , either in the sense of (3.19) or in the sense of (3.20), then the classical Markov semigroup $e^{tM}|_{\mathcal{P}}$ satisfies the DBC for $p = (p_1, \dots, p_n)$.*

THEOREM 3.13. *Consider the set-up of Theorem 3.7. Let e^{tm} satisfy the classical DBC for $p = (p_1, \dots, p_n)$. Then M defined by (3.14) satisfies both quantum versions of the DBC for $\rho := p_1 E_{11} + \dots + p_n E_{nn}$.*

The following theorem describes the DBC for K -invariant generators on the level of their Lindblad form. It is an extension of Theorem 3.10. (Note that (3.21), (3.22) are identical to (3.16), (3.17) of Theorem 3.10).

THEOREM 3.14. *Let $\nu \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$ and Y a self-adjoint operator on \mathfrak{h} such that*

$$M(A) = -\frac{1}{2}[\nu^* \nu, A]_+ + \nu^* A \otimes 1 \nu, \quad (3.21)$$

$$\nu K = (K \otimes 1 + 1 \otimes Y) \nu, \quad (3.22)$$

$$\text{Tr}_{\mathfrak{h}} \nu A \nu^* = \nu^* A \otimes e^{-\beta Y} \nu. \quad (3.23)$$

Then M is the generator of a K -invariant purely dissipative Markov c.p. semigroup satisfying the DBC for $\rho := e^{-\beta K} / \text{Tr } e^{-\beta K}$.

Proof. It follows from (3.17) that $\nu^* \nu$ commutes with $e^{-\beta K/2}$. Hence $[\nu^* \nu, \cdot]_+$ is self-adjoint for $(\cdot)_\rho$.

If M is a map on $B(\mathcal{K})$, then $M^{*\rho}$ will denote the adjoint for this scalar product. Let $M_1(A) = \nu^* A \otimes 1 \nu$. We compute:

$$\begin{aligned} M_1^{*\rho}(A) &= \text{Tr}_{\mathfrak{h}} e^{\beta K/2} \otimes 1 \nu e^{-\beta K/2} A e^{-\beta K/2} \nu^* e^{\beta K/2} \otimes 1 \\ &= \text{Tr}_{\mathfrak{h}} e^{\beta K/2} \nu^* (e^{-\beta K/2} A e^{-\beta K/2} \otimes e^{-\beta Y}) \nu e^{\beta K/2} \end{aligned} \quad (3.24)$$

$$= \nu^* A \otimes 1 \nu = M_1(A). \quad (3.25)$$

In (3.24) and (3.25) we used (3.23) and (3.22) respectively. ■

It is possible to replace the condition (3.23) with a different condition (3.26). Note that whereas (3.23) is quadratic in ν , (3.26) is linear in ν .

THEOREM 3.15. *Suppose that ϵ is an antiunitary operator on \mathfrak{h} such that*

$$(\phi \otimes w | \nu \psi) = (\nu \phi | \psi \otimes e^{-\beta Y/2} \epsilon w), \quad \phi, \psi \in \mathcal{K}, \quad w \in \mathfrak{h}. \quad (3.26)$$

Then (3.23) holds.

Proof. It is sufficient to assume that $A = |\psi\rangle\langle\psi|$ for some $\psi \in \mathcal{K}$. Let $\phi \in \mathcal{K}$. Let $\{w_i \mid i \in I\}$ be an orthonormal basis in \mathfrak{h} . Then

$$\begin{aligned} \text{Tr}_{\mathfrak{h}}(\phi | \nu A \nu^* \phi) &= \sum (\phi \otimes w_i | \nu \psi) (\nu \psi | \phi \otimes w_i) = \sum (\nu \phi | \psi \otimes e^{-\beta Y/2} \epsilon w_i) (\psi \otimes e^{-\beta Y/2} \epsilon w_i | \nu \phi) \\ &= (\nu \phi | |\psi\rangle\langle\psi| \otimes e^{-\beta Y} \nu \phi) = (\phi | \nu^* A \otimes e^{-\beta Y} \nu \phi). \quad \blacksquare \end{aligned}$$

There exists an extension of Theorem 3.11 to the Detailed Balance Condition. It can be viewed as a partial converse of Theorems 3.14 and 3.15:

THEOREM 3.16. *Let M be the generator of a K -invariant purely dissipative Markov c.p. semigroup satisfying the DBC for $e^{-\beta K} / \text{Tr} e^{-\beta K}$. Let \mathfrak{h}, ν realize its minimal Lindblad form (3.21). Let a self-adjoint operator Y on \mathfrak{h} satisfy (3.22). Then (3.23) is true and there exists a unique antiunitary operator ϵ on \mathfrak{h} such that (3.26) holds. Besides, $\epsilon Y \epsilon = -Y$ and $\epsilon^2 = 1$.*

Proof. Step 1. By the proof of Theorem 3.14, the DBC for $e^{-\beta K} / \text{Tr} e^{-\beta K}$ together with (3.22) imply (3.23).

Step 2. The next step is to prove that (3.23) and (3.8) imply the existence of an antiunitary ϵ on \mathfrak{h} satisfying (3.26).

