Three approaches for representing Lindblad dynamics by a matrix-vector notation

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Abstract. Markovian dynamics of open quantum systems are described by the L-GKS equation, known also as the Lindblad equation. The equation is expressed by means of left and right matrix multiplications. This formulation hampers numerical implementations. Representing the dynamics by a matrix-vector notation overcomes this problem. We review three approaches to obtain such a representation. The methods are demonstrated for a driven two-level system subject to spontaneous emission.

1. Introduction

An open system is a system that interacts with its environment. A full description has to account for all the degrees of freedom (DOF) of the entire system and its environment. Usually, only the system DOF are of interest. A reduced description attempts to describe only the system DOF explicitly, while the environment DOF are integrated out and affect the description implicitly. The goal is to reduce the description to a small number of variables and obtain a practical way to treat the system [1, 2, 3].

Open systems are often described by a stochastic process which in many cases becomes a simple Markov process. In brief, a Markov process is a stochastic process with a short time memory, i.e., the process state depends solely on the present state. Mathematically it can be constructed as the Chapman-Kolmogorov equation for the conditional joint probability [3]. For a Markov process the probability distribution $p_t(x)$ on a certain space, either real-space or phase-space, which could be continuous or discrete, follows the differential equation

$$\frac{d}{dt}p_t(x) = \mathcal{L}p_t(x),$$

(1)

The formal solution for Eq. (1) is given by,

$$p_t(x) = \Lambda_t p(x), \quad \Lambda_t = e^{\mathcal{L}t}, \quad t \geq 0,$$

(2)

where, without loss of generality, we define the initial time to be zero. The one-parameter family of maps $\{\Lambda_t, t \geq 0\}$ is a semigroup with the generator $\mathcal{L}$. The term semigroup implies that this family of maps does not form a full group. It lacks the negative range of
the parameter \( t \), which implies that the inverse property required by a group is missing. Physically, this property is the manifestation of irreversible dynamics which allows us to distinguish the future from the past. The map \( \Lambda_t \) is a positive map that satisfies the composition rule (Markov property) \( \Lambda_{t+s} = \Lambda_t \Lambda_s \quad t, s \geq 0 \), and preserves normalization of the probability density.

In the quantum scenario several modifications have to be made. The probability distribution \( p_t(x) \) is replaced by the density matrix \( \hat{\rho}(t) \). The property of positivity has to be strengthened to complete positivity. The dynamics follows the quantum master equation:

\[
\frac{d}{dt} \hat{\rho}(t) = \mathcal{L} \hat{\rho}(t). \tag{3}
\]

This is a direct consequence of the presence of entangled states \( \| \). To summarize, the quantum dynamical semigroup is a continuous one-parameter family of maps \( \{ \Lambda_t, t \geq 0 \} \), that satisfies \( [5] \):

(i) \( \Lambda_t \) is complete positive;
(ii) \( \Lambda_t \) is trace preserving;
(iii) \( \Lambda_{t+s} = \Lambda_t \Lambda_s \quad t, s \geq 0 \) semigroup (Markov) property;
(iv) \( \Lambda_t \) is strongly continuous.

Lindblad as well as Gorini, Kossakowski and Sudarshan (L-GKS) introduced the most general form of the quantum dynamical semigroup generator \( \mathcal{L} \) that satisfies these requirements \([6, 7]\). In the Lindblad form the Markovian master equation reads:

\[
\frac{d}{dt} \hat{\rho}(t) = \mathcal{L} \hat{\rho}(t) = -\frac{i}{\hbar} \left[ \hat{H}, \hat{\rho} \right] + \sum \gamma_i \left( \hat{A}_i \hat{\rho} \hat{A}_i^\dagger - \frac{1}{2} \{ \hat{A}_i^\dagger \hat{A}_i, \hat{\rho} \} \right) \equiv \mathcal{L}_H(\hat{\rho}) + \mathcal{L}_D(\hat{\rho}). \tag{4}
\]

Here, \( \hat{H} \) is the effective Hamiltonian of the system, \( \gamma_i \) are positive rates, and \( \{ \hat{A}_i \} \) are operators belonging to the Hilbert space of the system. We use the notation \( \mathcal{L}_H \) to represent the unitary part of the dynamics, and \( \mathcal{L}_D \) to represent the dissipative part. \( \mathcal{L}, \mathcal{L}_H \) and \( \mathcal{L}_D \) are linear operators that operate on the density matrix, usually referred to as super-operators.

