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LETTER TO THE EDITOR

Memory effects in long-time Lindblad motion

Klaus Dietz¹

Max Planck Institut für Physik komplexer Systeme, 01187 Dresden, Germany

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Abstract

It is shown that the Lindblad equation accounts for memory effects. That is to say, Lindblad operators can be constructed in a natural manner such that a memory term appears in the asymptotic (*time* $\rightarrow \infty$) region; at the same time the expectation values depend on the initial state. Furthermore, a procedure for extending the Lindblad equation to an equation of motion for an ideal Bose 'gas' of 'particles', i.e. systems with non-trivial internal structure, is described. Initially in some quantum state this collection of 'particles' will asymptotically turn into an equilibrium ensemble whose probability distribution is determined by the Lindblad operators building the dissipative part of the equation of motion.

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(A) The Lindblad generalization [1] of Schrödinger motion to dissipative motion hinges, apart from technical assumptions, only on very general physical notions:

- (i) The Abelian group of unitary Schrödinger motion generated by the Hamiltonian generalizes to a set of Abelian semigroups characterized by a collection of operators V_J , the Lindblad operators. The semigroup structure—the non-existence of time-reversed motion—accounts for absorption.
- (ii) Complete positivity, interpreted physically, means that positive motions in Hilbert space of states (system 1) can be extended to a positive motion in the product space resulting by adjoining a second Hilbert space (system 2), a construction leading to entanglement of both systems.

It should be noted that in the derivation of the Lindblad equation, concepts used in the derivation of master equations—for instance the decomposition of the space of states into a product '*system*' \otimes '*bath*'—do not play any role, at any place. Nor is there any conceptual relation with open systems. The relation of master equations with open systems and Lindblad equations has been clarified to some extent [2–7] and shown to be controlled by relative scales.

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¹ Permanent address: Physics Department, University of Bonn, 53115 Bonn, Germany.

We take up this observation and consider a system whose degrees of freedom interact with scale-dependent Hamiltonians and look for stationary states evolving from given initial states, i.e. we construct maps (ρ is the density operator of our system)

$$\tau(V) : \varrho|_{t=0} \mapsto \varrho|_{t=\infty} \tag{1}$$

and discuss their dependence on the Lindblad operators V_J which together with the Hamiltonian are supposed to differ for different scales—time scales, energy scales etc.

We present an explicit construction of asymptotic stationary states which will be seen to contain memory terms.

(B) In this section, we consider the case of only one Lindblad operator V and write the Lindblad equation of motion

$$\dot{B} = i[H, B] + V^{+}BV - \frac{1}{2}[V^{+}V, B]_{+}$$
(2)

where *H* is the Hamiltonian and *B* is an observable².

 $V = U\sqrt{V^+V}$

Using the polar decomposition (U is a unitary operator)

we rewrite (2) as (note that the assumption of unitarity of U excludes zero modes in V^+V)

$$\frac{1}{\sqrt{V+V}}\dot{B}\frac{1}{\sqrt{V+V}} = i\frac{1}{\sqrt{V+V}}[H,B]\frac{1}{\sqrt{V+V}} + U^{+}BU - \frac{1}{2}\left(\frac{1}{\sqrt{V+V}}B\sqrt{V+V} + \sqrt{V+V}B\frac{1}{\sqrt{V+V}}\right).$$
(4)

The observation (see below) that

$$W := \frac{1}{V^+ V} \tag{5}$$

is a (non-normalized) probability distribution leads us to the physically plausible assumption

$$W = W(H, \ldots) \tag{6}$$

where the dots indicate further observables commuting with H. Tracing the equation of motion we immediately see that the trace of the rhs of the equation of motion vanishes identically and hence

$$\operatorname{tr}(\dot{B}W) = 0 \tag{7}$$

or

$$tr(BW) = const \tag{8}$$

 $(\dot{W} = 0$ since W depends only on conserved quantities). Needless to say we tacitly assume W to be traceclass.

In [8] we have demonstrated the following asymptotic form for *B*:

(i) Irreducible V

$$B|_{t=\infty} = b(\infty)\mathbb{I} \tag{9}$$

where \mathbb{I} is the unit operator in \mathfrak{H} .

