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## On the parametrization of Lindblad equations

Klaus Dietz<sup>1</sup>

Sektion Physik, Universitaet Muenchen, Theresienstr. 37, 80333 Muenchen, Germany

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### Abstract

The structure of the Lindblad equation of motion of quantum states is discussed. General specifications for this motion to lead asymptotically into equilibrium states are given. Incomplete ‘thermalization’, i.e. the Lindblad motion of only a selected subset of quantum states leads to a reduced quantum system whose observables are explicitly constructed and seen to incorporate memory terms. It is shown that under rather general conditions the absolute value of Lindblad operators is given by the (inverse square root of the) grand-canonical probability distribution.

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The motion of finite, closed quantum systems is described by a one-parameter group of unitary transformations in an appropriate Hilbert space. Extending this concept to the description of irreversible processes—approach to equilibrium, for instance—the construction of a dynamical semigroup of time-dependent motions, i.e. maps acting on states (density operators) or observables, was introduced [1]. Assuming complete positivity—an assumption which allows the extension of positive maps, acting e.g. on a dynamical system  $\Sigma$ , to positive maps on an entangled dynamical system  $\Sigma \otimes \mathbb{C}^n$ , for all  $n$ , thus an assumption with important physical content—Lindblad [2] derived an explicit form of the (bounded) generators of this semigroup acting on  $\mathfrak{B}(\mathfrak{H})$  (the algebra of bounded operators on a separable Hilbert space  $\mathfrak{H}$ ).

The celebrated equations read (throughout the paper we use units  $\hbar = 1$ )

$$\dot{\varrho} = -i[H, \varrho] + \sum_J V_J \varrho V_J^\dagger - \frac{1}{2}(V_J^\dagger V_J \varrho + \varrho V_J^\dagger V_J) \quad (1)$$

for the density operator  $\varrho$  and

$$\dot{B} = i[H, B] + \sum_J V_J^\dagger B V_J - \frac{1}{2}[V_J^\dagger V_J, B]_+ \quad (2)$$

where  $\varrho$  is trace class and normalized to 1 and  $B$  is a bounded observable. The input is the Hamiltonian  $H$  and bounded operators  $V_J$ .

<sup>1</sup> Permanent address: Physics Department, University of Bonn, 53115 Bonn, Germany.

Whether these equations have anything to do with the description of the quantum dynamics of open systems is *a priori* unclear as can be seen from the following considerations. A theory of open systems should start from the concept of embedding the latter in a ('large') bath and considering the total 'system'  $\otimes$  'bath' as a closed system moving unitarily with the total Hamiltonian as a generator. The motion of an observable  $B$  of the open system is given as the map ( $\mathbb{I}$  is the unit operator on the 'bath')

$$B \longrightarrow \text{tr}_{\text{bath}}(\varrho_{\text{bath}} \mathfrak{U}(t)^+ (B \otimes \mathbb{I}) \mathfrak{U}(t)).$$

It is clear that these maps are completely positive; however, the formulation of general conditions under which these maps have the Markovian property, i.e. build up an Abelian semigroup, is a difficult task if rigorous answers are attempted. Physically speaking, the relative magnitude of timescales has been discovered to control the Markovian property of such maps (see [8]).

In this paper we study the asymptotic form of states  $\varrho$  assuming the semigroup property and the complete positivity of maps describing the motion of open systems or, equivalently, we study the asymptotics of the Lindblad equation (1). We show that under rather general circumstances the asymptotic form of states reveals a rather striking universality property: for a large class of Lindblad equations the asymptotic form of states is controlled by the Lindblad operators  $V_J$ , independently of the initial state—a situation typical for the approach to equilibrium.

In our method bath variables are tacitly assumed *implicitly* to be modelled by the Lindblad operators  $V_J$ . Very implicitly indeed, it is a formidable task to construct explicit relations even in very simple cases.