The operation of the super-operator \( \Lambda_t = e^{\mathcal{L}t} \) on the density matrix could be understood as repetitive operations of the super-operator \( \mathcal{L} \) as in the Taylor expansion:

\[
e^{\mathcal{L}t} \hat{\rho} \equiv \sum_k \frac{1}{k!} \mathcal{L}^k \hat{\rho}^k = \hat{\rho} + \mathcal{L} \hat{\rho} t + \frac{1}{2} \mathcal{L}^2 \hat{\rho} t^2 + \ldots \tag{5}
\]

Typically, the resulting dynamics of the system observables (expectation values and other correlation functions) \( c(t) \) will have the analytical form of sum of decaying oscillations\( \|^\):

\[
c(t) = \sum_m d_m e^{\lambda_m t}, \tag{6}
\]

\( ^\dagger \) There are special cases where the super-operator is not diagonalizable. In such cases, known as exceptional points, the exponential \( e^{\lambda t} \) is multiplied by a polynomial of \( t \). A study of exceptional points in L-GKS system can be found in Refs \([8, 9]\).
Three approaches for representing Lindblad dynamics by a matrix-vector notation

Here, $\lambda_m$ are the exponential coefficients and $d_m$ are the associated amplitudes, both can be complex. We may divide $\lambda_m$ into its real and imaginary parts, $\lambda_m = -\alpha_m + i\omega_m$, with $\alpha_m \geq 0 \in \mathbb{R}$ as the decay rates and $\omega_m \in \mathbb{R}$ as the oscillation frequencies. The coefficients $\lambda_m$ are the eigenvalues of the super-operator $L$, obtained by the eigenvalue equation:

$$L\hat{\sigma}_m = \lambda_m \hat{\sigma}_m.$$  \hspace{1cm} (7)

These eigenvalues can be used for the analysis of the L-GKS dynamics.

As noted above, the dynamics can be investigated by exponentiation of the super-operator $L$, Eq. (5), or by its eigenvalues, Eq. (7). The exponentiation and the eigenvalue problem of the (linear) super-operator $L$ are well defined. However, they are not suitable for numerical calculations. Calculations of the exponentiation and the eigenvalue equation of linear operators can be done by common numerical techniques if the linear operator is represented by a matrix. Therefore, a preferred representation of the dynamics, Eq. (4), is in a matrix-vector notation. This means that we are looking for a matrix $L$ and a vector $\vec{r}_s$ such that the dynamics are expressed as

$$\frac{d}{dt}\vec{r}_s = L\vec{r}_s.$$  \hspace{1cm} (8)

In this representation, the vector $\vec{r}_s$ represents the state of the system, or some information about it, e.g. a set of expectation values. Next, we describe three approaches for such a representation, and demonstrate them for a case of a driven two-level system with relaxation.

2. Matrix-vector representations

Suppose the density matrix $\hat{\rho}$ is an $n \times n$ matrix (if $\hat{\rho}$ is a function of continuous variables, e.g. $\hat{\rho}(r, r')$, these variables have to be discretized). The set of all $n \times n$ matrices form a linear space of dimension $n^2$. Under appropriate conditions, this linear space can have a Hilbert space construction, using the scalar product defined as

$$\langle \hat{\rho}_1, \hat{\rho}_2 \rangle = \text{Tr}\left\{\hat{\rho}_1^{\dagger}\hat{\rho}_2\right\}.$$  

Such a Hilbert space is called a Liouville space (also known as the Hilbert-Schmidt space). With such a construction we consider $\hat{\rho}$ as an $n^2$ vector. Similarly, we consider the super-operator $L$, which is an operator operating on elements in this linear space, as an $n^2 \times n^2$ matrix.

The above observation is the first step towards the representation we seek. In the following, we describe three approaches that use this concept to introduce such representation:

(i) **Vec-ing the density matrix** is the most natural way to construct an $n^2$ vector for the density matrix, and a suitable $n^2 \times n^2$ matrix for the super-operator.

(ii) **The Arnoldi method** approximates a large matrix in smaller dimensions, enabling simpler numerical calculations.
With the *Heisenberg picture* of the L-GKS equation we can search for a representation with a dimension smaller than \( n^2 \).

In the following, we describe these three approaches. Each of these approaches will be demonstrated in the case of the two-level system.

### 2.1. Vec-ing the density matrix

In this method, known as vec-ing \([10, 11, \text{Chapter 4}]\), the \( n \times n \) density matrix \( \hat{\rho} \) is flattened into an \( n^2 \) vector \( \vec{r} \). This flattening is done by ordering the columns of \( \hat{\rho} \) one below the other, so the \((a, b)\) entry of the matrix \( \hat{\rho} \) is the \((b - 1)n + a\) entry of the vector \( \vec{r} \). This is equivalent to choosing the representation basis as the set of matrices with all-zero entries, except one.

