Mathematical Structure of Steady-State Solutions for an Open Quantum System Consisting of Electrons in a Photon Cavity

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MATHEMATICAL STRUCTURE OF STEADY-STATE SOLUTIONS FOR AN OPEN QUANTUM SYSTEM CONSISTING OF ELECTRONS IN A PHOTON CAVITY

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16 ECTS thesis submitted in partial fulfillment of a
B.Sc. degree in Mathematics

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Abstract

The theory of open quantum systems strives to explain the behaviour of many-body systems obeying the laws of quantum mechanics, which are in some way controlled by the effects of its environment. Examples of open systems can be found across a broad range of scientific research and include cellular lifeforms, solar cells, and financial systems. In fact most realistic physical system can be modelled as an open many-body system. The question which one often aims to answer in the study of these systems, is how they evolve through time and whether they settle down to a state of equilibrium (i.e. reach their steady state). Investigation of the time evolution of open quantum many-body systems has been a long-standing problem of research in the past decades. Although the dynamics of these systems can theoretically be described, the resulting equations are in practice very difficult to solve due to the myriad of variables at hand.

In this thesis, we consider a rather general description of such a system, a many-level electron system in a photon cavity which is weakly coupled to its environment. Using a generalized master equation called the Nakajima-Zwanzig equation, we consider the steady-state of the system. We show that the assumption that the electron transport is a short-memory process induces a Dirac measure on the components of the dissipator in the equation. By investigating the relation between these components and their corresponding measures we use algebraic methods to represent these relations in terms of the physical operators at play. By casting the equation into the Liouville Tensor Space we obtain an eigenvalue problem in terms of the density operator. Within this framework we derive a computational model which solves the eigenvalue problem, thus allowing us to determine the steady-state of the system as well as an approximation of its transient behaviour over very long time scales.

Útdráttur

Hegðun fjöleinda kerfa sem lúta lögmálum skammtafræðinnar og ákvarðast stýrast af áhrifum ytra umhverfis er umfjöllunarefni eðlisfræði opinna skammtakerfa. Slík kerfi má finna á ýmsum sviðum vísinda og má sem dæmi nefna fjölfrumunga, sólarrafhlöður og fjármálakerfi. í raun er svo að flest öll raunveruleg kerfi eðlisfræðinnar má líta á sem opin fjöleindakerfi. Þær spurningar sem oft er leitast eftir að svara fyrir slík kerfi varðar þróun þeirra með tíma og hvort þau leiti í stöðugt ástand sem megi ákvarða. Rannsóknir á tímaþróun slíkra kerfa hefur reynst erfiðar viðfangs í nokkurra áratugi. Jafnvel þótt hreyfifræði slíkra kerfa megi fræðilega lýsa þá reynast jöfnurnar oft of flóknar til þess að hægt sé að leysa þær vegna hins gífurlega fjölda breyta sem þar fyrirfinnast.

Í þessari ritgerð athugum við fremur almenna lýsingu á slíku kerfi, þ.e. fjölstiga rafeindakerfi í ljóseindaholi sem er veiktengt við umhverfi sitt. Með því að nota skammtastýrijöfnu Nakajima og Zwanzig reynum við að athuga sístöðuástand kerfisins. Við sýnum að sú forsenda að kerfið búi við minnistap gefi af sér Dirac mál fyrir sérhvert stak þeirra staka sem lýsa orkutapi. Við nánari athugun má sjá að venslin milli þessara staka og tilheyrandi Dirac máls megi lýsa með algebraiskum aðferðum með tilliti til hinna eðlisfræðilegu virkja sem lýsa kerfinu. Með því að varpa jöfnunni í Liouville þinrúmið fáum við eigingildisverkefni sem lýsir þéttleikavirkjanum á gefnum tíma. Út frá þessari hugmyndafræði útbúum við líkan sem útbýr og leysir eigingildisverkefnið með tölvureikningum og leyfir okkur þar með að ákvarða sístöðuástand kerfisins ásamt því að gefa mat á hverfulu ástandi þessi.

Dedication

Firstly, I would like to express my sincere gratitude to Prof. Vidar Gudmundsson for offering me the opportunity to be involved in this project. This work has made me a better person, offering me a unique first insight into how scientific research is done, and making me understand what I love doing in my life. I am very thankful to other members of Vidar's team whom I have had the pleasure to work with, and to María Lára, Hólmfríður Hannesdóttir, Kristbjörg Anna, Tandri Gauksson and Alexander Poremba for great and interesting discussions that have improved my work immensely.