Identify \mathfrak{h} with \mathbb{C}^n , so that we have a complex conjugation $w \mapsto \bar{w}$ in \mathfrak{h} . We can assume that Y is diagonal, so that $\overline{Y \bar{w}} = Y w$, $w \in \mathfrak{h}$. Define ν^* by

$$(\phi \otimes w | \nu \psi) = (\nu^* \phi | \psi \otimes \bar{w}), \quad \phi, \psi \in \mathcal{K}, \quad w \in \mathfrak{h}. \quad (3.27)$$

(Note that \star is a different star from $*$ denoting the Hermitian conjugation, see [DF1]). We can rewrite (3.23) as

$$\nu^{*\star} A \otimes 1 \nu^* = \nu^* 1 \otimes e^{-\beta Y/2} (A \otimes 1) 1 \otimes e^{-\beta Y/2} \nu. \quad (3.28)$$

(3.28) defines a c.p. map. By the uniqueness part of Theorem 3.1 and (3.8), we obtain the existence of a unitary map U on \mathfrak{h} such that $\nu^* = 1 \otimes U e^{-\beta Y/2} \nu$. Now we set $\epsilon w = U^* \bar{w}$.

Step 3. We apply (3.23) twice:

$$(\phi \otimes w | \nu \psi) = (\nu \phi | \psi \otimes e^{-\beta Y/2} \epsilon w) = (\phi \otimes (e^{-\beta Y/2} \epsilon)^2 w | \nu \psi).$$

Using (3.8) we obtain $w = (e^{-\beta Y/2} \epsilon)^2 w$.

Step 4. Finally applying (3.23) together with (3.22) twice we obtain

$$(\phi \otimes w | \nu \psi) = (\nu e^{\beta K/2} \phi | e^{-\beta K/2} \psi \otimes \epsilon w) = (\phi \otimes \epsilon^2 w | \nu \psi).$$

Thus with help of (3.8) we get $w = \epsilon^2 w$. ■

Note that the above results show that for c.p. Markov semigroups that are K -invariant and satisfy the DBC for $e^{-\beta K} / \text{Tr } e^{-\beta K}$ we naturally obtain a certain algebraic structure on the “restricted reservoir” \mathfrak{h} that resembles closely the famous Tomita-Takesaki theory. The properties of $e^{-\beta Y}$ and ϵ are parallel to those of the *modular operator* and the *modular conjugations*—the basic objects of the Tomita-Takesaki formalism. (See also Subsection 4.3).

4. Bosonic reservoirs. In this section we recall basic terminology related to second quantization, see e.g. [De0]. We also introduce *Pauli-Fierz operators*—a class of models (known in the literature under various names) that are often used to describe realistic physical systems, see e.g. [DJ1, DJP].

4.1. Second quantization. Let \mathcal{H}_R be a Hilbert space describing 1-particle states. The corresponding bosonic Fock space is defined as

$$\Gamma_s(\mathcal{H}_R) := \bigoplus_{n=0}^{\infty} \otimes_s^n \mathcal{H}_R.$$

The vacuum vector is $\Omega = 1 \in \otimes_s^0 \mathcal{H}_R = \mathbb{C}$.

If $z \in \mathcal{H}_R$, then

$$a(z)\Psi := \sqrt{n}(z | \otimes 1^{(n-1)\otimes} \Psi \in \otimes_s^{n-1} \mathcal{H}_R, \quad \Psi \in \otimes_s^n \mathcal{H}_R,$$

is called the annihilation operator of z and $a^*(z) := a(z)^*$ is the corresponding creation operator. They are closable operators on $\Gamma_s(\mathcal{H}_R)$.

For an operator q on \mathcal{H}_R we define the operator $\Gamma(q)$ on $\Gamma_s(\mathcal{H}_R)$ by

$$\Gamma(q)|_{\otimes_s^n \mathcal{H}_R} = q \otimes \cdots \otimes q. \tag{4.1}$$

For an operator h on \mathcal{H}_R we define the operator $d\Gamma(h)$ on $\Gamma_s(\mathcal{H}_R)$ by

$$d\Gamma(h)|_{\otimes_s^n \mathcal{H}_R} = h \otimes 1^{(n-1)\otimes} + \cdots + 1^{(n-1)\otimes} \otimes h.$$

Note the identity $\Gamma(e^{ih}) = e^{itd\Gamma(h)}$.

4.2. Coupling to a bosonic reservoir. Let \mathcal{K} be a finite dimensional Hilbert space. We imagine that it describes a small quantum system interacting with a bosonic reservoir described by the Fock space $\Gamma_s(\mathcal{H}_R)$. The coupled system is described by the Hilbert space $\mathcal{H} := \mathcal{K} \otimes \Gamma_s(\mathcal{H}_R)$.

Let $V \in B(\mathcal{K}, \mathcal{K} \otimes \mathcal{H}_R)$. For $\Psi \in \mathcal{K} \otimes \otimes_s^n \mathcal{H}_R$ we set

$$a(V)\Psi := \sqrt{n}V^* \otimes 1^{(n-1)\otimes} \Psi \in \mathcal{K} \otimes \otimes_s^{n-1} \mathcal{H}_R.$$

$a(V)$ is called the annihilation operator of V and $a^*(V) := a(V)^*$ the corresponding creation operator. They are closable operators on $\mathcal{K} \otimes \Gamma_s(\mathcal{H}_R)$. Note in particular that if V is written in the form $\sum_j V_j \otimes |b_j\rangle$ (which is always possible), then

$$a^*(V) = \sum_j V_j \otimes a^*(b_j), \quad a(V) = \sum_j V_j^* \otimes a(b_j),$$

where $a^*(b_j)$, $a(b_j)$ are the usual creation/annihilation operators introduced in the previous subsection.

The following class of operators plays the central role in our article:

$$H_\lambda = K \otimes 1 + 1 \otimes d\Gamma(H_R) + \lambda(a^*(V) + a(V)). \quad (4.2)$$

Here K is a self-adjoint operator describing the free dynamics of the small system, $d\Gamma(H_R)$ describes the free dynamics of the reservoir and $a^*(V)/a(V)$, for some $V \in B(\mathcal{K}, \mathcal{K} \otimes \mathcal{H}_R)$, describe the interaction. Operators of the form 4.2 will be called *Pauli-Fierz operators*.