The next task is to find the suitable matrix that will represent the operation of the super-operator \( L \) on the density matrix. We make the following observations \([10, 11]\):  

(i) A left multiplication of the matrix \( \hat{\rho} \) by an \( n \times n \) matrix \( A \), i.e. \( A\hat{\rho} \), is equivalent to an operation on the vector \( \vec{r} \) by the \( n^2 \times n^2 \) matrix \( I \otimes A \), where \( I \) is the \( n \times n \) identity matrix, and \( \otimes \) is the Kronecker direct product.

(ii) Similarly, a right multiplication of the matrix \( \hat{\rho} \) by an \( n \times n \) matrix \( B \), i.e. \( \hat{\rho}B \), is equivalent to an operation on the vector \( \vec{r} \) by the \( n^2 \times n^2 \) matrix \( B^T \otimes I \). Here \( T \) denotes the transpose of the matrix.

(iii) Finally, a combination of left and right matrices multiplication, \( A\hat{\rho}B \), is equivalent to an operation on the vector \( \vec{r} \) by the \( n^2 \times n^2 \) matrix \( B^T \otimes A \).

The L-GKS super-operator is a sum of such right and left multiplications. Therefore, the construction of the \( n^2 \times n^2 \) matrix representation for the L-GKS generator has the parts as follows; for the commutator:

\[
\left[ \hat{H}, \hat{\rho} \right] \rightarrow \left( I \otimes \hat{H} - \hat{H}^T \otimes I \right) \vec{r}.
\]

For the dissipative part:

\[
\hat{A}_i \hat{\rho} \hat{A}_i^\dagger \rightarrow \left( \left( \hat{A}_i^\dagger \right)^T \otimes \hat{A}_i \right) \vec{r},
\]

\[
\hat{A}_i^\dagger \hat{A}_i \hat{\rho} \rightarrow \left( I \otimes \hat{A}_i^\dagger \hat{A}_i \right) \vec{r},
\]

\[
\hat{\rho} \hat{A}_i^\dagger \hat{A}_i \rightarrow \left( \left( \hat{A}_i^\dagger \hat{A}_i \right)^T \otimes I \right) \vec{r}.
\]

Then we write

\[
L = I \otimes \hat{H} - \hat{H}^T \otimes I + \sum_i \gamma_i \left( \left( \hat{A}_i^\dagger \right)^T \otimes \hat{A}_i - \frac{1}{2} \left( I \otimes \hat{A}_i^\dagger \hat{A}_i + \left( \hat{A}_i^\dagger \hat{A}_i \right)^T \otimes I \right) \right),
\]

and represent Eq. (4) as

\[
\frac{d}{dt} \vec{r} = L \vec{r}
\]

as desired.
The mapping of the density matrix into a density vector yields in a dramatic increment in the dimension of the problem, which becomes \( n^2 \) instead of \( n \). This yields unfavorable scaling of the desired computations with \( n \):

- **Eigenvalue approach.** Computation of the complete eigenvalue spectrum of \( L \) is performed via the diagonalization of \( L \). Diagonalization of a matrix scales as the cube of its dimension. Hence, the diagonalization of \( L \) scales as \( n^6 \).

- **Exponentiation methods.** The exponentiation of the matrix for time propagation, \( e^{Lt} \), can be computed via various ways \[12\]. Remarkably, two branches are of interest:
  
  (i) Directly employing the diagonalization of \( L \).
  
  (ii) By numerical approximations, which usually involve matrix-matrix multiplications.

Both diagonalization and matrix-matrix multiplications scale as the cube of the matrix dimension. Therefore, the overall scaling of the exponentiation is also \( n^6 \).

The calculation cost of the operation of the exponential \( e^{Lt} \) on an initial vector \( \vec{r}_0 \), i.e. \( e^{Lt}\vec{r}_0 \), can be reduced by employing matrix-vector multiplications, and therefore scales as \( n^4 \) \[13\].

For systems larger than a few degrees of freedom, such computations are expensive, and become practically impossible for systems larger than a few hundreds DOF.

The scaling problem suggests that we have to look for approaches that use a smaller number of dimensions. The following two approaches address this issue. The Arnoldi method uses a small-dimension approximation of a large matrix. The operator representation seeks for a small subset of variables that are sufficient to describe the quantities of interest. These two approaches are described in the next two sections.

