Exact density matrix of a discrete quantum system immersed in a thermal reservoir

A.J. van Wonderen and L.G. Suttorp*
Institute of Physics, University of Amsterdam,
Science Park 904, NL-1098 XH Amsterdam, The Netherlands

October 10, 2018

Abstract

Quantum dissipation is studied for a discrete system that linearly interacts with a reservoir of harmonic oscillators at thermal equilibrium. Initial correlations between system and reservoir are assumed to be absent. The dissipative dynamics as determined by the unitary evolution of system and reservoir is described by a Kraus map consisting of an infinite number of matrices. For all Laplace-transformed Kraus matrices exact solutions are constructed in terms of continued fractions that depend on the pair correlation functions of the reservoir.

1 Introduction

Recent years have witnessed a lot of research effort on non-Markovian dynamics of open quantum systems. Chruściński and Kossakowski [1], Semin and Petruccione [2], as well as Ferialdi [3] surmised that it might be very complicated to derive an exact non-Markovian master equation for the evolution of an open quantum system. In this manuscript we obtain an exact description of the non-Markovian evolution of an open quantum system. Rather than on a master equation, our description is based on a continued-fraction representation of the Kraus map for the density operator of the open quantum system.

In section 2 we derive a finite-temperature description of non-Markovian quantum dynamics on the basis of an infinite set of Kraus matrices [4]. Our starting-point is the dissipative map for the density operator that was obtained in [5]. Next, by embedding the set of Kraus matrices in a larger set of so-called matrix ratios and performing Laplace transformation, a closed hierarchy of nonlinear equations can be constructed, as has been shown in [6].

In section 3 we iterate the closed hierarchy for matrix ratios an arbitrary but finite number of times. Execution of this iteration happens in two steps, the first of which is carried out with relative ease. In contrast, the second step is technically most demanding. It provides us with a complicated expression for the matrix ratios in terms of matrix continued fractions.

The identity that is obtained in section 3 contains a matrix ratio of iterative order \( N \). In section 4 it is assumed that in the limit of \( N \rightarrow \infty \) this matrix ratio will be vanishing. By carrying out the limit of \( N \rightarrow \infty \) we thus obtain a continued-fraction solution for the matrix ratios in closed form. Since the Kraus matrices belong to the set of matrix ratios, we obtain the exact solution for the density operator of the open quantum system.

Throughout our paper the following assumptions are made: (i) the Hilbert space of the open quantum system is separable, i.e., it is spanned by a countable number of ket vectors; (ii) initial correlations between the open quantum system and the surrounding reservoir are absent, so that the initial composite density operator for system and reservoir factorizes; (iii) the reservoir consists of a continuum of harmonic oscillators that are initially at thermal equilibrium and that linearly interact with the system potentials.

*email: l.g.suttorp@uva.nl
In addition to the setting (i)-(iii), we furthermore assume that all of the infinite continued fractions occurring in this paper are convergent. We recall that the use of continued fractions in quantum optics goes back to early work on the Rabi model by Schwefel [7] and Swain [8].

In summary, our manuscript presents an alternative to master equations, namely an exact representation of the Kraus map for an open quantum system in terms of matrix continued fractions.

2 Kraus hierarchy

The evolution in time \( t \) of the density matrix \( \rho_S(t) \) of an open quantum system \( S \) with a discrete energy spectrum is governed by the map \[5\]

\[ \rho_S(t) = T e^{L(t)} \rho_S, \]

where \( \rho_S = \rho_S(t = 0) \) denotes the initial state of \( S \). The superoperator \( L \) is defined as

\[ L(t) \rho_S = K^{(+)}(t) \rho_S + \rho_S K^{(-)}(t) + \sum_{\alpha\beta} \int_0^t dv \int_0^t du \ c_{\beta\alpha}(v, u) V_\alpha(u) \rho_S V_\beta(v), \]

\[ K^{(\eta)}(t) = -\frac{1}{2} \sum_{\alpha\beta} \int_0^t dv \int_0^t du \ c_{\alpha\beta}^{(\eta)}(u, v) \eta \{V_\alpha(u)V_\beta(v)\}. \]

The prescription \( T \) orders products of system potentials \( \{V_\alpha(t)\}_\alpha \) according to

\[ T \left\{ \prod_{i=1}^m V_{\alpha_i}(t_{i_1}) \rho_S \prod_{j=1}^n V_{\alpha'_j}(t'_{j_1}) \right\} = T_+ \left\{ \prod_{i=1}^m V_{\alpha_i}(t_i) \right\} \rho_S T_- \left\{ \prod_{j=1}^n V_{\alpha'_j}(t'_{j}) \right\}, \]

\[ T_+ \left\{ \prod_{i=1}^m V_{\alpha_i}(t_i) \right\} = V_{\alpha_1}(t_1) \cdots V_{\alpha_m}(t_m), \]

\[ T_- \left\{ \prod_{j=1}^n V_{\alpha'_j}(t'_{j}) \right\} = V_{\alpha'_1}(t'_{1}) \cdots V_{\alpha'_n}(t'_{n}), \]

where the inequalities \( t_1 > \cdots > t_m \) and \( t'_1 > \cdots > t'_n \) are assumed. The dependence on time of the system potentials is determined by the unperturbed system Hamiltonian \( H_S \) as \( V_\alpha(t) = \exp(iH_st)V_\alpha \exp(-iH_st) \).