Note that operators of the form (4.2) or similar are very common in the physics literature and are believed to give an approximate description of realistic physical systems in many circumstances (e.g. an atom interacting with radiation in the dipole approximation), see e.g. [DJ1].

4.3. Thermal reservoirs. In this subsection we will discuss thermal reservoirs. We fix a positive number β having the interpretation of the inverse temperature.

Recall that the free Hamiltonian is $H_0 := K \otimes 1 + 1 \otimes d\Gamma(H_R)$. To have a simpler formula for the Gibbs state of the small system we assume that $\text{Tr} e^{-\beta K} = 1$. We set

$$\tau_t(C) := e^{itH_0} C e^{-itH_0}, \quad \omega_\beta(C) := \text{Tr} e^{-\beta K} \otimes |\Omega\rangle\langle\Omega|, \quad C \in B(\mathcal{H}).$$

THEOREM 4.1. *The following are equivalent:*

- 1) For any $D_1, D_2, D'_1, D'_2 \in B(\mathcal{K})$ and

$$B_j := D_j \otimes 1 (a^*(V) + a(V)) D'_j \otimes 1, \quad j = 1, 2,$$

and for any $t \in \mathbb{R}$ we have

$$\omega_\beta(\tau_t(B_1)B_2) = \omega_\beta(B_2\tau_{t+i\beta}(B_1)). \quad (4.3)$$

- 2) For any function f on the spectrum of $\text{sp}H_R$ and $A \in B(\mathcal{K})$, we have

$$\text{Tr}_{\mathcal{H}_R} 1 \otimes \bar{f}(-H_R) V A V^* = V^* A \otimes e^{-\beta H_R} f(H_R) V. \quad (4.4)$$

Proof. The left hand side of (4.3) equals

$$\text{Tr} e^{-\beta K + itK} D_1 V^* (D'_1 e^{-itK} D_2 \otimes e^{-itH_R}) V D'_2.$$

The right hand side of (4.3) equals

$$\text{Tr} D_2 V^* (D'_2 e^{-\beta K + itK} D_1 \otimes e^{(-\beta + it)H_R}) V D'_1 e^{-itK}.$$

Now we set $A_1 := D'_2 e^{-\beta K + itK} D_1$, $A_2 := D'_1 e^{-itK} D_2$, and use the cyclicity of the trace. We obtain

$$\text{Tr} A_2 \otimes e^{-itH_R} V A_1 V^* = \text{Tr} A_2 V^* A_1 \otimes e^{-\beta H_R + itH_R} V.$$

By the Fourier transformation we get

$$\text{Tr} A_2 \otimes \bar{f}(-H_R) V A_1 V^* = \text{Tr} A_2 V^* A_1 \otimes e^{-\beta H_R} f(H_R) V.$$

This implies (4.4). ■

We will say that the reservoir is thermal at the inverse temperature β iff the conditions of Theorem 4.1 are true.

(4.3) is just the β -KMS condition for the state ω_β , the dynamics τ and appropriate operators. Note that (4.3) is satisfied for Pauli-Fierz semi-Liouvillians constructed with

help of the Araki-Woods representations of the CCR, where we use the terminology of [DJP, De0]. Theorem 4.1 describes a substitute of the KMS condition without invoking explicitly operator algebras.

The KMS condition is closely related to the Tomita-Takesaki theory. One of the objects introduced in this theory is the modular conjugation. It turns out that the set-up of Theorem 4.1 is sufficient to introduce a substitute for the modular conjugation without talking about operator algebras.

Define

$$\mathcal{H}_{\bar{R}} := \{(\phi|\otimes f(H_R) V\psi : \phi, \psi \in \mathcal{K}, f \in C_c(\mathbb{R})\}^{\text{cl}}.$$

(cl denotes closure). Clearly, $\mathcal{H}_{\bar{R}}$ is a subspace of \mathcal{H}_R invariant with respect to the 1-particle reservoir Liouvillean H_R . It describes the part of \mathcal{H}_R that is coupled to the small system. Let $H_{\bar{R}}$ denote the operator H_R restricted to the space $\mathcal{H}_{\bar{R}}$.

THEOREM 4.2. *Suppose that the reservoir is thermal at inverse temperature β . Then there exist a unique antiunitary operator $\epsilon_{\bar{R}}$ on $\mathcal{H}_{\bar{R}}$ such that*

$$(\phi\otimes w|V\psi) = (V\phi|\psi\otimes e^{-\beta H_{\bar{R}}}\epsilon_{\bar{R}}w). \quad (4.5)$$

It satisfies $\epsilon_{\bar{R}}^2 = 1$ and $\epsilon_{\bar{R}}H_{\bar{R}}\epsilon_{\bar{R}} = -H_{\bar{R}}$.

Proof. For $f \in C_c(\mathbb{R})$, $\phi, \psi \in \mathcal{K}$, we set

$$\epsilon_{\bar{R}}((\phi|\otimes e^{-\beta H_{\bar{R}}/2} f(H_{\bar{R}}) V\psi) := (\psi|\otimes \bar{f}(-H_{\bar{R}})V\phi.$$

(4.4) implies that $\epsilon_{\bar{R}}$ is a well defined antiunitary map. ■

5. Quantum Langevin dynamics. Suppose that we are given a c.p. Markov semigroup e^{tM} on $B(\mathcal{K})$. We will describe a certain class of self-adjoint operators Z on a larger Hilbert space such that $e^{-itZ} \cdot e^{itZ}$ is a dilation on e^{tM} . We will use the name *quantum Langevin* (or *stochastic*) *dynamics* for $e^{-itZ} \cdot e^{itZ}$. The unitary group e^{-itZ} will be called a *Langevin* (or *stochastic*) *Schrödinger dynamics*.