The asymptotic form of states has been studied in the literature proposing various 'system'  $\otimes$  'bath' models and different dynamical ansätze. For example in [9], asymptotic quantum Brownian motion has been studied in the quantum diffusion picture (stochastic Langevin–Itô equation) and by using the path integral representation of the Green function for the density operator. Another example relevant in our context is found in [10]. The authors discuss the relation between the dynamics of classical and quantum systems under the influence of a measuring process. The latter is modelled by coupling a set of oscillators, thermally distributed or selectively coupled. Elimination of the measurement process leads to a Lindblad equation similar to the one set up to describe the dynamics of a single atom maser [11], asymptotic solutions are given. However, it has to be noted that this equation is beyond the scope of Lindblad equations considered in this paper: the absolute value of its Lindblad operators is not bounded and admits a zero mode contrary to our assumptions. A tangible consequence of this fact is that the parametrization of the absolute value of a Lindblad operator by the Gibbs distribution, derived in this paper, is obviously not possible.

In the following discussion, we consider the case of only one Lindblad operator  $V$  and return to the general case at the end of the paper, in section D.

We have shown in [3] that the polar decomposition [4]

$$V = U|V|$$

plays a key role in the interpretation of the motion generated by the Lindblad generator. The absolute value  $|V|$  is a nonnegative self-adjoint (s.a.) operator

$$|V| = (V^+V)^{1/2}$$

and  $U$  is a partial isometry. We assume  $V^+V$  is positive (for a collection of the assumptions discussed in [3, 5] and implicitly used here see the appendix)

$$V^+V > 0$$

and, hence,  $U$  is unitary. Defining

$$W = (V^+ V)^{-1}$$

and

$$\tilde{\varrho} = W^{-1/2} \varrho W^{-1/2}$$

we rewrite the Lindblad equations as

$$W^{1/2} \dot{\tilde{\varrho}} W^{1/2} = -iW^{1/2} [H, \tilde{\varrho}] W^{1/2} + U \tilde{\varrho} U^+ - \frac{1}{2} (W^{1/2} \tilde{\varrho} W^{-1/2} + W^{-1/2} \tilde{\varrho} W^{1/2}) \tag{3}$$

and

$$W^{1/2} \dot{B} W^{1/2} = iW^{1/2} [H, B] W^{1/2} + U^+ B U - \frac{1}{2} (W^{1/2} B W^{-1/2} + W^{-1/2} B W^{1/2}) \tag{4}$$

where we used the key assumption

$$[W, H] = 0 \tag{5}$$

which is *a posteriori* justified by observing that  $W$  figures as the (operator of the) probability distribution (non-normalized) of final states in the ensemble into which an arbitrarily given initial state develops by Lindblad motion. For the sake of clarity we reiterate the argument given in [3] in greater detail. Let us begin with the discussion of the motion of an arbitrary state  $\varrho_0$  (which is trace class by the very notion of a quantum state and  $\text{tr}(\varrho_0) = 1$ ). We see that by assumption (5) the trace of the rhs of (3) vanishes identically in  $\tilde{\varrho}$  so that we reproduce the normalization condition ( $\text{tr}$  denotes the trace in  $\mathfrak{H}$ )

$$\text{tr}(\tilde{\varrho} W) = \text{const} = 1.$$

Furthermore, we see by inspection of (3) and (4) that a multiple of the identity is a stationary solution. The completely dissipative [2] character of the Lindblad generator leads to (for details see [5])

$$\tilde{\varrho} \longrightarrow \text{const} \times \mathbb{I}$$

and

$$B \longrightarrow b(\infty) \mathbb{I} \tag{6}$$

with

$$b(\infty) = \frac{\text{tr}(B|_{t=\infty} W)}{\text{tr}(W)}$$

for  $t \rightarrow \infty$ , so that, in particular

$$\text{tr}(\tilde{\varrho}_0 W) = \text{tr}(\varrho) = \text{const} \times \text{tr}(W)$$

and, hence

$$\tilde{\varrho} \longrightarrow \frac{\mathbb{I}}{\text{tr}(W)}$$

or

$$\begin{aligned} \varrho|_{t=\infty} &= \frac{W}{\text{tr}(W)} \\ &:= P_W \end{aligned} \tag{7}$$

for all initial states  $\varrho_0$  :  $W/\text{tr}(W)$  is the probability distribution of pure states in the final state  $\varrho|_{t=\infty}$ , Lindblad motion transports an arbitrary quantum state  $\varrho_0$ —in particular any pure state—into the state  $P_W$  which has lost any trace of the structure of the initial state.