Since the system Hilbert space is spanned by a countable number of ket vectors, the interaction with the reservoir can be described by the Hamiltonian \( \sum_\alpha V_\alpha \otimes U_\alpha \). The dummy \( \alpha \) takes on a countable number of values. The reservoir is made up by a continuum of e.m. modes, so the set of potentials \( \{U_\alpha\} \) consists of ladder operators. If the reservoir is in a thermal state \( \rho_R \) at time zero, Wick’s theorem can be employed to express reservoir correlation functions of arbitrary order in terms of three pair correlation functions. These are given by

\[ c_{\alpha_1\alpha_2}(t_1, t_2) = \text{Tr}_R[U_{\alpha_1}(t_1)U_{\alpha_2}(t_2)\rho_R], \]

\[ c_{\alpha_1\alpha_2}^{(+)}(t_1, t_2) = c_{\alpha_1\alpha_2}(t_1, t_2) \theta(t_1 - t_2) + c_{\alpha_2\alpha_1}(t_2, t_1) \theta(t_2 - t_1), \]

\[ c_{\alpha_1\alpha_2}^{(-)}(t_1, t_2) = c_{\alpha_1\alpha_2}(t_1, t_2) \theta(t_2 - t_1) + c_{\alpha_2\alpha_1}(t_2, t_1) \theta(t_1 - t_2), \]

where \( \theta(t) \) is the Heaviside step function. It should be pointed out that \( 1 \) is valid if the initial state of system and reservoir can be written as \( \rho_{SR} = \rho_S \otimes \rho_R \), where \( \rho_R \) denotes a thermal state.

By working out \( 1 \) with the help of \( 3 \) one can expand the density matrix of \( S \) as

\[ \rho_S(t) = \sum_{q=0}^{\infty} \sum_{\alpha_1, \cdots, \alpha_q, \alpha'_1, \cdots, \alpha'_q} \int_0^t dt_1 \cdots \int_0^{t_{q-1}} dt_q \int_0^t dt'_1 \cdots \int_0^{t'_{q-1}} dt'_q. \]
We sum over all permutations $P$ and $Q$ of the integers \{1, \ldots, q\}. The Kraus matrices $\{W_q^{(\pm)}\}_{q \geq 0}$ satisfy the infinite hierarchy

$$W_0^{(+)}(t) = 1_S - \sum_{\alpha \beta} \int_0^t du \int_0^u dv \, c_{\alpha \beta}(u, v) \, V_\alpha(u) W_1^{(+)}(u; v)_\beta,$$

$$W_q^{(+)}(t; t_1, \ldots, t_q)_{\alpha_1 \cdots \alpha_q} = V_{\alpha_1}(t_1) W_{q-1}^{(+)}(t_1; t_2, \ldots, t_q)_{\alpha_2 \cdots \alpha_q}$$

$$- \sum_{j=1}^{q+1} \sum_{\alpha \beta} \int_{t_1}^t du \int_{t_{j-1}}^{t_j} dv \, c_{\alpha \beta}(u, v) V_\alpha(u) W_q^{(+)}(u; t_1, \ldots, t_{j-1}, v, t_j, \ldots, t_q)_{\alpha_1 \cdots \alpha_j \alpha_{j+1} \cdots \alpha_q},$$

with $t > t_1 > \cdots > t_q > 0$. In evaluating the boundaries of the integral over $v$ one has to choose $t_0 = u$ and $t_{q+1} = 0$. From the solution for $W_q^{(+)}$ and the symmetry relation

$$W_q^{(-)}(t; t_1, \ldots, t_q)_{\alpha_1 \cdots \alpha_q} = \left[ W_q^{(+)}(t; t_1, \ldots, t_q)_{\alpha_1 \cdots \alpha_q} \right]^\dagger$$

the solution for the Kraus matrices $W_q^{(-)}$ can be found. On the right-hand side of (7) the replacements $V_{\alpha_j} \rightarrow V_{\alpha_j}^\dagger$ must be made for $1 \leq j \leq q$, as indicated by the subscripts $\alpha_j^\dagger$.

The material presented in (11)-(7) constitutes a repetition of the treatment developed in (5). In this article, we shall solve the Kraus hierarchy (3). To that end, we represent the system potentials by means of the orthonormal basis of eigenkets $\{|k\rangle\}_{k \geq 1}$ of $H_S$, with eigenvalues $\{\omega_k\}_{k \geq 1}$. We thus make the transition

$$\alpha \rightarrow (kl), \quad V_\alpha(t) \rightarrow |k\rangle \langle l| \exp[i\omega(kl)t],$$

where the shorthand $\omega(kl) = \omega_k - \omega_l$ is used.