In Subsection 5.1 we will restrict ourselves to a subclass of quantum Langevin dynamics involving only the so-called linear noises. Actually, at present our results on the extended weak coupling limit are limited only to them.

In Subsection 5.2 we will describe a more general class of quantum Langevin dynamics, which also involve *quadratic noises*. Our construction involving quadratic noises is related to the operator-theoretic approach of Chebotarev [Ch, ChR], and especially of Gregoratti [Gr].

We expect that our approach to the extended weak coupling limit can be improved to cover also this larger class. Within the approach of [AFL] there exist partial results in this direction [Go].

The history of the discovery of quantum Langevin dynamics is quite involved. The construction can be traced back to [AFLe], and especially [HP] where the quantum stochastic calculus was introduced. But apparently only in [Fr] and [Maa] it was independently realized that this leads to a dilation of Markov c.p. semigroups. Let us also mention [At, Me, Fa] for more recent presentations of the quantum stochastic calculus.

5.1. Linear noises. Apart from a c.p. Markov semigroup e^{tM} let us fix some additional data. More precisely, we fix an operator Υ , an auxiliary Hilbert space \mathfrak{h} and an operator ν from \mathcal{K} to $\mathcal{K} \otimes \mathfrak{h}$ such that

$$-i\Upsilon + i\Upsilon^* = -\nu^*\nu$$

and M is given by

$$M(A) = -i(\Upsilon A - A\Upsilon^*) + \nu^* A \otimes 1 \nu, \quad A \in B(\mathcal{K}).$$

In other words, we fix a concrete Lindblad form of M .

Introduce the Hilbert space $\mathcal{Z}_R := \mathfrak{h} \otimes L^2(\mathbb{R})$. The enlarged Hilbert space is $\mathcal{Z} := \mathcal{K} \otimes \Gamma_s(\mathcal{Z}_R)$.

Let Z_R be the operator of multiplication by the variable x on $L^2(\mathbb{R})$. Let $(1|, |1)$ be defined as in (2.2).

We choose a basis (b_j) in \mathfrak{h} , so that we can write

$$\nu = \sum \nu_j \otimes |b_j). \quad (5.1)$$

(Note that at the end the construction will not depend on the choice of a basis). Set

$$\nu_j^+ = \nu_j, \quad \nu_j^- = \nu_j^*.$$

For $t \geq 0$ we define the quadratic form

$$\begin{aligned} U_t &:= e^{-itd\Gamma(Z_R)} \sum_{n=0}^{\infty} \int_{t \geq t_n \geq \dots \geq t_1 \geq 0} dt_n \cdots dt_1 \\ &\times (2\pi)^{-\frac{n}{2}} \sum_{j_1, \dots, j_n} \sum_{\epsilon_1, \dots, \epsilon_n \in \{+, -\}} (-i)^n e^{-i(t-t_n)\Upsilon} \nu_{j_n}^{\epsilon_n} e^{-i(t_n-t_{n-1})\Upsilon} \cdots \nu_{j_1}^{\epsilon_1} e^{-i(t_1-0)\Upsilon} \\ &\times \prod_{k=1, \dots, n: \epsilon_k = +} a^*(e^{it_k Z_R} b_{j_k} \otimes |1)) \prod_{k'=1, \dots, n: \epsilon_{k'} = -} a(e^{it_{k'} Z_R} b_{j_{k'}} \otimes |1)); \\ U_{-t} &:= U_t^*. \end{aligned}$$

We will denote by $I_{\mathcal{K}}$ the embedding of $\mathcal{K} \simeq \mathcal{K} \otimes \Omega$ in \mathcal{Z} .

THEOREM 5.1. U_t extends to a strongly continuous unitary group on \mathcal{Z} such that

$$I_{\mathcal{K}}^* U_t I_{\mathcal{K}} = e^{-it\Upsilon}, \quad I_{\mathcal{K}}^* U_t A \otimes 1 U_{-t} I_{\mathcal{K}} = e^{tM}(A).$$

Thus U_t is a unitary dilation of $e^{-it\Upsilon}$, and $U_t \cdot U_t^*$ is a dilation of e^{tM} .

As every strongly continuous unitary group, U_t can be written as e^{-itZ} for a certain self-adjoint operator Z . Note that formally (and also rigorously with an appropriate regularization)

$$Z = \frac{1}{2}(\Upsilon + \Upsilon^*) + d\Gamma(Z_R) + (2\pi)^{-\frac{1}{2}} a^*(\nu \otimes |1)) + (2\pi)^{-\frac{1}{2}} a(\nu \otimes |1)).$$

Thus Z has the form of a Pauli-Fierz operator with a rather singular interaction.

Let us present an alternative variation of the above construction, which is actually closer to what can be found in the literature. Let \mathcal{F} be the Fourier transformation on $\mathcal{Z}_R = \mathfrak{h} \otimes L^2(\mathbb{R})$ defined as in (2.6). The operator Z transformed by $1_{\mathcal{K}} \otimes \Gamma(\mathcal{F})$ will be

denoted by

$$\hat{Z} := 1_{\mathcal{K}} \otimes \Gamma(\mathcal{F}) Z 1_{\mathcal{K}} \otimes \Gamma(\mathcal{F}^*). \quad (5.2)$$

It equals

$$\hat{Z} = \frac{1}{2}(\Upsilon + \Upsilon^*) \otimes 1 + 1 \otimes d\Gamma(D_\tau) + a(\nu \otimes |\delta_0\rangle) + a^*(\nu \otimes |\delta_0\rangle),$$

where δ_0, D_τ are defined as in (2.8), (2.9).