**Remark:** The density matrix \( \hat{\rho} \) is hermitian. Therefore there are only \( n(n+1)/2 \) unique entries and not \( n^2 \). This fact can be used to reduce the size of the vectors and matrices, known as a half-vectorization \[14\] Chapter 11]. However, we will not discuss this here.

### 2.2. Arnoldi method

The Arnoldi method is a method to approximate a large matrix \( A \) in a smaller dimension \[15\]. This is done by choosing an appropriate set of a small number of vectors, which should be representative of the relevant subspace for a specific problem. Then the desired matrix is represented in the reduced subspace which is spanned by the chosen vectors. The method starts with an initial vector \( \vec{v} \) and creates set of \( K + 1 \) vectors by the repetitive operation of the matrix \( A \): \( \{\vec{v}, A\vec{v}, A^2\vec{v}, \ldots, A^K\vec{v}\} \). Then an orthonormal set is generated from this set by the Gram-Schmidt process. This orthonormal vectors set spans a subspace with dimension \( K + 1 \), and the matrix \( A \) is represented in this subspace by a \((K+1) \times (K+1)\) matrix. This smaller matrix can be used for the efficient evaluation of functions of the matrix \( A \), e.g. the exponential \[16\] or the eigenvalues \[17\].
In our case we try to approximate the linear super-operator $L$ by a matrix which is smaller than $n^2 \times n^2$. Conceptually, we start with the initial density matrix $\hat{\rho}_0 \equiv \hat{\rho}_s(0)$, and operate $K$ times with $L$ to get the set $\{\hat{\rho}_0, L\hat{\rho}_0, L^2\hat{\rho}_0, \ldots, L^K\hat{\rho}_0\}$ which is the starting point for orthogonalization and $(K + 1) \times (K + 1)$-dimension matrix representation of $L$. We note that the operation of $L$ involves $n \times n$ matrix-matrix multiplications, which scales as $n^3$. Therefore, it is more efficient to use the operation of $L$ for the procedure than to use the vec-ing matrix $L$ (Eq. (9)) described in Sec. 2.1 above.

The actual procedure follows, adapted to the notation of a super-operator and density matrices:

(i) Begin with the normalized density matrix $\hat{\rho}_0$.

(ii) for $j = 0$ to $K$

(a) Compute a non-orthonormalized new density matrix by setting: $\hat{\rho}_{j+1} := L\hat{\rho}_j$

(b) for $i = 0$ to $j$

1. Set: $L_{i,j} := \langle \hat{\rho}_i^\dagger, \hat{\rho}_{j+1} \rangle = \text{Tr}\left\{\hat{\rho}_i^\dagger L\hat{\rho}_{j+1}\right\}$
2. Subtract the projection on $\hat{\rho}_i$: $\hat{\rho}_{j+1} := \hat{\rho}_{j+1} - L_{i,j}\hat{\rho}_i$

(c) end for

(d) Set: $L_{j+1,j} := \|\hat{\rho}_{j+1}\| \equiv \sqrt{\text{Tr}\left\{\hat{\rho}_{j+1}^\dagger \hat{\rho}_{j+1}\right\}}$

(e) Normalize $\hat{\rho}_{j+1}$ by setting $\hat{\rho}_{j+1} := \frac{\hat{\rho}_{j+1}}{L_{j+1,j}}$

(iii) end for

The procedure yields

$$L_{i,j} = \text{Tr}\left\{\hat{\rho}_i^\dagger L\hat{\rho}_j\right\} \quad i \leq j + 1$$

For $i > j + 1$, the expression in the RHS vanishes. Thus, we can define a $(K+1) \times (K+1)$ matrix which its general element is given by a matrix element of $L$ in the Liouville space:

$$L_{i,j} = \text{Tr}\left\{\hat{\rho}_i^\dagger L\hat{\rho}_j\right\}$$

(Note that the procedure also yields $\hat{\rho}_{K+1}$ and $L_{K+1,K}$ which are not necessary for our purposes). $L$ represents the operation of the super-operator $L$ on the subspace that is spanned by the density matrices $\{\hat{\rho}_0, \hat{\rho}_1, \hat{\rho}_2, \ldots, \hat{\rho}_K\}$. The matrix $L$ is referred to as the Hessenberg matrix of $L$. The density matrix has to be approximated by its projection on the subspace: $\hat{\rho} \approx r_0\hat{\rho}_0 + r_1\hat{\rho}_1 + r_2\hat{\rho}_2 + \ldots + r_K\hat{\rho}_K$. The vector

$$\vec{r} \equiv (r_0, r_1, r_2, \ldots, r_K)^T$$

is the representation of the density matrix in this subspace. The dynamics of the vector $\vec{r}$ is generated by the matrix $L$ that was constructed in step (2) of the above procedure:

$$\frac{d}{dt}\vec{r} = L\vec{r}.$$
The Arnoldi algorithm usually becomes problematic when a large dimension approximation is required, i.e. when $K$ is large. In such a case, a restarted Arnoldi algorithm should be used instead (see, for example, [18]). This topic is beyond the scope of this paper.