For matrix elements of $W_q^{(+)}$ the notation

$$\langle k | W_q^{(+)}(t; t_1, \ldots, t_q)_{(t_1 k_2) \cdots (t_q k_{q+1})} | l \rangle_{q+1} = W_q(t; t_1, \ldots, t_q)_{(k_1 k_2 \cdots k_{q+1}) (l_1 l_2 \cdots l_{q+1})}$$

will be introduced. Furthermore, the abbreviations

$$K_q^n = (k_{n+1} k_{n+2} \cdots k_q), \quad K_q = K_q^0, \quad T_q^n = t_{n+1}, t_{n+2}, \ldots, t_q, \quad T_q = T_q^0, \quad \delta_{k_1 \cdots k_s} = \prod_{s=1}^q \delta_{k_s l_s},$$

$$\int_0^t dt_1 \cdots \int_0^{t_{n+1}} dt_{n+2} \cdots \int_0^{t_{q-1}} dt_q, \quad Z_n^+ = z + z_1 + z_2 + \cdots + z_n$$

will be employed. Last, the Laplace transform

$$\hat{W}_q(z; Z_q)_{K_{q+1} L_{q+1}} = (-i)^{q+1} \int_0^\infty dt \int_0^t dt_q \, \exp[izt + iZ_q \cdot T_q] W_q(t; T_q)_{K_{q+1} L_{q+1}}$$

will be invoked, with $\text{Im} z > 0$ and $\text{Im} z_j > 0$ for $1 \leq j \leq q$. For $q = 0$ the integration over $T_q$ and the variable $Z_q$ must be omitted.

Transformation of the Kraus hierarchy (6) provides us with

$$\hat{W}_q(z - \omega_k; Z_q)_{K_{q+1} L_{q+1}} = \delta_{k_1 l_1} (z - \omega_k)^{-1} \hat{W}_{q-1}(z + z_1 - \omega_k)_{Z_q^1}^{K_{q+1} L_{q+1}}$$

(12)
\[
\sum_{j=1}^{q+1} \int_C \frac{dy}{2\pi i} (z - \omega_k)^{-1} \hat{c}(k, l)(m) (y) \hat{W}_{q+1} (z - y - \omega_k; Z_{j-1}, y, Z_{q+1}^{-1}) (kK_{j+1}) (L_{j-1} L_{q+1}^{-1}) ,
\]

where for \( q = 0 \) the convention \( \hat{W}_{-1} = 1 \) is in force. The transform \( \hat{f}(z) \) is given by \(-i \int_0^\infty d\exp[izt] f(t)\), with \( f \) any smooth function. The contour \( C \) is parametrized as \(-\infty < \Re y < \infty\), with \( \Im y \) fixed and \( \Im z > \Im y > 0\).

To get a clue about how \([12]\) must be solved we consider a simplified version, namely, \( \hat{W}_q = A\hat{W}_{q-1} + B\hat{W}_{q+1} \), with constant matrices \( A \) and \( B \). Since on the right-hand side the index \( q \) both increases and decreases, solution by direct iteration is rather awkward. However, the size of the iterative solution can be significantly reduced if the matrix ratio \( R_q = \hat{W}_q \hat{W}_{q-1}^{-1} \) is introduced. We then obtain the identity \( R_q = [1 - BR_{q+1}]^{-1} \), the iteration of which yields a matrix continued fraction. As continued fractions frequently occur in quantum mechanics, and more specifically quantum optics \([7]-[8]\), it seems that we have found a natural path for solving the Kraus hierarchy. Even more so because at zero temperature employment of the ratio \( R_q \) in \([12]\) reproduces the well-known and exact density matrix for decay of a two-level atom \([9]\).

At finite temperature, additional preparations have to be made in order to work with matrix ratios. We have to iterate \([12]\) so as to replace it by the more general hierarchy

\[
\hat{W}_q (z - \omega_k; Z_q) \hat{K}_{q+1} L_{q+1} = \delta_{KqLn} \prod_{s=1}^n (Z_{s+1}^{-1} - \omega_{ks}^{-1})^{-1} \hat{W}_{-n} (Z_n^{-1} - \omega_{k_{n+1}}; Z_q^n) \hat{K}_{q+1} L_{q+1}^{-1}
\]

\[
- \sum_{p=0}^{n-2} \sum_{j=p+2}^{q+1} \sum_{klm} \int_C \frac{dy}{2\pi i} \delta_{K_{p+1} L_{p+1}} \prod_{s=1}^{p+2} (Z_{s+1}^{-1} - \omega_{ks}^{-1})^{-1} \hat{c}(k_{p+2}) (l)(m) (y) \hat{W}_{q+p} (Z_{p+1}^{-1} - y - \omega_k; Z_{j-1}, y, Z_q^{-1}) (kK_{j+2} mK_{q+1}) (L_{p+1} L_{q+1}^{-1}) ,
\]