I am extremely thankful to my girlfriend, Arnbjörg Soffía, who has often had to show me a great deal of patience during long nights when I had to work on an "idea". At other times she has offered me love and mathematical insights that have progressed my way of thinking about delightful abstract concepts.

I thank my family for offering me the environment in which I have prospered.

I thank my friends who have shaped my views and ideas, burning the midnight oil with me while frantically figuring out a way to learn about our universe.

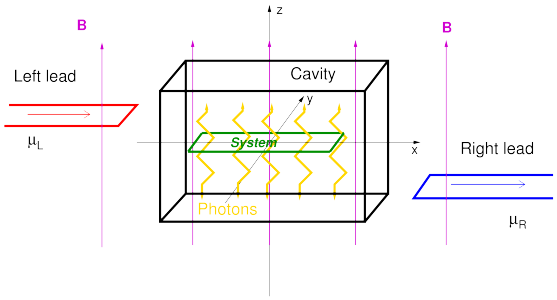
Finally, I would like to thank the teachers that have taught me mathematics and physics in both college and university, for inspiring me to think about science and mathematics. I hope this document is the first of many for which I can seek that inspiration.

1 Introduction

1.1 The Physical Model

An important problem in physics is the description of an open system, i.e. a central system, coupled to external reservoirs. Here, we will especially consider an electron system on the nanometer scale , weakly coupled to external leads. Originally, for time $t < 0$, the three subsystems are not coupled and are each in an equilibrium state. In the leads the electrons occupy the energy levels according to the Fermi distribution with a definite chemical potential. After the coupling, the difference in the chemical potentials (the bias), drives a current through the central system. At

Figure 1.1: A photon cavity, weakly coupled to its leads.



any given time a measurement on the system yields information about an ensemble of states. But as the measurement is intrinsically probabilistic, to describe the system we consider the probability of measuring, at any given time, any mixture of states. For a many-body system, such a description is given by the density operator [1].

$$\rho(t) = \sum_i p_i |\Psi_i(t)\rangle\langle\Psi_i(t)|, \tag{1.1}$$

where p_i is the probability of the system being in the pure state Ψ_i at time t. In the study of quantum many-body systems, the Banach space considered is a direct sum of Hilbert spaces containing any number of many-body states. This space is called the Fock space.

In order to understand the mathematical construction of this model, we shall give an introduction to the underlying mathematical theory.

1.2 Stochastic Processes & Master Equations

The transport of electrons through a photon cavity can be viewed as a stochastic process. A brief review of stochastic processes will give us the necessary insights to model an open quantum system.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. A family of random variables on the space $(X_t)_{t\in T}$, where T is an ordered subset of $\mathbb{R}$, is called a stochastic process. One can also represent it as the map $X : \Omega \times T \longrightarrow \mathbb{R}$.

We say that a stochastic process has a short memory if its future state depends only on its most recent state. This is also called the Markov property.

The Markov property can be expressed in terms of the conditional probability measure [2],

$$\mathbb{P}(X_{t_{n+1}} = x_{n+1} | X_{t_0} = x_0, \ldots, X_{t_n} = x_n) = p_{x_n x_{n+1}}(t_{n+1} - t_n). \tag{1.2}$$

Where $p_{x_n x_{n+1}}(t_{n+1} - t_n)$ is the probability of finding a process starting in state x_n, in state x_{n+1} in the time $t_{n+1} - t_n$. We now introduce the concept of a semigroup of operators. In such a framework we obtain a generalization of the Cauchy problem in terms of a propagator. Let X be a Banach Space, a semigroup of operators on X is a family of operators $(T(t))_{t \geq 0}$ such that,

- $T(t + s) = T(t)T(s)$,
- $T(0) = I$,
- $T(t)x \to x$ for $t \to 0^+$,

where I is the Identity operator on X. We can think of a given sample of a stochastic process as a path within a subspace of Ω. All such paths are described by the transition matrix or the propagator. Its components are given by

$$P(t)_{i,j} = p_{i,j}(t), \tag{1.3}$$

where the probability p is defined as in 1.2. The propagator is a semigroup.