### 2.3. The Heisenberg representation

Not always the full state of the system will be of concern. In most cases we will be interested only in the expectation values of some measured quantities. This fact can reduce significantly the dimensions of the problem. For example, in the standard thermalizing master equation the population and the coherences are decoupled, and the population of a certain level is given by solving a single differential equation [19]. The full state of the system can be reconstructed by calculating all the expectation values of the Lie algebra of the system. Generally, a full reconstruction of the state will scale as the Vec-ing of the density matrix introduced in Sec. 2.1. Nevertheless, in many cases we can use symmetries to reduce the dimensions of the problem. For example, if the initial state of harmonic oscillator is a Gaussian state, then it will stay Gaussian along the dynamics and only the first two moments are necessary to retrieve the full state [20]. Another example is coupled two qubits in which the full dimension of the system is 16, but only 3 operators are sufficient to define the energy and coherence of the system [21].

To describe the dynamics of the expectation values, it is common to use the master equation in the Heisenberg representation. The operator $\hat{X}$ belonging to dual Hilbert space of the system follows the dynamics [4, 19]:

$$\hat{X}(t) = e^{\mathcal{L}^\dagger t} \hat{X}(0),$$

which in its differential form is written explicitly as

$$\frac{d}{dt}\hat{X} = \mathcal{L}^\dagger \hat{X} \equiv \frac{i}{\hbar} \left[\hat{H}, \hat{X}\right] + \sum_i \gamma_i \left(\hat{A}_i^\dagger \hat{X} \hat{A}_i - \frac{1}{2} \left\{\hat{A}_i^\dagger, \hat{A}_i, \hat{X}\right\}\right).$$

If there is a a set of operators $\{\hat{X}_k\}_{k=1}^M$, $M < n^2$, that forms a closed set under the operation of $\mathcal{L}^\dagger$, meaning

$$\mathcal{L}^\dagger \hat{X}_k = \sum_{j=1}^M l_{kj} \hat{X}_j$$

then we can write a closed linear system of coupled differential equations. The expectation values $x_k \equiv \langle \hat{X}_k \rangle$ will have the corresponding set of coupled differential equations. The analytical form of their dynamics will follow the form of Eq. (6). We define the vector of expectation values $\vec{R} \equiv (x_1, x_2, \ldots)^T$. This system can be represented in a matrix-vector notation,

$$\frac{d}{dt} \vec{R} = \mathcal{L}^\dagger \vec{R},$$

where the matrix $\mathcal{L}^\dagger$ is defined by the equation set Eq. (13), $(\mathcal{L}^\dagger)_{kj} = l_{kj}$. The dimension of this matrix is $M^2$. Note that eigenvalues of the matrix $\mathcal{L}^\dagger$ are complex conjugates of a subset of the eigenvalues of the super-operator $\mathcal{L}$ of Eq. (1).
3. Example: The two-level system master equation

3.1. The model

As an example, we consider a driven two-level system (TLS) with spontaneous emission [22, 23].

We use the following definitions:

\[
\hat{S}_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.
\]

In addition:

\[
\hat{S}_+ \equiv \hat{S}_x + i\hat{S}_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{S}_- \equiv \hat{S}_x - i\hat{S}_y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.
\]

The commutation relations are:

\[
[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk}\hat{S}_k,
\]

where \(\epsilon_{ijk}\) is the Levi-Civita symbol, defined as:

\[
\epsilon_{ijk} = \begin{cases} +1 & \text{if } ijk \text{ is cyclic permutation of } xyz \\ -1 & \text{if } ijk \text{ is anti-cyclic permutation of } xyz \\ 0 & \text{if } i = j \text{ or } j = k \text{ or } k = i. \end{cases}
\]

The system Hamiltonian is

\[
\hat{H}_S = \omega_s\hat{S}_z,
\]

with \(\omega_s\) as the system transition frequency. The system is driven by the external field \(f(t) = \varepsilon e^{-i\omega_L t}\), with the carrier frequency \(\omega_L\) and amplitude \(\varepsilon\). The coupling to the driving field is expressed by the matrix

\[
\hat{V} = \begin{pmatrix} 0 & f(t) \\ f^*(t) & 0 \end{pmatrix}.
\]

In order to work within a time-independent Hamiltonian, we move to an interaction picture according to \(\omega_L\hat{S}_z\), obtaining

\[
\hat{H} = \Delta\hat{S}_z + \varepsilon\hat{S}_x,
\]

where \(\Delta \equiv \omega_s - \omega_L\) is the detuning between the system and the field frequencies.