with the conditions \( q \geq 0 \) and \( 0 \leq n \leq q + 1 \). Now it can be recognized that a set of matrix ratios must be defined according to

\[
R_{q,n} (z; Z_q) \hat{K}_{q+1} L_{q+1} = \sum_{M_{q+1}} \hat{W}_q (z - \omega_k; Z_q) \hat{K}_{q+1} M_{q+1} \hat{W}_{-n} (Z_{q}^{-1} - \omega_{m_{n+1}}; Z_q^n) M_{q+1} L_{q+1}^{-1} ,
\]

for \( 0 \leq n \leq q + 1 \). On the right-hand side a matrix inverse is taken, so one has \( R_{q,0} = \delta_{K_{q+1} L_{q+1}} \).

On the left-hand side of \([13]\) the unit matrix appears upon multiplying from the right by \( \hat{W}_q^{-1} (z - \omega_k; Z_q) \hat{K}_{q+1} L_{q+1}^{-1} \). On the right-hand side we insert the identity \( I^{-1} I = 1 \) in order to get a closed set of equations in terms of matrix ratios. The intermediate matrix must be chosen as

\[
I (z; Z_q) \hat{K}_{q+1} L_{q+1} = \delta_{K_{q+1} L_{q+1}} \hat{W}_{q-j} (Z_{j+1}^{-1} - \omega_{k_{j+1}}; Z_q) \hat{K}_{q+1} L_{q+1}^{-1} .
\]

We then find

\[
R_{q,n}^{-1} (z; Z_q) \hat{K}_{q+1} L_{q+1} = \delta_{K_{q+1} L_{q+1}} \prod_{s=1}^n (Z_{s+1}^{-1} - \omega_{ks}^{-1}) + \sum_{p=0}^{n-2} \sum_{j=p+2}^{q+1} \sum_{klm} \int_C \frac{dy}{2\pi i} \delta_{K_{p+1} L_{p+1}} \prod_{s=1}^{p+2} (Z_{s+1}^{-1} - \omega_{ks}^{-1})^{-1} \hat{c}(k_{p+2}) (l)(m) (y) \hat{W}_{q+p} (Z_{p+1}^{-1} - y - \omega_k; Z_{j-1}, y, Z_q^{-1}) (kK_{j+2} mK_{q+1}) (L_{p+1} L_{q+1}^{-1}) ,
\]

with \( q \geq 0 \) and \( 0 \leq n \leq q + 1 \). The boundaries of the summations over \( p \) and \( j \) guarantee that both \( R_{q-p,j-p} \) and \( R_{q,j} \) satisfy the afore-mentioned conditions, so indeed we have a closed set in our hands. Its solution directly produces the Kraus matrices, in view of the property \( R_{q+1} (z; Z_q) \hat{K}_{q+1} L_{q+1} = \hat{W}_q (z - \omega_k; Z_q) \hat{K}_{q+1} L_{q+1}^{-1} \).
3 Continued fractions

In the previous section, we have replaced the Kraus hierarchy (6) by the closed set (16) for matrix ratios. Construction of the iterative solution of (16) goes in two steps: we start by eliminating $R^{-1}$ on the right-hand side of (16). Then, in the ensuing equation we perform a finite iteration in $R$.

From (16) we obtain an expression for $R_{q,jo}^{-1}(z; Z_q)_{m_{q+1}M_{q+2}}$ that is substituted on the right-hand side. Continuation of this process ad infinitum brings us to

\[
R_{q,jo}^{-1}(z; Z_q)_{K_{q+1},K_{q+2}} = \prod_{s=1}^{q+1} (Z_{s-1}^+ - \omega[s, 1]) \prod_{s=1}^{q+1} \delta(s, 1; s, 2)
\]

\[+ \sum_{h_1=1}^{\infty} \sum_{j_1=1}^{p_{(1)}} \cdots \sum_{j_q=1}^{p_{(q)}} \delta(s, m_1 + 2; s, m_1 + 3) \prod_{s=p(m_1)+3}^{j(m_1-1)} (Z_{s-1}^+ - \omega[s, m_1 + 2]) \prod_{m_1=1}^{j(m_1-1)} \left( K_{q,a} \right) \]

\[\times \left\{ \sum_{q=0}^{N} R_{q-p(m_1),j(m_1)-p(m_1)}(Z_{p(m_1)+1}^+ - z_q + m_1; Z_{j(m_1)-1}^+ - z_q + m_1; Z_{j(m_1)-1}^+ - z_q + m_1; \right\} \]

\[\left( L' L'' \right) \]  \( \text{(17)} \)