Denote

$$\mathfrak{D} = [Q_\gamma | \gamma = 0, 1, 2, \dots] \tag{8}$$

with

$$[Q_\alpha, Q_\beta] = 0$$

all  $\alpha, \beta = 0, 1, \dots$ , a set of mutually commuting operators (the Hamiltonian  $H$  is taken as  $Q_0 : H = Q_0$ ) defining a complete measurement, and note that because of (5) we have

$$W = W(H, Q_1, \dots)$$

a relation we shall exploit in the next section. Here this relation leads us to the following naive realization of equilibrium states: the stationary state, reached asymptotically from any initial state by Lindblad motion whose probability distribution depends only on constants of motion will be dubbed equilibrium state.

Roughly speaking, relation (6) which holds for any (bounded) operator tells us that, asymptotically, the system 'looses' all dynamical variables which is another way of noting the equilibrium nature of asymptotic Lindblad states.

In [3], we have seen that these observations generalize to cases where only a selected subset of quantum states undergoes 'Lindbladization', i.e. are asymptotically eliminated. This partial elimination of a selected set of degrees of freedom via the construction of asymptotic solutions of (1) or (2) leaves us with a reduced set of observables of the resulting system. The Lindblad equation thus provides a physically motivated procedure for the elimination of selected degrees of freedom, the physical motivation hinging on the already mentioned notions of complete positivity and semigroup structure of dynamical maps. To be more specific on the precise meaning of the degrees of freedom to be eliminated let us decompose the Lindblad operator in the following way

$$V = ((\tilde{V}_{ik}) \otimes \mathbb{I})$$

the indices  $(ik)$  enumerate a selected set of quantum numbers of certain degrees of freedom. Physically two selection criteria apply:

- (i) The partial elimination of  $K$  degrees of freedom  $Q_\lambda : (ik)$  denote quantum numbers separated from the rest of the spectrum by scales. For example, consider the energy spectrum of a molecule where electronic, vibrational and rotational components differ by scales of an order of magnitude.
- (ii) The total elimination of degrees of freedom  $Q_\lambda$ . Here the indices  $(ik)$  run over all of the spectrum. A typical example is the elimination of variables describing the dynamics of a (heat-) bath.

We now perform the trace, with respect to the levels to be eliminated, of equation (4) and denote this operation by  $\tilde{\text{Tr}}$ . Separating the levels to be eliminated we endow the Hamiltonian with a product structure and write

$$H = ((\tilde{H}_{ik}) \otimes \mathbb{H})$$

to obtain [3]

$$\tilde{\text{Tr}}(BW) = C + \int_0^t (\mathbb{H} \tilde{\text{Tr}}(\tilde{W} \tilde{H} B(t)) - \tilde{\text{Tr}}(\tilde{W} B(t) \tilde{H}) \mathbb{H}) dt$$

where

$$W = ((\tilde{W}_{ik}) \otimes \mathbb{I})$$

and

$$\tilde{W} = (\tilde{V}^+ \tilde{V})^{-1}.$$

We immediately see that the second term contains the history  $B(t)$  of the quantum evolution of the initial configuration  $B|_{t=0}$ . It is, however, important to note that the integrand of the memory term is different from zero only in the initial phase of the time evolution.

$B$  tends to  $c\mathbb{I}$  for times exceeding the relaxation time (equation (6)), hence

$$[\mathbb{H}, B(t)] = 0$$

for

$$t \gg t_{\text{relaxation}}$$

and

$$[\tilde{H}, \tilde{W}] = 0$$

because of

$$[H, W] = 0.$$

Thus  $\tilde{\text{Tr}}(BW)$  is a constant of motion for times larger than the relaxation time and contains a contribution which relates to the history pertaining only to the approach to equilibrium. It is therefore small for small relaxation times. The statement sometimes found in the literature, namely that the Lindblad equation is a ‘Markovian equation of motion’ has to be seen *cum grano salis*, with a big grain of salt indeed.

In this section we shall address the problem of finding a physically adequate interpretation, and in the following a parametrization with parameters which can be measured in independent experiments and thus have relevance for physical processes not related to the relaxation process considered. We are trying to establish a natural relation of Lindblad operators to observables relevant for the description of equilibrium states.