 $^{^2}$ V is assumed to be invertible; B, H are bounded operators acting in a separable Hilbert space for which the Lindblad equation has been proved. This fact allows us to use interchangeably the notions 'operator' and 'matrix' and treat the question of dimensions—finite or infinite—in a rather cavalier way.

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(ii) Reducible V, i.e.

$$V = \sum_{\alpha} \oplus V_{\alpha} \tag{10}$$

where the V_{α} are matrices in orthogonal subspaces \mathfrak{H}^{α} of \mathfrak{H} , yield

$$B|_{t=\infty} = \sum_{\alpha} \oplus b^{\alpha}(\infty) \mathbb{I}^{\alpha}.$$
 (11)

In the following, we consider only the irreducible case and derive

$$B|_{t=\infty} = \frac{\operatorname{tr}(B|_{t=0}W)}{\operatorname{tr}(W)}\mathbb{I}.$$
(12)

The expectation value of the asymptotic configuration then is

$$\langle B|_{t=\infty} \rangle = \operatorname{tr}(B|_{t=0}\varrho_0) = \frac{\operatorname{tr}(B|_{t=0}W)}{\operatorname{tr}(W)}$$
(13)

for all states ρ_0 , i.e. the expectation value is independent of the initial state, no memory effects are present. We see that

$$P_W = \frac{W}{\text{tr}(W)} \tag{14}$$

is a normalized probability distribution derived from the Lindblad operator V. Translating this result into the Schrödinger picture we derive that any initial state ρ_0 tends to P_W for $t \to \infty$, i.e.

$$\tau(V) : \varrho_0 \mapsto \varrho_0|_{t=\infty} = P_W \tag{15}$$

for all initial states ρ_0 .

We now turn to the question of memory effects. To show that they can be incorporated we extend the Lindblad equation, without changing its formal content, to an equation of motion for quantum subsystems separated, e.g. by scales, from the system built up by these subsystems. As an example we could take a molecule: the subsystems are spanned by the states corresponding to the inner degrees of freedom of the atoms composing the molecule, the system—the molecule—is built up by the atomic states of outer shells.

To realize this construction we endow the input matrices V and H with a direct product structure and, to simplify matters, choose the ansätze

$$V = (\tilde{V}_{ik}\mathbb{I})\sqrt{n} \tag{16}$$

$$H = (\tilde{H}_{i,k} \mathbb{H}) \tag{17}$$

$$\tilde{V}_{ik}, \tilde{H}_{ik} \in \mathbb{C} \tag{18}$$

where \mathbb{I} is the $n \times n$ unit matrix and \mathbb{H} is an $n \times n$ matrix sub-Hamiltonian, identical for all sites (i, k), i.e. \tilde{V} and \tilde{H} are matrices with $n \times n$ matrix valued entries indexed by (i, k). Our ansatz for V guarantees that, in the terms of our example, the Lindblad operator leaves the inner degrees of freedom unaffected. The observable B is written as a matrix of $n \times n$ matrices B_{ik}

$$B = (B_{ik}). (19)$$

The probability distribution is then

$$W = ((\tilde{V}^{+}\tilde{V})^{-1} \otimes \mathbb{I}) =: (\tilde{W}_{ik} \otimes \mathbb{I}).$$
⁽²⁰⁾

V has the polar decomposition $V = U\sqrt{V^+V} = V$

$$= U\sqrt{V^{+}V} = (\tilde{U} \otimes \mathbb{I})\sqrt{\tilde{V}^{+}\tilde{V} \otimes \mathbb{I}}.$$
(21)

Tracing the equation of motion with respect to the indices (i, k) then yields instead of (7)

$$\tilde{\mathrm{Tr}}(\dot{B}W) = \mathbb{H}\,\tilde{\mathrm{Tr}}(\tilde{W}\tilde{H}B) - \tilde{\mathrm{Tr}}(\tilde{W}B\tilde{H})\mathbb{H}$$
(22)

which leads to

$$\tilde{\mathrm{Tr}}(BW) = C + \int_0^t (\mathbb{H} \; \tilde{\mathrm{Tr}}(\tilde{W}\tilde{H}B(t)) - \tilde{\mathrm{Tr}}(\tilde{W}B(t)\tilde{H})\mathbb{H}) \,\mathrm{d}t.$$
(23)