We used the following notations:

\[
K_{q,a} = (k_{1,a}k_{2,a} \cdots k_{q,a}) ,
\]

\[
\omega[a, b] = \omega_{k_{a,b}}, \quad \delta(a, b; c, d) = \delta_{k_{a,b}k_{c,d}} , \quad m(n) = m_n ,
\]

\[
\{a, b; c, d; e, f; g, h\}_{N} = \hat{c}_{(k_{a,b}k_{c,d})(k_{e,f}k_{g,h})}(z_q + m_{N+1}) .
\]

Furthermore, the indices $L'$ and $L''$ must be replaced by

\[
L' = k_{q+3,m_1+2}k_{p(m_1)+3,m_1+2} \cdots k_{j(m_1)-1,m_1+3}k_{q+4,m_1+3}k_{j(m_1)-1,m_1+3} \cdots k_{q+1,m_1+2} ,
\]

\[
L'' = k_{p(m_1)+2,m_1+3} \cdots k_{j(m_1)-1,m_1+3}k_{q+2,m_1+3}k_{j(m_1)-1,m_1+3} \cdots k_{q+1,m_1+3} .
\]

Identity (17) marks the completion of step one.

Step two is much harder and consists of performing for (17) a finite number of iterations in $R_{q,jo}$. In order to cast (17) into a form that indeed allows for iteration, we define a number of permutations. The permutations $C_{j, q}$ and $D_{N, q}$ are given by

\[
C_{j, q}(i) = \begin{cases} 
  i & \text{if } i \leq j - 1 , \\
  q + 1 & \text{if } i = j , \\
  i - 1 & \text{if } j + 1 \leq i \leq q + 1 , \\
  i & \text{if } q + 2 \leq i , 
\end{cases}
\]

\[
D_{N, q}(i) = \begin{cases} 
  i & \text{if } i \leq p_{m_N} + 2 , \\
  q + 3 & \text{if } i = p_{m_N} + 3 , \\
  i - 1 & \text{if } p_{m_N} + 4 \leq i \leq j_{m_N} + 1 , \\
  q + 4 & \text{if } i = j_{m_N} + 2 , \\
  i - 2 & \text{if } j_{m_N} + 3 \leq i \leq q + 4 , \\
  i & \text{if } q + 5 \leq i ,
\end{cases}
\]

with $N = 1, 2, 3, \ldots$. We furthermore define

\[
E_{N, q}(i) = C_{j(m(N)), q}(i) ,
\]

\( \text{(21)} \)
with \( N = 1, 2, 3, \ldots \). For \( N = 0 \) the definitions \( D_{0,q}(i) = i - 2 \) if \( 3 \le i \le q + 3 \) and \( E_{0,q}(i) = i - 1 \) if \( 2 \le i \le q + 2 \) will be employed. The permutation \( F_{N,q} \) must be constructed from

\[
F_{N,q}(i) = C_j(m(1),q+m(1)-1) (C_j(m(2))+1,q+m(2)+1) \cdots \left( \cdots C_j(m(N)) + N-1,q+m(N)-1(i) \cdots \right) .
\]

(22)

For \( N = 0 \) one has \( F_{0,q}(i) = i \) for all integers \( i \).

Furthermore, we introduce some rules for writing up long expressions in a concise manner. We shall make use of the following notation:

\[
\bar{n} = \bar{n} + N + 1, \quad \bar{m} = m + N + 1,
\]

\[
\bar{z}_{n,i} = z + \sum_{i=1}^{n} z_{F_{N,q}(i)} - \sum_{i=1}^{N} z_{q + m_i}, \quad \int_{N} = \int_{C} \left( \int_{C} \int_{C} \cdots \int_{C} \right) \frac{1}{(2\pi i)^{N+1-m_n}} d\bar{z}_{q+m+1} \cdots d\bar{z}_{q+m+n} \cdot
\]

\[
q' = q - p(m+n), \quad j' = j(m+n) - p(m+n), \quad \bar{z}' = \bar{z}_{p(m+n+1,n+1)} ;
\]

\[
K'' = (k_{D_{N+1,q},m+n+1+2} m(n+1)+4), m+n+1+2 \cdots k_{D_{N+1,q},q+3}, m+n+1+2) ;
\]

\[
K'' = (k_{E_{N+1,q},m+n+1+3} k_{E_{N+1,q},m+n+1+3} k_{E_{N+1,q},m+n+1+3} \cdots k_{E_{N+1,q},q+3}, m+n+1+3) ;
\]

\[
Z'' = z_{F_{N+1,q},m+n+1+2} z_{F_{N+1,q},m+n+1+2} \cdots z_{F_{N+1,q},q+3}, m+n+1+3) ,
\]

(23)

where the permutations \( D_{N,q}, E_{N,q}, \) and \( F_{N,q} \) are specified in \([20]–[22]\).