The spontaneous emission is expressed by a dissipative term, and the L-GKS master equation takes the form [22, 23]:

\[
\frac{d}{dt}\hat{\rho}_S = -i\left[\hat{H}, \hat{\rho}_S\right] + \gamma \left(\hat{S}_-\hat{\rho}_S\hat{S}_+ - \frac{1}{2}\left\{\hat{S}_+\hat{S}_-, \hat{\rho}_S\right\}\right),
\]

where \(\gamma\) is the spontaneous emission rate.
3.2. Matrix-vector representation of the TLS dynamics

In the following we will implement the different approaches discussed above, for the relaxed driven TLS.

3.2.1. Vec-ing the density matrix

We use the procedure presented in Sec. (2.1) for the L-GKS of the two-level system with relaxation, Eq. (14).

The basis for the representation is the trivial set of matrices:
\[ \left\{ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\}. \]

To represent the commutator as a \( n^2 \times n^2 \) matrix, we use the procedure to get:
\[
-i \Delta \left( I \otimes \hat{S}_z - \hat{S}_z^T \otimes I \right) = -i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Delta & 0 & 0 \\ 0 & 0 & -\Delta & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\]
\[
-i \epsilon \left( I \otimes \hat{S}_x - \hat{S}_x^T \otimes I \right) = -\frac{i}{2} \begin{pmatrix} 0 & \epsilon & -\epsilon & 0 \\ \epsilon & 0 & 0 & -\epsilon \\ -\epsilon & 0 & 0 & \epsilon \\ 0 & -\epsilon & \epsilon & 0 \end{pmatrix}.
\]

For the dissipator we have:
\[
\gamma \left( \hat{S}_+^T \otimes \hat{S}_- \right) - \frac{\gamma}{2} \left( I \otimes \left( \hat{S}_+ \hat{S}_- \right) + (\hat{S}_+ \hat{S}_-)^T \otimes I \right) = \gamma \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \]

We combine all parts to get:
\[
L = \begin{pmatrix} -\gamma & -i \frac{\epsilon}{2} & i \frac{\epsilon}{2} & 0 \\ -i \frac{\epsilon}{2} & - \frac{1}{2} \gamma - i \Delta & 0 & i \frac{\epsilon}{2} \\ i \frac{\epsilon}{2} & 0 & -\frac{1}{2} \gamma + i \Delta & -i \frac{\epsilon}{2} \\ \gamma & i \frac{\epsilon}{2} & -i \frac{\epsilon}{2} & 0 \end{pmatrix}. \tag{15}
\]

3.2.2. Arnoldi method

The Arnoldi method that was presented in Sec. 2.2 and we use it here to find a representation of the two-level system super-operator. Note that generally the Arnoldi method is used for the approximation of large matrices. Here we have a small-size problem \((n^2 = 4)\), and we create an exact matrix, which represents the two-level system super-operator on a basis that spans the entire space.

We start with an initial density matrix \( \rho_0 \) (chosen arbitrary):
\[
\rho_0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \]
Then we follow the Arnoldi iteration procedure to get the basis \( \{ \hat{\rho}_0, \hat{\rho}_1, \hat{\rho}_2, \hat{\rho}_3 \} \):
\[
\left\{ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \frac{1}{\Omega} \begin{pmatrix} \varepsilon & \Delta \\ \Delta & 0 \end{pmatrix}, \frac{1}{\sqrt{2}\Omega} \begin{pmatrix} -2\Delta & \varepsilon \\ \varepsilon & 0 \end{pmatrix} \right\},
\]
with the definition: \( \Omega = \sqrt{2\Delta^2 + \varepsilon^2} \). This implies that the initial vector in this basis is \( \vec{r}(0) = (1, 0, 0, 0)^T \).