It has to be stated that taking the trace of this $n \times n$ matrix, we obtain a vanishing result

$$Tr(\dot{B}W) = tr_n \, \tilde{T}r(\dot{B}W) = 0 \tag{24}$$

$$0 = [W, H] = [\tilde{W}, \tilde{H}] \otimes \mathbb{H}$$
⁽²⁵⁾

and, thus

$$[\tilde{W}, \tilde{H}] = 0. \tag{26}$$

Following the derivation given in [8] we find for the asymptotic configuration

$$B|_{t=\infty} = b(\infty)(\delta_{ik}) \tag{27}$$

where $b(\infty)$ is now an $n \times n$ matrix which reads

$$b(\infty) = \frac{1}{(\tilde{\mathrm{Tr}}\,\tilde{W})} \left(\tilde{\mathrm{Tr}}(B|_{t=0}W) + \int_0^\infty (\mathbb{H}\,\tilde{\mathrm{Tr}}(\tilde{W}\tilde{H}B(t)) - \tilde{\mathrm{Tr}}(\tilde{W}B(t)\tilde{H})\mathbb{H})\,\mathrm{d}t \right).$$
(28)

We note the explicit appearance of a memory term. Calculating the expectation value of $B|_{t=\infty}$ in some state ρ_0 written as

$$\varrho_{(0)} = \left(\varrho_{ik}^{(0)}\right) \tag{29}$$

where the $\varrho_{ik}^{(0)}$ are $n \times n$ matrices, we find

$$\langle B|_{t=\infty} \rangle = \sum_{i} \operatorname{tr}_n \left(\varrho_{ii}^{(0)} b(\infty) \right) \tag{30}$$

and observe that now the asymptotic expectation value does depend on the initial state in concordance with the appearance of a memory term.

So we have seen that a simple and intuitively clear generalization of the Lindblad equation to an equation for dynamical degrees of freedom of subsystems leads to memory effects; the asymptotic subsystem variables given in equations (23) should be interpreted as the new dynamical subsystem variables obtained from an asymptotic averaging procedure over those degrees of freedom of the total system living on 'lower' scales; equations (23) are clearly seen as an elimination procedure for 'environment' variables separated into a statistical average and a memory term.

(C) We now turn to the case of more than one, say N, Lindblad operators. We take N finite with the provision of eventually letting $N \to \infty$ as certain physical models might require. The equation of motion then reads

$$\dot{B} = i[H, B] + \sum_{J} \left(V_{J}^{+} B V_{J} - \frac{1}{2} \left[V_{J}^{+} V_{J}, B \right]_{+} \right).$$
(31)

We rewrite this equation as an equation operating in a direct sum of identical spaces

$$\mathfrak{H}_N = \sum_{1 \to N} \oplus \mathfrak{H}$$
(32)

and define

$$B_N := B\mathbb{I}_N \tag{33}$$

$$H_N := H \mathbb{I}_N \tag{34}$$

$$V_N := \sqrt{N} (V_J \delta_{JK}) \tag{35}$$

to arrive at

$$\dot{B}_N = i[H_N, B_N] + V_N^+ B_N V_N - \frac{1}{2} [V_N^+ V_N, B_N]_+.$$
(36)

The polar decompositions

$$V_J = U_J \sqrt{V_J^+ V_J} \tag{37}$$

lead to the polar decomposition

$$V_N = U_N \sqrt{V_N^+ V_N} \tag{38}$$

where

$$U_N = (U_J \delta_{JK}) \tag{39}$$

is unitary. Employing the same procedure as above we have

$$\frac{1}{\sqrt{V_N^+ V_N}} \dot{B}_N \frac{1}{\sqrt{V_N^+ V_N}} = i \frac{1}{\sqrt{V_N^+ V_N}} [H_N, B_N] \frac{1}{\sqrt{V_N^+ V_N}} + U_N^+ B U_N - \frac{1}{2} \left(\sqrt{V_N^+ V_N} B_N \frac{1}{\sqrt{V_N^+ V_N}} + \frac{1}{\sqrt{V_N^+ V_N}} B_N \sqrt{V_N^+ V_N} \right).$$
(40)