As a final abbreviation we introduce the symbol \( \sum_{N} \) to indicate a summation over integers \( h_{N+1}, \{ j_i, p_i \}_{m+n+1}^{h_{N+1}+1} \) and \( \{ k_{a,b} \}_{a=m+n+1}^{h_{N+1}+1} b=m_n+2 \), except for \( \{ k_{q+2}, m+n+2, k_{q+3}, h_{N+1+1}, k_{q+4}, h_{N+1+1} \} \), with boundaries given by

\[
m+n+1 \le h_{N+1} < \infty, \quad \{ p_{m+n} - 1 \le p_i \le j_i - 2, p_i + 2 \le j_i \le q + 1 \}^{h_{N+1}+1}_{n=m+n+1} .
\]

(24)

In the summation with horizontal bar each integer \( k_{a,b} \) runs over the same values as the label \( k \) of the eigenket \( |k \rangle \) of \( H_S \). It should be stressed that the prescriptions for sum and integral with horizontal bar should be transferred in facsimile to formulas that are completely written out. The only component that may be adapted is integer \( N \), which may take on any nonnegative value. Last, the special choices \( m_0 = p_0 = 0 \) are in force.

With the above instruments in hand we can shorten our continued fractions considerably. Instead of \([17]\) we may write

\[
R_{q,j_0}(z; q)_{K_{N+1},N+1,2} = A_0 + B_0 R_{q,j_0}(z; q)_{K_{N+1},N+1} K_{N+1}, K_{N+1},
\]

(25)

where the prescription for the new components reads

\[
A_N = \left[ \prod_{s=p(m+n)+3}^{q+3} \delta(D_{N,q}(s), m+n; E_{N,q+1}(s-1), m+n+1) \prod_{s=p(m+n)+3}^{q+3} (Z_{s+n+3,N} - \omega[D_{N,q}(s), m+n]) \right]
\]

\[
B_{N} = \sum_{N} \int_{N} \prod_{s=p(m+n)+3}^{q+3} \delta(D_{N,q}(s), m+n; s-2, m+n+2) \delta(s-2, h_{N+1}; E_{N,q+1}(s-1), m+n+1)
\]

\[
\times \left[ \prod_{s=p(m+n)+1}^{h_{N+1}} (Z_{s+n+1,N} - \omega[s, h_{N+1}+1]) \right]
\]

\[
\times \prod_{m+n+1}^{p(m+n)+1} \{ p_{m+n+1} + 2, m+n+1; q+3, m+n+1; q+2, m+n+1+1; q+4, m+n+1 \}
\]

\[
\times \prod_{s=p(m+n)+1}^{h_{N+1}} \delta(s, m+n+1; m+n+1) \prod_{s=p(m+n)+3}^{q+3} (Z_{s+n+3,N} - \omega[s, m+n+1]) \right] .
\]

(26)
Again, these components must be implemented in facsimile, the integer $N \geq 0$ being the only variable that may be modified.

Iteration of (25) gives

$$R_{q,j_0}(z; Z_q)_{K_{q+1}K_{q+1}} = \left\{ A_0 + B_0 \left\{ A_1 + B_1 \left\{ A_2 + \cdots \right\} \right\} \right\}_{N, -1} \right\} -1$$

with $N = 0, 1, 2, \ldots$. The superscript $-1$ of each right bracket indicates that a matrix inverse must be taken.

From (25) it follows that on the right-hand side of (25) a product over $m_1$ must be carried out. We stress that this product over $m_1$ pertains to the full expression $B_0R$, where indices and arguments of the matrix $R$ have been omitted. For the sum $\sum_{N=0}^{\infty}$ and integral $\frac{1}{N=0}$ figuring on the right-hand side of (25) the same remark applies. Consequently, iteration of (25) produces in (27) a most complicated analytic structure.

The proof of (27) is based on induction in $N$. Upon substituting the relation

$$R_{q_1,q_2}(z'; Z_{q_2})_{K_{q_1}K_{q_2}} = \left\{ A_{N+1} + B_{N+1}R_{q_1,q_2}K_{q_1}K_{q_2} \right\}_{N, -1}$$

into (27), we indeed reproduce (27) with the replacement $N \rightarrow N + 1$ made. Therefore, it is sufficient to verify that (25) holds true. This can be shown by carrying out a suitable set of consecutive transformations of the variables and labels in (17). Last, by choosing $N = -1$ in (28) we reproduce (25), as required. We thus have demonstrated that a finite iteration of (25) provides us with (27).

4 Density matrix

If the conditions $\text{Im}(z + z_1 + \cdots + z_j) > \gamma_j$ are fulfilled for $0 \leq j \leq q$, then all matrix ratios $R_{q,j_0}(z; Z_q)$ are analytic in $z$ and $z_1, z_2, \ldots, z_q$. Hence, it is reasonable to assume that the matrix continued fraction (27) converges for $N \rightarrow \infty$ as long as the inequalities $\text{Im}(z + z_1 + \cdots + z_j) > \gamma_j$ are satisfied for $0 \leq j \leq q$. The fixed numbers $\{\gamma_j\}_{j=0}^{q}$ depend on such parameters as the coupling constant for the interaction between system and thermal reservoir; in this work the set $\{\gamma_j\}_{j=0}^{q}$ will not be specified any further.