The representation of the super-operator \( L \) in this basis is the matrix obtained by the procedure:
\[
L = \begin{pmatrix}
\frac{\varepsilon}{\sqrt{2}} & -\frac{\varepsilon\gamma}{\Omega} & -\frac{\sqrt{2}\gamma\Delta}{\Omega} & 0 \\
\frac{\varepsilon}{\sqrt{2}} & -\frac{\varepsilon\gamma}{\Omega} & -\frac{\sqrt{2}\gamma\Delta}{\Omega} & 0 \\
0 & -\frac{\gamma}{\sqrt{2}} & \frac{\gamma\Delta^2 + \varepsilon^2}{\Omega} & \frac{\gamma\varepsilon}{\sqrt{2}\Omega} \\
0 & 0 & \frac{\varepsilon\Delta}{\sqrt{2}\Omega} & \frac{\varepsilon^2}{\Omega} - \gamma
\end{pmatrix}.
\]

3.2.3. The Heisenberg representation
For the system described above, the L-GKS equation in the Heisenberg picture is:
\[
\frac{d}{dt} \hat{X} = i \left[ \hat{H}, \hat{X} \right] + \gamma \left( \hat{S}_+ \hat{X} \hat{S}_- - \frac{1}{2} \left\{ \hat{S}_+ \hat{S}_-, \hat{X} \right\} \right).
\]
As a set of basis operators we choose the set:
\[
\left\{ \hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{I} \right\}.
\]
The L-GKS equation for the operators of the basis gives:
\[
\begin{align*}
\frac{d}{dt} \hat{S}_x &= i \left[ \hat{H}, \hat{S}_x \right] + \gamma \left( \hat{S}_+ \hat{S}_x \hat{S}_- - \frac{1}{2} \left\{ \hat{S}_+ \hat{S}_-, \hat{S}_x \right\} \right) \\
&= -\Delta \hat{S}_y - \frac{1}{2} \gamma \hat{S}_x,
\end{align*}
\[
\begin{align*}
\frac{d}{dt} \hat{S}_y &= i \left[ \hat{H}, \hat{S}_y \right] + \gamma \left( \hat{S}_+ \hat{S}_y \hat{S}_- - \frac{1}{2} \left\{ \hat{S}_+ \hat{S}_-, \hat{S}_y \right\} \right) \\
&= \Delta \hat{S}_y - \varepsilon \hat{S}_z - \frac{1}{2} \gamma \hat{S}_y,
\end{align*}
\[
\begin{align*}
\frac{d}{dt} \hat{S}_z &= i \left[ \hat{H}, \hat{S}_z \right] + \gamma \left( \hat{S}_+ \hat{S}_z \hat{S}_- - \frac{1}{2} \left\{ \hat{S}_+ \hat{S}_-, \hat{S}_z \right\} \right) \\
&= \varepsilon \hat{S}_y - \gamma \hat{S}_z - \frac{1}{2} \gamma \hat{I},
\end{align*}
\]
and, of course:
\[
\frac{d}{dt} \hat{I} = 0.
\]
The expectation values of these operators, will follow the same dynamics. We denote the vector of this expectation values as \( \vec{R} \equiv \{ s_x, s_y, s_z, I \} \). The dynamics of this vector is given by
\[
\frac{d}{dt} \vec{R} = L^\dagger \vec{R},
\]
with the matrix:
\[
L^\dagger = \begin{pmatrix}
-\frac{1}{2} \gamma & -\Delta & 0 & 0 \\
\Delta & -\frac{1}{2} \gamma & -\varepsilon & 0 \\
0 & \varepsilon & -\gamma & -\frac{1}{2} \gamma \\
0 & 0 & 0 & 0
\end{pmatrix}.
\]
3.3. Comparison

We demonstrated the three approaches for representing the L-GKS dynamics with a matrix-vector notation. For the relaxed two-level system we obtained three different matrices. However, they are all equivalent, representing the dynamics by different bases or in different spaces. A simple verification is calculating the eigenvalues for different values of the parameters. As a neat example, for the values of \( \Delta = \sqrt{\frac{1}{108}} \gamma \), \( \varepsilon = \sqrt{\frac{8}{108}} \gamma \), we know from a previous study [8] that we get a third order non-hermitian degeneracy of the eigenvalue \( \lambda = -\frac{2}{3} \gamma \). Substituting these values to the three matrices yield the same non-hermitian degeneracy.

4. Discussion

There is a heavy conceptual and computational price for the reduced description of open quantum systems in Liouville space. To pave the way to overcome this difficulty, it is desirable to represent the dynamics in the more familiar matrix vector notation.

Significant simplification can be identified in the Heisenberg representation, when a set of operators which is closed to the equation of motion is found. For the Hamiltonian part, a closed set is obtained when the operators form a closed compact Lie algebra and the Hamiltonian is a linear combination of these operators [24]. Additional requirements are needed for the set to be also closed to the dissipative part [20, Appendix A].