Similarly to the operator of Section 2.1 denoted with the same symbol, the operator \hat{Z} (as well as Z) has a number of intriguing properties. Let us describe one of them.

Let $\mathcal{D}_0 := \mathfrak{h} \otimes H^1(\mathbb{R})$. (Recall that $H^1(\mathbb{R})$ is the first Sobolev space). Let $\mathring{\Gamma}_s^{\text{al}}(\mathcal{D}_0)$, denote the corresponding algebraic Fock space and $\mathcal{D}_1 := \mathcal{K} \otimes \mathring{\Gamma}_s^{\text{al}}(\mathcal{D}_0)$. Introduce the (non-self-adjoint) sesquilinear form

$$\hat{Z}^+ = \Upsilon \otimes 1 + 1 \otimes d\Gamma(D_\tau) + a(\nu \otimes |\delta_0\rangle) + a^*(\nu \otimes |\delta_0\rangle). \quad (5.3)$$

Let $\psi, \psi' \in \mathcal{D}_1$. Then

$$\lim_{t \downarrow 0} \frac{1}{t} (\psi | e^{-it\hat{Z}} - 1) \psi' = -i(\psi | \hat{Z}^+ \psi'). \quad (5.4)$$

Thus it seems that $\hat{Z}^+ = \hat{Z}$, which is true only if Υ is self-adjoint and hence there are no off-diagonal terms in Z . Clearly, the explanation of the above paradox is similar as in Subsect. 2.1: $(\psi | e^{-it\hat{Z}} \psi')$ is not differentiable at zero. This is related to the fact that ψ, ψ' do not belong to $\text{Dom} Z$. Thus \hat{Z}^+ can again be called a *false form*.

In the literature, the Langevin Schrödinger dynamics $e^{-it\hat{Z}}$ is usually introduced through the so-called *Langevin* (or *stochastic*) *Schrödinger equation* satisfied by

$$\hat{W}(t) := e^{itd\Gamma(D_\tau)} e^{-it\hat{Z}}. \quad (5.5)$$

To write this equation recall the decomposition (5.1) and note that. Then, in the sense of quadratic forms on \mathcal{D}_1 , we have

$$i \frac{d}{dt} \hat{W}(t) = (\Upsilon \otimes 1 + a^*(\nu \otimes |\delta_t\rangle)) \hat{W}(t) + \sum_j \nu_j^* \hat{W}(t) a(b_j \otimes |\delta_t\rangle). \quad (5.6)$$

Note that $a(\nu \otimes |\delta_0\rangle)$ and $a^*(\nu \otimes |\delta_0\rangle)$ appearing in \hat{Z} and \hat{Z}^+ are quantum analogs of a classical *white noise*. They are “localized” at $\tau = 0$. Besides, they are (formally) given by a linear expression in terms of creation/annihilation operators. Therefore, they are often called *linear quantum noises*.

5.2. Quadratic noises. This subsection is outside of the main line of this article. It is closely related to Subsect. 2.2. It is not needed for the description of the weak coupling limit, as given in the next section.

Clearly, $\Psi \in \mathcal{K} \otimes (\otimes_s^n \mathfrak{h} \otimes L^2(\mathbb{R})) \simeq \mathcal{K} \otimes (\otimes_s^n L^2(\mathbb{R}, \mathfrak{h}))$ can be identified with a function $\Psi(\tau_1, \dots, \tau_n)$ with values in $\mathcal{K} \otimes (\otimes^n \mathfrak{h})$ and the arguments satisfying $\tau_1 < \dots < \tau_n$.

Let S be a unitary operator on $\mathcal{K} \otimes \mathfrak{h}$. Let $S_{(j)}$ be this operator acting on $\mathcal{K} \otimes \otimes^n \mathfrak{h}$, where it is applied to the j 'th “leg” of the tensor product $\otimes^n \mathfrak{h}$. We define an operator $\Lambda(S)$ on $\mathcal{K} \otimes (\otimes_s^n L^2(\mathbb{R}, \mathfrak{h}))$ as follows: If $\tau_1 < \dots < \tau_k < 0 < \tau_{k+1} < \dots < \tau_n$, then

$$(\Lambda(S)\Psi)(\tau_1, \dots, \tau_n) := S_{(k+1)} \cdots S_{(n)} \Psi(\tau_1, \dots, \tau_n).$$

Clearly, $\Lambda(S)$ is a unitary operator. If $\mathcal{K} = \mathbb{C}$, then it coincides with $\Gamma(\gamma(S))$, where $\gamma(S)$ was defined in (2.15) and Γ is the *functor of the second quantization* defined in (4.1).

Introduce the operator $\hat{Z}_{S,0}$ on $\mathcal{K} \otimes \Gamma_s(\mathcal{Z}_R)$ by

$$\hat{Z}_{S,0} := \Upsilon + \Lambda(S)^* 1 \otimes d\Gamma(D_\tau) \Lambda(S). \quad (5.7)$$

The operator (5.7) is very singular and contains a ‘‘delta interaction at $\tau = 0$ ’’.