Convergence of (27) implies that we may set $R_{q_j,q_j}(z)$ equal to zero for large $N$ and the inequalities $\text{Im}(z + z_1 + \cdots + z_j) > \gamma_j$ true, with $0 \leq j \leq q$. The solution for the Kraus matrices is thus found as

$$\hat{W}_q(z - \omega_{k_1}; Z_q)_{K_{q+1}K_{q+1}} = R_{q_{q+1}}(z; Z_q)_{K_{q+1}K_{q+1}} =$$

$$\lim_{N \rightarrow \infty} \left\{ A_0 + B_0 \left\{ A_1 + B_1 \left\{ A_2 + \cdots + B_{N-1} \left\{ A_N \right\}_{N, -1} \right\}_{N, -1} \right\}_{N, -1} \right\}_{j_0=q+1}.$$  

The components $A_N$ and $B_N$, defined in (26), must be implemented in facsimile.

The solution for the Kraus operators being available, we can return to the density matrix as given by (5). In order to express (5) in terms of Laplace transforms throughout, we substitute the inverse of the transformation (11). Next, the Laplace representation of the correlation functions can be found with the help of the identity $c_{\alpha'\alpha}(t', t) = c_{\alpha'\alpha}(t' - t, 0)$ and the relations

$$c_{\alpha'\alpha}(t, 0) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dy \exp(-i\nu t) \hat{c}_{\alpha'\alpha}(y),$$

$$\hat{c}_{\alpha'\alpha}(y) = \hat{c}_{\alpha'\alpha,+}(y) + \hat{c}_{\alpha'\alpha,-}(y),$$

$$\hat{c}_{\alpha'\alpha}(y) = -i \int_{0}^{\infty} dt \exp(i\nu t) c_{\alpha'\alpha}(\eta t, 0),$$

\begin{equation}
\end{equation}
with $\eta = \pm 1$. Note that the difference $t' - t$ can become negative, so we do need the backward transform $\hat{c}_{\alpha'\alpha}(-y)$.

Once we have switched to Laplace representation, the temporal integrals of Eq. (5) become elementary. We must evaluate the repeated integral

$$J_q(t; Z_q) = (-i)^q \int_0^t \! dT_q \exp(iZ_q \cdot T_q),$$

with $q = 1, 2, 3, \ldots$. The answer reads

$$J_q(t; Z_q) = \sum_{p=0}^{q} (-1)^p \exp[i(Z_p^+ - z)t] \prod_{k=1}^{p} (Z_p^+ - Z_{k-1}^+)^{-1} \prod_{k=p+1}^{q} (Z_k^+ - Z_p^+)^{-1},$$

a result that can be proved by means of induction in $q$. Note that in Eq. (5) time arguments of correlation functions are paired in all possible ways by the permutations $P$ and $Q$ of the integers $\{1, 2, \ldots, q\}$. All of these pairings can be transferred to the Laplace variables via the identity

$$\sum_{j=1}^{q} z_j t_{P(j)} = \sum_{j=1}^{q} z_{P^{-1}(j)} t_j,$$

where of course $P$ may be replaced by $Q$.

With the foregoing technical preparations completed we can present the elements of the exact density matrix as

$$\langle k_1 | \rho_S(t) | k'_1 \rangle = \sum_{q=0}^{\infty} \sum_{PQ} \sum_{p=0}^{q} \frac{Q_{q+1}^1 L_{q+1}^1 K_{q+1}^1 L_{q+1}^1}{2\pi} \int_{C_0} \int_{C_1} \cdots \int_{C_q} \int_{C_0} \int_{C_1} \cdots \int_{C_q} \frac{dz_0}{2\pi} \frac{dz_1}{2\pi} \cdots \frac{dz_q}{2\pi} \exp[-iz_0 t + iz_0' t'] J_q(t; \{y_{p^{-1}(j)} - z_j\}_{j=1}^{q}) J_q(t; \{-y_{Q^{-1}(j)} + z'_j\}_{j=1}^{q})$$

$$\times \hat{W}_q(z_0; Z_q)_{K_{q+1}^1 L_{q+1}^1} \langle l_{q+1}^1 | \rho_S | l_{q+1}^1 \rangle [\hat{W}_q(z'_0; Z_q)_{L_{q+1}^1 K_{q+1}^1}]^\dagger$$

$$\times \frac{1}{q!} \prod_{j=1}^{q} \hat{c}_{(Q(j) + 1_{Q(j)})} (l_{P(j)} k_{P(j)} + 1) (y_j).$$