When a closed set of operators cannot be found one has to resort to approximate methods. The idea is to construct a representative subset of operators. This set is generated from the initial state with successive applications of the dynamical generator \( \mathcal{L} \). The initial idea can be traced to Lanczos [25] who applied it to obtain iterative solutions to eigenvalue problems of a hermitian operator \( \mathbf{A} \). Since the eigenvalues of \( \mathcal{L} \) are complex, the iterative approach is modified to the Arnoldi method [17]. The Arnoldi approach is effective in the reduction of a large scale problem into a relatively small approximation space. Therefore, it should be considered as a standard approach for the treatment of large-scale L-GKS problems.

Bibliography

[1] Karl Kraus. General state changes in quantum theory. *Annals of Physics*, 64(2):311–335, 1971.
[2] Edward Brian Davies. Quantum theory of open systems. IMA, 1976.
[3] Crispin W Gardiner et al. Handbook of stochastic methods, volume 4. Springer Berlin, 1985.
[4] Robert Alicki and Mark Fannes. Quantum dynamical systems. Oxford university press, 2001.
[5] Robert Alicki and Karl Lendi. Quantum Dynamical Semigroups and Applications, volume 717 of Lecture Notes in Physics. Springer Berlin Heidelberg, 2007.
[6] Goran Lindblad. On the generators of quantum dynamical semigroups. *Communications in Mathematical Physics*, 48(2):119–130, 1976.
[7] Vittorio Gorini, Andrzej Kossakowski, and Ennackal Chandy George Sudarshan. Completely positive dynamical semigroups of n-level systems. *Journal of Mathematical Physics*, 17(5):821–825, 1976.
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[8] Morag Am-Shallem, Ronnie Kosloff, and Nimrod Moiseyev. Exceptional points for parameter estimation in open quantum systems: analysis of the bloch equations. *New Journal of Physics*, 17(11):113036, 2015.

[9] Morag Am-Shallem, Ronnie Kosloff, and Nimrod Moiseyev. Parameter estimation in atomic spectroscopy using exceptional points. *arXiv preprint arXiv:1511.07205*, 2015.

[10] Machnes, Shai and Penio, Martin B. Surprising interactions of markovian noise and coherent driving. *arXiv:1408.3056v1*, 2014.

[11] Horn Roger and R Johnson Charles. *Topics in matrix analysis*. Cambridge University Press, 1994.

[12] Cleve Moler and Charles Van Loan. Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. *SIAM Review*, 45(1):3–49, 2003.

[13] Awad H. Al-Mohy and Nicholas J. Higham. Computing the action of the matrix exponential, with an application to exponential integrators. *SIAM Journal on Scientific Computing*, 33(2):488–511, 2011.

[14] Karim M Abadir and Jan R Magnus. *Matrix algebra*, volume 1. Cambridge University Press, 2005.

[15] Lloyd N Trefethen and David Bau III. *Numerical linear algebra*, volume 50. Siam, 1997.

[16] Y. Saad. Analysis of some krylov subspace approximations to the matrix exponential operator. *SIAM Journal on Numerical Analysis*, 29(1):209–228, 1992.

[17] Walter Edwin Arnoldi. The principle of minimized iterations in the solution of the matrix eigenvalue problem. *Quarterly of Applied Mathematics*, 9(1):17–29, 1951.

[18] Hillel Tal-Ezer. On restart and error estimation for Krylov approximation of $w = f(A)v$. *SIAM Journal on Scientific Computing*, 29(6):2426–2441, 2007.

[19] Breuer, HP and Petruccione, F. *Open quantum systems*. Oxford university press, 2002.

[20] Yair Rezek and Ronnie Kosloff. Irreversible performance of a quantum harmonic heat engine. *New Journal of Physics*, 8(5):83, 2006.

[21] Ronnie Kosloff and Tova Feldmann. Discrete four-stroke quantum heat engine exploring the origin of friction. *Phys. Rev. E*, 65:055102, May 2002.

[22] GS Agarwal. Master-equation approach to spontaneous emission. *Physical Review A*, 2(5):2038, 1970.

[23] Claude Cohen-Tannoudji, Jacques Dupont-Roc, and Gilbert Grynberg. *Atom-Photon Interactions: Basic Process and Applications*. Wiley-VCH Verlag GmbH, Weinheim, Germany, 1998.

[24] Y Alhassid and RD Levine. Connection between the maximal entropy and the scattering theoretic analyses of collision processes. *Physical Review A*, 18(1):89, 1978.

[25] Cornelius Lanczos. *An iteration method for the solution of the eigenvalue problem of linear differential and integral operators*. United States Governm. Press Office, 1950.