Let us now define the dynamics $\hat{U}_{S,t}$ that generalizes \hat{U}_t . Let $S_{ij} \in B(\mathcal{K})$ be defined by

$$S = \sum_{i,j} S_{ij} \otimes |b_i\rangle\langle b_j|. \quad (5.8)$$

Set

$$\nu_{S,j}^+ = \nu_j, \quad \nu_{S,j}^- = \sum_i \nu_i^* S_{ij}.$$

Then we introduce the quadratic form

$$\begin{aligned} \hat{U}_{S,t} &:= \sum_{n=0}^{\infty} \int_{t \geq t_n \geq \dots \geq t_1 \geq 0} dt_n \cdots dt_1 \\ &\quad \sum_{j_1, \dots, j_n} \sum_{\epsilon_1, \dots, \epsilon_n \in \{+, -\}} (-i)^n \prod_{k=1, \dots, n: \epsilon_k = +} a^*(b_{j_k} \otimes |\delta_{t_k - t}\rangle) \\ &\quad \times e^{-i(t-t_n)\hat{Z}_{S,0}} \nu_{S,j_n}^{\epsilon_n} \otimes 1 e^{-i(t_n-t_{n-1})\hat{Z}_{S,0}} \dots \nu_{S,j_1}^{\epsilon_1} \otimes 1 e^{-i(t_1-0)\hat{Z}_{S,0}} \\ &\quad \times \prod_{k'=1, \dots, n: \epsilon_{k'} = -} a(b_{j_{k'}} \otimes |\delta_{t_{k'}}\rangle); \\ \hat{U}_{S,-t} &:= \hat{U}_{S,t}^*. \end{aligned}$$

One can check that $\hat{U}_{S,t}$ extends to a strongly continuous unitary group. Therefore, one can define a self-adjoint operator \hat{Z}_S such that $\hat{U}_{S,t} = e^{-it\hat{Z}_S}$. It satisfies

$$I_{\mathcal{K}}^* \hat{U}_{S,t} I_{\mathcal{K}} = e^{-it\Upsilon}, \quad I_{\mathcal{K}}^* \hat{U}_{S,t} A \otimes 1 \hat{U}_{S,-t} I_{\mathcal{K}} = e^{tM}(A).$$

It is awkward to write a formula for \hat{Z}_S in terms of creation/annihilation operators, even formally. There exists however an alternative formalism that is commonly used in the literature to define the group $e^{-it\hat{Z}_S}$. Let $\psi, \psi' \in \mathcal{D}_1$. Introduce the cocycle

$$\hat{W}_S(t) := e^{itd\Gamma(D_\tau)} e^{-it\hat{Z}_S}. \quad (5.9)$$

Then, in the sense of the quadratic form on \mathcal{D}_1 , the cocycle satisfies the differential equation

$$i \frac{d}{dt} \hat{W}_S(t) = (\Upsilon \otimes 1 + a^*(\nu \otimes |\delta_t\rangle)) \hat{W}_S(t) \quad (5.10)$$

$$+ \sum_{ij} i(1 - S_{ij}) \otimes a^*(b_i \otimes |\delta_t\rangle) \hat{W}_S(t) a(b_j \otimes |\delta_t\rangle) \quad (5.11)$$

$$+ \sum_j \nu_{S,j}^- \hat{W}_S(t) a(b_j \otimes |\delta_t\rangle). \quad (5.12)$$

This formula is the *quantum Langevin (stochastic) equation* for the cocycle $\hat{W}_S(t)$ in the sense of [HP, Fa, Pa, At, Maa, Fr, Bar, Me], which includes all three kinds of noises. In the literature, the dilation $e^{-it\hat{Z}_S}$ is usually introduced through a version of (5.12).

5.3. Total energy operator. Let us analyze the impact of the invariance of a c.p. semi-group on its quantum Langevin dynamics.

Suppose now that K is a self-adjoint operator on \mathcal{K} and Y a self-adjoint operator on \mathfrak{h} . Assume that they satisfy

$$\nu K = (K \otimes 1 + 1 \otimes Y)\nu, \quad \left[\frac{1}{2}(\Upsilon + \Upsilon^*), K \right] = 0. \quad (5.13)$$

This implies in particular that M is K -invariant. Define the self-adjoint operator on \mathcal{Z}

$$E := K \otimes 1 + 1 \otimes d\Gamma(Y \otimes 1). \quad (5.14)$$

Then it is easy to see that the quantum Langevin dynamics commutes with this operator:

$$[E, e^{-itZ}] = 0. \quad (5.15)$$

E will be called the *total energy operator*, which is a name suggested by the physical interpretation that we attach to E .

Next we discuss the implications of the DBC of a c.p. semigroup on its quantum Langevin dynamics. We set

$$\begin{aligned} \sigma_t(C) &:= e^{itE} C e^{-itE}, \\ \omega_\beta(C) &:= \text{Tr} e^{-\beta K} \otimes |\Omega\rangle\langle\Omega| C / \text{Tr} e^{-\beta K}, \quad C \in B(\mathcal{Z}). \end{aligned}$$

We will see that the DBC for $e^{-\beta K} / \text{Tr} e^{-\beta K}$ is related to a version of the β -KMS condition for the dynamics σ_t and the state ω_β .

THEOREM 5.2. *Assume (5.14). Then the following statements are equivalent:*

1) For any $D_1, D_2, D'_1, D'_2 \in B(\mathcal{K})$, $f_1, f_2 \in L^2(\mathbb{R})$ and

$$B_j := D_j \otimes 1 (a^*(\nu \otimes |f_j\rangle) + a(\nu \otimes |f_j\rangle)) D'_j \otimes 1, \quad j = 1, 2.$$

and for any $t \in \mathbb{R}$ we have

$$\omega_\beta(\sigma_t(B_1)B_2) = \omega_\beta(B_2\sigma_{t+i\beta}(B_1)). \quad (5.16)$$

2)

$$\text{Tr}_{\mathfrak{h}} \nu A \nu^* = \nu^* A \otimes e^{-\beta Y} \nu, \quad (5.17)$$

(This implies in particular that M satisfies the DBC for $e^{-\beta K} / \text{Tr} e^{-\beta K}$).