(34)

The contours $\{C_j, C^*_j\}_{j=0}^{q}$ run parallel to the real axis from $-\infty$ to $+\infty$, obeying the conditions $\text{Im}(z_0 + z_1 + \cdots + z_j) > \gamma_j$ and $\text{Im}(z'_0 + z'_1 + \cdots + z'_j) < -\gamma_j$ for $0 \leq j \leq q$. The set $\{\gamma_j\}_{j=0}^{q}$ is made up of fixed positive numbers. The adjoint Kraus operator must be found from

$$[\hat{W}_q(z_0^*; Z_q^*)_{L_{q+1}^1 K_{q+1}^1}]^\dagger = [\hat{W}_q(z_0^*; Z_q^*)_{L_{q+1}^1 K_{q+1}^1}]^\dagger.$$

(35)

For the Kraus operators one must substitute the solution (29) in terms of matrix continued fractions.

The result (34) can be seen as the solution of the time-ordering problem posed by (11). In its turn, the concise representation (11) relies on the possibility of factorizing reservoir correlation functions with the help of Wick’s theorem. A reservoir for which Wick’s theorem indeed holds true is given by a continuum of harmonic oscillators at temperature $\beta^{-1}$. For such a setting the reservoir potentials come out as

$$U_{(kl)} = \int_0^\infty \! d\omega \lambda(\omega)_{(kl)} a(\omega) + \int_0^\infty \! d\omega \lambda(\omega)_{(kl)} a^\dagger(\omega),$$

(36)

where $a(\omega)$ and $a^\dagger(\omega)$ are the ladder operators of the mode of frequency $\omega$. By $\lambda(\omega)_{(kl)}$ we denote the coupling constant for the transition $|l\rangle \rightarrow |k\rangle$ within $S$ as induced by the reservoir
mode of frequency \( \omega \). Starting from (36) and adopting the Laplace representation (30), we derive for the reservoir correlation functions the expressions

\[
\hat{c}_{(kl)(mn)}(y) = 2\pi i \int_0^\infty d\omega \lambda(\omega)_{(kl)} \lambda(\omega)_{(mn)}^* \left(e^{-\beta \omega} - 1\right)^{-1} \delta(y - \omega) \\
+ 2\pi i \int_0^\infty d\omega \lambda(\omega)_{(lk)} \lambda(\omega)_{(mn)} (1 - e^{\beta \omega})^{-1} \delta(y + \omega),
\]

with \( \delta(\omega) \) the Dirac delta function. Therefore, after insertion of (37) into (34) we can exchange the integrals over \( \{ y_j \}_{j=1}^q \) for integrals over mode frequencies.

5 Conclusion

In this work, we have obtained the Kraus map for the density operator of a quantum system that exchanges energy with a large reservoir. The assumptions on which our result relies have been described in the Introduction.

The Kraus matrices making up the Kraus map possess a most complex analytic structure, determined by matrix continued fractions of a very sophisticated form. Moreover, in order to compute the density operator of the open quantum system one must still carry out an infinite sum over the set of Kraus matrices. Therefore, one may seriously doubt the existence of an exact master equation for the density operator itself. This last judgment has also been put forward in the literature [1]–[3].

In summary, we conclude that the system-reservoir formalism provides us with a viable description of quantum dissipative processes as long as the coupling between system and reservoir is weak. In that case, the memory time of the reservoir is much shorter than the time scale on which the system evolves. Consequently, a perturbation theory can be set up in which Kraus matrices are factorized from a certain order onwards. For the perturbed density matrix of the system conservation of trace and positivity can be explicitly proved [6].

In contrast, if one refrains from making any approximations, then the dissipative evolution of the system must be found from (34). In view of the fact that the structure of this equation is extremely difficult, the system-reservoir approach seems to be unsuited if it comes to performing practical computations for a system that is strongly coupled to a reservoir.

References

[1] D. Chruściński and A. Kossakowski Phys. Rev. Lett. 111 (2013) 050402
[2] V. Semin and F. Petruccione EPL 113 (2016) 20004
[3] L. Ferialdi Phys. Rev. A 95 (2017) 020101
  L. Ferialdi Phys. Rev. A 95 (2017) 069908(E)
[4] K. Kraus Ann. Phys., NY 64 (1971) 311
[5] A.J. van Wonderen and L.G. Suttorp EPL 102 (2013) 60001
[6] A.J. van Wonderen and L.G. Suttorp J. Phys. A: Math. Theor. 51 (2018) 175304
[7] S. Schweber Ann. Phys., NY 41 (1967) 205
[8] S. Swain J. Phys. A: Math. Nucl. Gen. 6 (1973) 192
  S. Swain J. Phys. A: Math. Nucl. Gen. 6 (1973) 1919
[9] W.H. Louisell Quantum Statistical Properties of Radiation (Wiley, New York, 1973) p. 288, eq. (5.3.16)