Semigroups can "generate" solutions to differential equations on Banach spaces. Given a function u_0 and a linear operator $\mathcal{A}$ on Banach space X.

$$\begin{cases} \dfrac{\partial}{\partial t} u(x,t) = \mathcal{A}u(x,t), \quad \text{for } t \geq 0 \\ \\ u(x,0) = u_0(x). \end{cases} \tag{1.4}$$

This is called the abstract Cauchy Problem. Its solution can be given in terms of a semigroup of operators T as $T(t)u_0(x) = u(x,t)$. In this case the relation between T and $\mathcal{A}$ is simply,

$$T(t) = e^{t\mathcal{A}} \tag{1.5}$$

In general the relation between T and $\mathcal{A}$ is given by the limit,

$$\mathcal{A}x = \lim_{t \to 0^+} \frac{1}{t}(T(t) - I)x, \tag{1.6}$$

where x is some point in X, and $\mathcal{A}$ is called the infinitesimal generator of the semigroup. Thus, the solution $u(x,t)$ may be found by solving the operator equation

$$\frac{\partial T}{\partial t} = \mathcal{A}T \tag{1.7}$$

In functional analysis equations of this form are called evolution equations.

Now if we consider again the propagator $P(t)$. If it is differentiable with respect to time, we can consider the differential Chapman-Kolmogorov equation or the master equation

$$\frac{\partial P_t}{\partial t} = \mathcal{A}P_t, \tag{1.8}$$

where $\mathcal{A}$ is the generator of a semigroup of operators $\{P_t | t \geq 0\}$.

Therefore, given an initial time t_0, at time t_1 we have

$$P_{t_1} = e^{t\mathcal{A}} P_{t_0}, \tag{1.9}$$

where $t = t_1 - t_0$.

Master equations describe systems that are in exactly one state at any given time and the switching between states is described probabilistically. If we consider jump processes as well, we get what is called the Liouville master equation,

$$\frac{\partial P}{\partial t} = \mathcal{L}P + \int_0^t \Lambda(P) dt' \tag{1.10}$$

Where Λ describes dissipation of the process in the system. The solution to equation 1.10 when $\dfrac{\partial P}{\partial t} = 0$ describes the steady state of the process.

1.3 Quantum Master Equations

Analogously to how master equations are defined for conditional transition probability we can define quantum master equations for the density operator. The Nakajima-Zwanzig approach is to introduce the Liouville-Von Neumann quantum master equation,

$$\frac{\partial \rho(t)}{\partial t} = \mathcal{L}(t)\rho(t). \tag{1.11}$$

The Liouville operator, $\mathcal{L}$, is defined as $\mathcal{L}\rho = \frac{-i}{\hbar}[H, \rho]$, where H is the Hamiltonian of the central system $\mathcal{H}$. It is the generator of a quantum dynamical semigroup [3], $V(t)$, defined as,

$$\mathcal{L}\rho = \lim_{\epsilon \to 0^+} \frac{1}{\epsilon}(V(t) - I)\rho. \tag{1.12}$$

From equation 1.11 we get,

$$V(t)\rho = e^{t\mathcal{L}}\rho. \tag{1.13}$$

Such an equation is of the Lindblad form if

$$\mathcal{L}\rho = \frac{-i}{\hbar}\mathcal{L}\rho + \frac{1}{2}\sum_{\alpha} \left\{ \left[A_\alpha \rho, A_\alpha^\dagger\right] + \left[A_\alpha, \rho A_\alpha^\dagger\right] \right\}, \tag{1.14}$$

The operators A_α are called the Lindblad operators. The generator of the semigroup associated with it is bounded. Furthermore the semigroup is assumed to be completely positive meaning that for any natural number n its tensor product with the identity element I_n maps positive elements to positive elements.[3] The latter condition was introduced by G. Lindblad in 1976 to describe irreversible processes in quantum mechanics [4].

1.4 The Nakajima-Zwanzig Equation

The open quantum system we consider is described with the Liouville-von Neumann equation for the time-evolution of the density operator ρ. However, the continuous state space of the leads is too large to allow an effective calculation. A way out of this dilemma was suggested by Nakajima and Zwanzig who invented a scheme to project the dynamics of the whole system onto the open central system. We can make a projection of dynamics to give a generalization of the quantum master equation describing the relevant part of the open system [5, 6, 7]. By doing this we obtain what is called the Nakajima-Zwanzig Equation.