6. Weak coupling limit for Pauli-Fierz operators. In this section we describe the main results of this article. They are devoted to a rather large class of Pauli-Fierz operators in the weak coupling limit. In the first subsection we recall the well known results about the reduced dynamics, which go back to Davies [Da1, Da2, Da3]. In the second subsection we describe our results that include the reservoir [DD2]. They are inspired by [AFL]. Finally, we discuss the case of thermal reservoirs.

6.1. Reduced weak coupling limit. We consider a Pauli-Fierz operator

$$H_\lambda = K \otimes 1 + 1 \otimes d\Gamma(H_R) + \lambda(a^*(V) + a(V)).$$

We assume that \mathcal{K} is finite dimensional and for any $A \in B(\mathcal{K})$ we have $\int \|V^* A \otimes 1 e^{-itH_0} V\| dt < \infty$. The following theorem is essentially a special case of a result of Davies [Da1, Da2, Da3], see also [DD2].

THEOREM 6.1 (Reduced weak coupling limit for Pauli-Fierz operators). *There exists a K -invariant Markov c.p. semigroup e^{tM} on $B(\mathcal{K})$ such that*

$$\lim_{\lambda \searrow 0} e^{-itK/\lambda^2} I_{\mathcal{K}}^* e^{itH_\lambda/\lambda^2} A \otimes 1 e^{-itH_\lambda/\lambda^2} I_{\mathcal{K}} e^{itK/\lambda^2} = e^{tM}(A),$$

and a contractive semigroup $e^{-it\Upsilon}$ on \mathcal{K} such that $[\Upsilon, K] = 0$ and

$$\lim_{\lambda \searrow 0} e^{itK/\lambda^2} I_{\mathcal{K}}^* e^{-itH_\lambda/\lambda^2} I_{\mathcal{K}} = e^{-it\Upsilon}.$$

If the reservoir is at inverse temperature β , then M satisfies the DBC for the state $e^{-\beta K} / \text{Tr} e^{-\beta K}$.

The operator $\Upsilon \in B(\mathcal{K})$ arising in the weak coupling limit equals

$$\Upsilon := -i \sum_{\omega} \sum_{k-k'=\omega} \int_0^\infty 1_k(K) V^* 1_{k'}(K) e^{-it(H_R-\omega)} V 1_k(K) dt.$$

In order to write an explicit formula for M it is convenient to introduce an additional assumption, which anyway will be useful later on in the extended weak coupling limit.

ASSUMPTION 6.2. *Suppose that for any $\omega \in \text{sp}K - \text{sp}K$ there exist an open $I_\omega \subset \mathbb{R}$ and a Hilbert space \mathfrak{h}_ω such that $\omega \in I_\omega$ and*

$$\text{Ran} 1_{I_\omega}(H_R) \simeq \mathfrak{h}_\omega \otimes L^2(I_\omega, dx),$$

$1_{I_\omega}(H_R) H_R$ is the multiplication operator by the variable $x \in I_\omega$ and, for $\psi \in \mathcal{K}$,

$$1_{I_\omega}(H_R) V \psi \simeq \int_{I_\omega}^\oplus v(x) \psi dx.$$

Assume that I_ω are disjoint for distinct ω and $x \mapsto v(x) \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h}_\omega)$ is continuous at ω .

Thus we assume that the reservoir 1-body Hamiltonian H_R and the interaction V are well behaved around the *Bohr frequencies*, the differences of eigenvalues of K .

Let $\mathfrak{h} := \bigoplus_{\omega} \mathfrak{h}_\omega$. We define $\nu_\omega \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h}_\omega)$ by

$$\nu_\omega := (2\pi)^{\frac{1}{2}} \sum_{\omega=k-k'} 1_k(K) v(\omega) 1_{k'}(K)$$

and $\nu \in B(\mathcal{K}, \mathcal{K} \otimes \mathfrak{h})$ by

$$\nu := \sum_{\omega} \nu_\omega.$$

Note that

$$\begin{aligned} i\Upsilon - i\Upsilon^* &= \sum_{\omega} \sum_{k-k'=\omega} \int_{-\infty}^{\infty} 1_k(K) V^* 1_{k'}(K) e^{-it(H_R-\omega)} V 1_k(K) dt \\ &= \sum_{\omega} \sum_{k-k'=\omega} 1_k(K) v^*(\omega) 1_{k'}(K) v(\omega) 1_k(K) = \nu^* \nu. \end{aligned}$$

The generator of a c.p. Markov semigroup that arises in the reduced weak coupling limit, called sometimes the Davies generator, is

$$\begin{aligned} M(A) &= -i(\Upsilon A - A\Upsilon^*) + \nu^* A \otimes 1 \nu \\ &= -i \left[\frac{\Upsilon + \Upsilon^*}{2}, A \right] - \frac{1}{2} [A, \nu^* \nu]_+ + \nu^* A \otimes 1 \nu, \quad A \in B(\mathcal{K}). \end{aligned} \quad (6.1)$$

6.2. Energy of the reservoir in the weak coupling limit. Introduce the operator Y on \mathfrak{h} by setting

$$Y = \omega \quad \text{on} \quad \mathfrak{h}_\omega. \quad (6.2)$$

The operator Y has the interpretation of the asymptotic energy of the restricted reservoir.

THEOREM 6.3.

1) *The operator ν constructed in the weak coupling limit satisfies*

$$\nu K = (K \otimes 1 + 1 \otimes Y) \nu. \quad (6.3)$$

This implies in particular that M is K -invariant.

2) *If the reservoir is at inverse temperature β , then ν satisfies*

$$\text{Tr}_{\mathfrak{h}} \nu A \nu^* = \nu^* A \otimes e^{-\beta Y} \nu, \quad (6.4)$$

This implies in particular that M satisfies the DBC for $e^{-\beta K} / \text{Tr} e^{-\beta K}$.