As a first step we evoke the KMS condition [6] for the correlation function in an equilibrium state  $\varrho_e$

$$\langle A(t)B(0) \rangle = \langle B(0)A(t + i\beta) \rangle$$

with

$$\langle A \rangle = \text{tr}(\varrho_e A).$$

This condition has been used as a starting point for the definition of an equilibrium state [7] and plays a central role in the theory of thermal equilibrium. In particular, it implies that the density operator for an equilibrium state is proportional to the canonical probability distribution [6]

$$\varrho_e \propto \exp(-\beta H)$$

in addition it shows that the (symmetrized) two-point correlation function is periodic with period  $i\beta$  and is holomorphic in the strip  $0 \leq \Im(t) < \beta$ .

It is clear that any of the observables  $Q_i, Q_i \in \mathfrak{D}$  specified in (8), generates a group of automorphisms  $\Psi$

$$\Psi : A_0 \mapsto A_\sigma = \exp(-i\sigma Q_i) A_0 \exp(i\sigma Q_i)$$

via the equation

$$\partial_\sigma = -i[Q_i, A]$$

where  $\sigma$  is some real parameter. If we continue  $\sigma$  to purely imaginary values

$$\sigma \mapsto i\tau$$

we have

$$\partial_\tau = [Q_i, A]$$

and  $\Psi$  is no longer a Hermitian map ( $\Phi$  is Hermitian if  $\Phi(A^+) = \Phi^+(A)$ ,  $\Phi \in \mathfrak{B}(\mathfrak{H})$ ).

Define

$$\Xi : A_0 \mapsto A_\tau = \exp(-\tau Q_i) A_0 \exp(\tau Q_i) + \exp(\tau Q_i) A_0 \exp(-\tau Q_i)$$

a Hermitian map  $\mathfrak{B}(\mathfrak{H}) \rightarrow \mathfrak{B}(\mathfrak{H})$ .

The  $Q_i$  also generate another type of transformation via the equation

$$\partial_\mu = -[Q_i, A]_+$$

i.e. the Hermitian map

$$\Lambda : A_0 \mapsto A_\mu = \exp(-\mu Q_i) A_0 \exp(-\mu Q_i).$$

We are now in the position to interpret the Lindblad operator in terms of these transformations. Let  $B$  be an observable whose Lindblad motion we are going to consider

$$\dot{B} = \mathfrak{L}_L(B).$$

The Lindblad equation can then be written as

$$\Lambda(\dot{B} - [H, B]) = \mathfrak{L}_D.$$

We have to guarantee that

$$\mathfrak{L}_L(B^+) = \mathfrak{L}_L^+(B)$$

and

$$\mathfrak{L}_L(\mathbb{I}) = 0 \tag{9}$$

which of course means that  $\mathfrak{L}_L$  is Hermitian and the generated map maps  $\mathbb{I}$  into  $\mathbb{I}$ . The generator  $\mathfrak{L}_D$  is connected with the transformation  $\Xi$  which complies with the first condition, to fulfil the second requirement we introduce an arbitrary unitary operator  $U$  and write

$$\mathfrak{L}_D(B) = U^+ B U - \frac{1}{2} \Xi_\sigma(B)$$

so that the Lindblad equation now reads

$$\Lambda_\sigma(\dot{B}) - [H, \Lambda_\sigma(B)] = U^+ B U - \frac{1}{2} \Xi_\sigma(B).$$

It is clear that instead of considering only one generator  $Q_i$  we can take some of the generators  $Q_j$ ,  $j = 0, 1, \dots, M$  and construct generalized operations  $\Lambda$  and  $\Xi$  generated by the equations

$$\begin{aligned} \partial_{\sigma_j} A &= [Q_j, A] \\ \partial_{\sigma_j} A^+ &= -[Q_j, A^+] \end{aligned} \tag{10}$$

$$\partial_{\tau_j} A = [Q_j, A]_+ \quad j = 1, \dots, M \tag{11}$$

so that

$$\begin{aligned} \Xi : A_{00\dots 0} \mapsto A_{\sigma_0 \sigma_1 \dots \sigma_M} &= \exp\left(\sum \sigma_j Q_j\right) A_{00\dots} \exp\left(-\sum \sigma_j Q_j\right) \\ &+ \exp\left(-\sum \sigma_j Q_j\right) A_{00\dots} \exp\left(\sum \sigma_j Q_j\right) \end{aligned}$$

$$\Lambda : A_{00\dots 0} \mapsto A_{\sigma_0 \sigma_1 \dots \sigma_M} = \exp\left(-\sum \sigma_j Q_j\right) A_{00\dots} \exp\left(-\sum \sigma_j Q_j\right)$$

and

$$\begin{aligned} \partial_t \Lambda_{\sigma_0 \dots \sigma_M}(B(0, \dots, t)) &= i[H, \Lambda_{\sigma_0 \dots \sigma_M}(B(0, \dots, t))] \\ &+ U^\dagger B(0, \dots, t) U - \frac{1}{2} \Xi_{\sigma_0 \dots \sigma_M}(B(0, \dots, t)). \end{aligned} \tag{12}$$