$$\frac{\partial \rho}{\partial t} = \mathcal{P}\mathcal{L}\rho + \int_0^t \mathcal{K}(t, t')\rho(t')dt' \tag{1.15}$$

where, $\mathcal{P}$ is a projection operator which projects the Liouville operator onto to relevant part of the system dynamics. The dissipation term Λ can be written as [5]

$$\Lambda(\Omega, \tau, \chi, t) = \frac{1}{\hbar^2}\int dq \chi(t) \left\{ [\tau, \Omega] + h.c. \right\}. \tag{1.16}$$

For our system the Nakajima-Zwanzig equation takes the form [8, 9, 10, 11].

$$\partial_t \rho = \mathcal{L} - \sum_l \Lambda(\Omega, \tau, \chi, t)_l. \tag{1.17}$$

Here the sum is over the leads that are coupled to the system and for each lead we have

$$\Lambda(\Omega, \tau, \chi, t) = \frac{1}{\hbar^2}\int dq \chi(t) \left\{ [\tau, \Omega] + h.c. \right\}, \tag{1.18}$$

where q is a continuous quantum number representing the momentum and the subband index in a lead and the operator τ is the coupling tensor of the lead. The coupling tensor is carried

out smoothly in time by the switching function χ, turning on the electron transport through the system. The operator Ω is given by,

$$\Omega(t) = \int_0^t ds\chi(s)U(t-s)\left\{\tau^\dagger\rho(s)(1-F) - \rho(s)\tau^\dagger F\right\}U^\dagger(t-s)e^{i(s-t)\epsilon}. \tag{1.19}$$

Where F is the Fermi function which describes the equilibrium distribution of particles over the energy states before the subsystems are coupled together. $U(t-s) = \exp\{-i(t-s)H/\hbar\}$ is the unitary time-evolution operator for the closed central system.

Previously, we have mainly been interested in observing electron-photon interaction in the transient regime. We have studied systems with non-trivial geometry. To do this we have needed a large truncated Fock many-body state space to solve the Nakajima-Zwanzig equation. The dissipative terms in the equation are not in a Lindblad form.

1.5 Problem Outline

The objective of this thesis is to provide a method of solving equation 1.17 when $\partial_t\rho = 0$ i.e. the steady-state of the system.

The solution consists of the following main parts.

- We explain how we can express the intergrand, Λ, in the dissipation term in terms of the density operator as is done in [8].
- By representing the density of states in the leads numerically, we transform the integrand of Λ with respect to q to the energy domain. [10] We show that defining a matrix of Dirac measures gives us a way to solve an approximative form of the equation exactly.
- The kernel of the integro-differential equation contains numerous terms with the reduced density operator sandwiched between operators. These operators are represented as matrices in the Fock many-body space of interacting electrons and possibly photons. We will use a Kronecker tensor product to transform these terms into a standard linear algebra problem in Liuoville space [12, 13, 14, 15].
- For the transient regime we have used a non-Markovian version of the Nakajima-Zwanzig equation. In order to find the steady state we relax this condition and seek the Markovian form of Ω. Our aim is to minimize the approximations needed and allow for the possibility to calculate the Markovian time-evolution of the system in addition to the non-Markovian one. However using this approach we can calculate far beyond the transient regime [16].

2 The Mathematical Model

2.1 The Markov Approximation

We begin by obtaining an expression for the components of the Ω operator. Its utility will become evident as it will give us a mathematically natural way to express the Markov approximation.

The Ω operator is given by,

$$\Omega(t) = \int_0^t ds\chi(s)U(t-s)\left\{\tau^\dagger\rho(s)(1-F) - \rho(s)\tau^\dagger F\right\}U^\dagger(t-s)e^{i(s-t)\epsilon}. \tag{2.1}$$

We shall let the switch-on function of the leads be $\chi(s) = 1$. The matrix components of the unitary time-evolution operator, U, in the Fock-space of the Hamiltonian describing the central system, are given by

$$U(t-s)_{\alpha\beta} = e^{-i(t-s)E_\alpha/\hbar}\delta_{\alpha\beta}, \tag{2.2}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta symbol. Now, for component α, β of the Ω operator we have

$$\Omega_{\alpha\beta}(t) = \int_0^t ds\left\{(1-F)U(t-s)_{\alpha\lambda}\tau^\dagger_{\lambda\sigma}\rho(s)_{\sigma\gamma}U(t-s)^\dagger_{\gamma\beta} - FU(t-s)_{\alpha\lambda}\rho(s)_{\lambda\sigma}\tau^\dagger_{\sigma\gamma}U(t-s)^\dagger_{\gamma\beta}\right\}e^{i(s-t)\epsilon}.$$

We define the following functionals,

$$\mathcal{S}[\rho(s)] = \pi(1-F)\tau^\dagger\rho(s),$$
$$\mathcal{R}[\rho(s)] = \pi F\rho(s)\tau^\dagger.$$

The reason for the inclusion of π will become apparent when we make the Markov approximation.