Assuming either independence of W_J on J (U_J does depend on J in general) or, alternatively, V_J positive and in analogy with (6)

$$W_J := \frac{1}{V_J^+ V_J} = W_J(H, \ldots)$$
 (41)

and taking the total trace (tr_N pertains to the matrix indices of the $N \times N$ matrices introduced above, tr₅ to the operators on \mathfrak{H}) we find

$$\operatorname{tr}_{\mathfrak{H}}\operatorname{tr}_{N}(\dot{B}_{N}W_{N}) = 0 \tag{42}$$

and thus

$$\operatorname{tr}_{\mathfrak{H}}\left(\dot{B}\sum_{1\to N}W_{J}\right)=0\tag{43}$$

and

$$\langle B|_{t=\infty} \rangle = \frac{\operatorname{tr}_{\mathfrak{H}}(B|_{t=0}W)}{\operatorname{tr}_{\mathfrak{H}}(W)}$$
(44)

$$W = \sum_{J} W_{J}.$$
(45)

To illustrate this result we take V_J as positive and assume the following specific ansatz:

$$W_J (V^+ V)^J \qquad J = 1, 2, \dots$$
 (46)

and put

$$V = \exp\left(-\frac{\beta H}{2}\right). \tag{47}$$

The expectation value for B reaches asymptotically

$$\langle B|_{t=\infty} \rangle = \frac{1}{\bar{N}} \operatorname{tr}_{\mathfrak{H}} \left(\frac{B|_{t=0}}{\exp(\beta H) - 1} \right)$$
(48)

which is simply the expectation value of the 'particle' observable *B* in an ideal Bose 'gas' of, on average, \bar{N} 'particles' at inverse temperature β ; 'particle' is just a more intuitive name for the physical object dubbed 'system' up to now.

This interpretation deserves further clarifications. To this end we reformulate equation (40) as an equation in Fock space \mathfrak{H}_F , aiming at the Bose nature of the ideal gas to be introduced. We define

$$\mathfrak{H}_F := \sum_J \oplus \mathfrak{H}^{\otimes J} \tag{49}$$

and

$$V_F := \sum_J \oplus V^{\otimes J} \tag{50}$$

so that

$$W_F = V_F^+ V_F = \sum_J \oplus (V^+ V)^{\otimes J}.$$
(51)

In the product space $\mathfrak{H}^{\otimes J}$ we select as physically relevant states symmetric states which we take as superpositions of symmetric 'system' product states—we introduce many-'particle' boson states. The observable *B* is extended to a symmetrically operating operator

$$B_F = \sum_{J} \oplus (\dots \otimes \mathbb{I} \otimes B \otimes \dots)$$
(52)

where *B* stands consecutively on all positions of the *J*-fold product.

1

The expectation value at $t = \infty$ is, in strict analogy with (13) and (44)

$$\langle B_F|_{t=\infty} \rangle = \frac{\operatorname{tr}_{\mathfrak{H}_F}(B_F|_{t=0}W_F)}{\operatorname{tr}_{\mathfrak{H}_F}(W_F)}$$
(53)

where the trace is now to be calculated with a symmetric product basis in $\mathfrak{H}^{\otimes J}$ for all *J*. Computing this trace one encounters disconnected terms (matrix elements now pertain to \mathfrak{H})

$$\sum_{i_1,\dots,i_L} \langle i_1 | BV^J | i_1 \rangle \langle i_2 | V^J | i_2 \rangle \cdots \langle i_L | V^{J_k} | i_L \rangle$$
(54)

$$\sum_{l} J_{l} = J. \tag{55}$$

All these terms sum up to the same common factor in the numerator and denominator—the connected cluster theorem—so that we reproduce (48) with $W_J = (V^+V)^J$. We conclude that any symmetric quantum many-particle state composed of whatever complex quantum systems—a Bose many-particle state—is transported by Lindblad motion into an equilibrium ensemble with a probability distribution

$$W_{\rm Bose} = \frac{1}{W_{55} - 1} \tag{56}$$

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where

$$W_{\mathfrak{H}} = \frac{1}{V^+ V} \tag{57}$$

is an operator acting in the space of the system's states. This derivation is a first step towards a dissipative quantum field theory: the case of free fields, although we never explicitly introduced this concept. I shall return to the extension to more complicated cases in a forthcoming publication.

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