Comparing with (4) we have

$$W = \exp\left(-\sum \sigma_j Q_j\right)$$

and

$$P_W = \frac{\exp(-\beta H - \beta \sum \alpha_j Q_j)}{Z(\beta, \alpha_1, \dots)}$$

for the probability distribution of the final state (7); the partition function for the asymptotic equilibrium system is then

$$Z(\beta, \alpha_1, \alpha_2, \dots) = \text{tr}\left(\exp\left(-\beta H - \beta \sum \alpha_i Q_i\right)\right) \tag{13}$$

where we identified  $\sigma_0$  with the inverse temperature and the  $\alpha_i$  with the chemical potentials corresponding to the observables  $Q_1, \dots, Q_M$ . We have thus found a parametrization of the Lindblad operator  $V$

$$V = U \exp\left(1/2\left(\beta H + \beta \sum \alpha_i Q_i\right)\right)$$

suggested by the interpretation of

$$\text{tr}((V^\dagger V)^{-1})(V^\dagger V)^{-1} = P_W$$

as the asymptotic density operator—the absolute value of  $V$  is given as the inverse square root of the grand-canonical distribution, its ‘phase’ is given by a (unspecified) unitary  $U$ .

We now turn to the case of several Lindblad operators  $V_j$ ,  $j = 1, \dots$ . In this case there is a plethora of possibilities, some models have already been discussed in [3]. In the following we propose an ansatz which seems reasonable for physical phenomena where the dynamics of many physically different systems is controlled by one and the same Hamiltonian. Quantum electrodynamics is an important example for such a situation: practically all phenomena in the range between the Lambshift or the g-2 effect to electron–positron pair production (energies around 1 MeV) are described by one Hamiltonian—atomic, molecular and solid-state effects. One of the processes we envisage in the context of this paper is the disintegration of a molecule into some of its constituents. The disintegration dynamics for such processes is controlled by projections onto subsystems corresponding to these constituents and which are selected by the required number of electrons in the nonrelativistic, by the total electron charge in the relativistic case. In this case it seems reasonable to assume that the absolute value of *all* Lindblad operators is determined by the Hamiltonian of the total system—the QED Hamiltonian in our example. The same holds true for the other operators  $Q_i$  introduced in (8). With these specifications we write

$$V_J = U_J \exp\left(1/2\left(\beta H + \beta \sum \alpha_i Q_i\right)\right).$$

The Lindblad equation now reads

$$\begin{aligned} \partial_t (\Lambda_{\sigma_0 \sigma_1 \dots}(B(0, \dots, t))) &= i[H, \Lambda_{\sigma_0 \sigma_1 \dots}(B(0, \dots, t))] \\ &+ \sum_J U_J^\dagger B(0, \dots, t) U_J - N/2 \Xi_{\sigma_0 \sigma_1 \dots}(B(0, \dots, t)) \end{aligned} \tag{14}$$

a similar equation holds for the density operator.

*Summary.* The key element in our treatment of the Lindblad equations (1) and (2) was to rewrite them in the form (3) and (4) using the polar decomposition of the Lindblad operators  $V_j$ . The trace of the rhs's of the latter equations is immediately seen to vanish identically in  $\tilde{Q}$  and  $B$ , respectively. Take one of the  $Q_j$  introduced in (8) which is a constant under Hamiltonian motion, Lindblad motion on the other hand leaves only

$$\mathrm{tr}(Q_j(t)W) = \mathrm{const}$$

invariant. Furthermore, we derived that any initial state  $\varrho_0$  develops into the equilibrium distribution  $P_W$

$$\varrho_0 \longrightarrow P_W = W/\mathrm{tr}(W)$$

so that the asymptotic expectation value is given in terms of the initial ( $t = 0$ ) configuration as