6.3. Extended weak coupling limit. Recall that given $(\Upsilon, \nu, \mathfrak{h})$ we can define the space $\mathcal{Z}_{\mathbb{R}}$ and the Langevin Schrödinger dynamics e^{-itZ} on the space $\mathcal{Z} := \mathcal{K} \otimes \Gamma_{\mathfrak{s}}(\mathcal{Z}_{\mathbb{R}})$, as in Subsect. 5.1.

For $\lambda > 0$, we define the family of partial isometries $J_{\lambda, \omega} : \mathfrak{h}_\omega \otimes L^2(\mathbb{R}) \rightarrow \mathfrak{h}_\omega \otimes L^2(I_\omega) \subset \mathcal{H}_{\mathbb{R}}$:

$$(J_{\lambda, \omega} g_\omega)(y) = \begin{cases} \frac{1}{\lambda} g_\omega\left(\frac{y-\omega}{\lambda^2}\right), & \text{if } y \in I_\omega; \\ 0, & \text{if } y \in \mathbb{R} \setminus I_\omega. \end{cases}$$

We set $J_\lambda : \mathcal{Z}_{\mathbb{R}} \rightarrow \mathcal{H}_{\mathbb{R}}$, defined for $g = (g_\omega)$ by

$$J_\lambda g := \sum_{\omega} J_{\lambda, \omega} g_\omega.$$

Note that J_λ are partial isometries and $\text{s-lim}_{\lambda \searrow 0} J_\lambda^* J_\lambda = 1$.

Set $Z_0 := d\Gamma(\mathcal{Z}_{\mathbb{R}})$. The following theorem [DD2] was inspired by [AFL]:

THEOREM 6.4 (Extended weak coupling limit for Pauli-Fierz operators).

$$\text{s}^* \text{-lim}_{\lambda \searrow 0} \Gamma(J_\lambda^*) e^{i\lambda^{-2}tH_0} e^{-i\lambda^{-2}(t-t_0)H_\lambda} e^{i\lambda^{-2}t_0H_0} \Gamma(J_\lambda) = e^{itZ_0} e^{-i(t-t_0)Z_0} e^{-it_0Z_0}.$$

The extended weak coupling limit can be used to describe interesting physical properties of non-equilibrium quantum systems, see e.g. [DM]. The following corollary, which generalizes the results of [Du], describes the asymptotics of correlation functions for observables of the form $\Gamma(J_\lambda) A \Gamma(J_\lambda^*)$, where A are observables on the asymptotic space.

COROLLARY 6.5 (Asymptotics of correlation functions). *Suppose that $A_\ell, \dots, A_1 \in B(\mathcal{Z})$ and $t, t_\ell, \dots, t_1, t_0 \in \mathbb{R}$. Then*

$$\begin{aligned} & s^* \text{-} \lim_{\lambda \searrow 0} I_{\mathcal{K}}^* e^{i\lambda^{-2}tH_0} e^{-i\lambda^{-2}(t-t_\ell)H_\lambda} e^{-i\lambda^{-2}t_\ell H_0} \Gamma(J_\lambda) A_\ell \Gamma(J_\lambda^*) \\ & \quad \dots \Gamma(J_\lambda) A_1 \Gamma(J_\lambda^*) e^{i\lambda^{-2}t_1 H_0} e^{-i\lambda^{-2}(t_1-t_0)H_\lambda} e^{-i\lambda^{-2}t_0 H_0} I_{\mathcal{K}} \\ & = I_{\mathcal{K}}^* e^{itZ_0} e^{-i(t-t_\ell)Z} e^{-it_\ell Z_0} A_\ell \dots A_1 e^{it_1 Z_0} e^{-i(t_1-t_0)Z} e^{-it_0 Z_0} I_{\mathcal{K}}. \end{aligned}$$

The following corollary is interesting since it describes how reservoir Hamiltonians converge to operators whose dynamics under the quantum Langevin dynamics $U_{-t} \cdot U_t$ is well-studied, see e.g. [Bar].

COROLLARY 6.6 (Asymptotic reservoir energies). *Consider the operator $Y : \mathfrak{h} \mapsto \mathfrak{h}$ defined in (6.2). The operator $E := K \otimes 1 + 1 \otimes d\Gamma(Y \otimes 1)$ plays the role of “asymptotic total energy operator”, i.e.*

$$[E, e^{itZ}] = 0. \quad (6.5)$$

Moreover, for $\kappa_1, \dots, \kappa_\ell \in \mathbb{R}$,

$$\begin{aligned} & s^* \text{-} \lim_{\lambda \searrow 0} I_{\mathcal{K}}^* e^{i\lambda^{-2}tH_0} e^{-i\lambda^{-2}(t-t_\ell)H_\lambda} e^{-i\lambda^{-2}t_\ell H_0} e^{i\kappa_\ell d\Gamma(H_R)} \\ & \quad \dots e^{i\kappa_1 d\Gamma(H_R)} e^{i\lambda^{-2}t_1 H_0} e^{-i\lambda^{-2}(t_1-t_0)H_\lambda} e^{-i\lambda^{-2}t_0 H_0} I_{\mathcal{K}} \\ & = I_{\mathcal{K}}^* e^{itZ_0} e^{-i(t-t_\ell)Z} e^{-it_\ell Z_0} e^{i\kappa_\ell d\Gamma(Y \otimes 1)} \dots e^{i\kappa_1 d\Gamma(Y \otimes 1)} e^{it_1 Z_0} e^{-i(t_1-t_0)Z} e^{-it_0 Z_0} I_{\mathcal{K}}. \end{aligned}$$

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