$$\langle Q_j(t) \rangle \longrightarrow \mathrm{tr}(Q_j(0)P_W)$$

for  $t \longrightarrow \infty$ . We now take the standpoint that our system is Lindblad-transported into the equilibrium state  $P_W$ , evoke the KMS condition for the latter and conclude [6] its proportionality to the canonical distribution. It is clear that any of the  $Q_j \in \mathfrak{D}$  generates a corresponding motion in some parameter, hence we expect a KMS condition to hold for the analytic continuation in this parameter: we conclude the proportionality of  $P_W$  to the corresponding equilibrium distribution ( $\sigma_j$  denotes the imaginary part)

$$P_W \propto \exp(-\sigma_j Q_j).$$

Assuming the KMS condition for a selection of some  $Q_j$  dictated by the physics of the process under consideration we end up with the grand-canonical distribution

$$P_W = \frac{\exp(-\beta H - \sum \beta \alpha_j Q_j)}{Z(\beta, \alpha_1, \dots)}.$$

The motions generated by the  $Q_j$  for purely imaginary parameters have a physical interpretation: the form of (3) and (4) suggests that their structural elements derive from the corresponding equations of motion (10) and (11), as is clear from the construction of the maps  $\Lambda$  and  $\Xi$ . Starting from a configuration  $B(0, 0, \dots, 0)$  at time 0 we endow this configuration with an (inverse) temperature  $\beta$  and chemical potentials  $\alpha_j$  by transforming

$$B(0, 0, \dots, t) \longmapsto B_\Lambda(\beta, \beta \alpha_1, \dots, t) = (\Lambda B)(0, 0, \dots, t)$$

and

$$B(0, 0, \dots, t) \longmapsto B_\Xi(\beta, \beta \alpha_1, \dots, t) = (\Xi B)(0, 0, \dots, t)$$

the Lindblad equation (12), seen as an equation for  $B(0, 0, \dots, t)$ , finally defines the initial value problem leading asymptotically to the equilibrium state determined by the inverse temperature and the chemical potentials introduced by these transformations. The approach to equilibrium is controlled by a unitary operator  $U$  which entered the scene because of the condition (9) and stands for the unitary in the polar decomposition of the Lindblad operator  $V$ . This discussion immediately generalizes to the case of several  $V_j$  as is seen in (14).

## Appendix

It seems worthwhile to recollect the assumptions formulated in [3, 5] which lead to the result (7). First of all the Lindblad operators  $V$  are assumed to be bounded in the uniform metric; furthermore, it is essential to assume that  $V^+V$  be invertible, i.e.  $V^+V > 0$ , and trace class.

The latter assumption simply means that we stipulate normalizable probability distributions (7). Relation (6) finally was derived under the assumption of irreducibility of the Lindblad equations: there is *no* basis in the underlying Hilbert space in which the Lindblad equation disintegrates into a set of independent equations (see [5])—as we discussed in this reference this is the generic case. In the reducible case the dissipative Lindblad term in (1) or (2) can be represented as a direct sum of (irreducible) operators so that the asymptotic solution (6) is now a direct sum of multiples of unit operators acting in the irreducible subspaces in which these independent Lindblad equations operate. In terms of formulae we have

$$\tilde{\varrho} \longrightarrow \bigoplus_{\alpha} b_{\alpha}(\infty) \mathbb{P}_{\alpha}$$

where

$$\mathbb{P}_{\alpha} = \sum_k |k\rangle_{\alpha} \langle k|_{\alpha}$$

is the projector on the irreducible subspace  $\mathfrak{H}_{\alpha}$ . For the asymptotic state we then have instead of (7)

$$\varrho|_{t=\infty} = \sum_{\alpha} P_W^{\alpha} N_{\alpha}$$

where

$$P_W^{\alpha} = W_{\alpha} / \text{tr}(W_{\alpha})$$

is the normalized probability distribution for the system ( $\alpha$ ),

$$W_{\alpha} = \mathbb{P}_{\alpha} W \mathbb{P}_{\alpha}$$

and

$$N_{\alpha} = \text{tr}(W_{\alpha}) / \text{tr}(W)$$

is the probability weight of  $\mathfrak{H}_{\alpha}$  in  $\mathfrak{H}$ . Written in this form the asymptotic state has a clear probabilistic interpretation. The irreducibility assumption excludes Hermitian Lindblad operators and in particular the choice  $U = 1$  in the polar decomposition defined above.

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