Thus,

$$\Omega_{\alpha\beta}(t) = \frac{1}{\pi}\int_0^t ds\left\{e^{-i(t-s)E_\alpha}\delta_{\alpha\lambda}\mathcal{S}[\rho(s)]_{\lambda\gamma}e^{i(t-s)E_\beta}\delta_{\gamma\beta} - e^{-i(t-s)E_\alpha}\delta_{\alpha\lambda}\mathcal{R}[\rho(s)]_{\lambda\gamma}e^{i(t-s)E_\beta}\delta_{\gamma\beta}\right\}e^{i(s-t)\epsilon}.$$

We make a change of variables, such that $s = t - s'$, then $ds' = -ds$ and obtain

$$\Omega_{\alpha\beta}(t) = \frac{1}{\pi}\int_0^t ds'\left\{\mathcal{R}[\rho(t-s')]_{\alpha\beta} - \mathcal{S}[\rho(t-s')]_{\alpha\beta}\right\}e^{is'(E_\beta - E_\alpha - \epsilon)}. \tag{2.3}$$

We now make the Markov approximation. Assuming that $\rho(t-s')$ is independent of the quantum fluctuations of the system with a period corresponding to $\hbar/(E_\beta - E_\alpha - \epsilon)$ during the time evolution, i.e. when $s' \in [0, t]$. This assumption holds true for $t >> \hbar/(E_\beta - E_\alpha - \epsilon)$. Thus, $\rho(t-s) \sim \rho(t) \equiv \rho$ and

$$\Omega_{\alpha\beta} = \left\{\mathcal{R}[\rho(t)]_{\alpha\beta} - \mathcal{S}[\rho(t)]_{\alpha\beta}\right\}\int_0^t ds' e^{is'(E_\beta - E_\alpha - \epsilon)} \tag{2.4}$$

The upper limit of the time integral can then be approximated with $t \to \infty$. Via the Markov approximation the integral becomes the Dirac Delta functional, i.e.

$$\Omega_{\alpha\beta} = \left\{\mathcal{R}[\rho(t)]_{\alpha\beta} - \mathcal{S}[\rho(t)]_{\alpha\beta}\right\}\delta\left(E_\beta - E_\alpha - \epsilon\right). \tag{2.5}$$

We have thus obtained an expression for the components of the Ω operator.

Although this expression looks simple enough, it is rather non-trivial how one should write a corresponding matrix representation. As one can see the value of each component of this operator has a very specific dependence on its component number. Later in this chapter we will show how to solve this dilemma.

The main reason we seek for a matrix representation of the equation, is that we want to be able to construct an efficient computational model which can solve the Nakajima-Zwanzig equation for our system. Furthermore, we do so with a large number of many-body states in the central system. We have made several attempts to make such a construction using only the component representation of the equation but such an attempt quickly spirals into the abyss of confusion.

2.2 Changing the Domain of the Integral Transformation

Revisiting equation 1.18 we consider how we can solve the integral over the quantum number q.

For any operator A in the many-body Fock space and its product by Ω, component α, β can be represented as

$$\int dq A(q)_{\alpha\lambda}\Omega_{\lambda\beta} = \int d\epsilon \left(\frac{dq}{d\epsilon}\right) A(\epsilon)_{\alpha\lambda}\Omega_{\lambda\beta}, \tag{2.6}$$

where $|\frac{dq}{d\epsilon}| \equiv D(\epsilon)$ is the density of states in the energy bands.

It should be apparent now that the Markov approximation allows us to solve this integral in an exact way.

Last section's result yields

$$\int d\epsilon D(\epsilon) A(\epsilon)_{\alpha\lambda}\Omega_{\lambda\beta} = \int D(\epsilon)\, A(\epsilon)_{\alpha\lambda} \left\{\mathcal{R}[\rho(t)]_{\lambda\beta} - \mathcal{S}[\rho(t)]_{\lambda\beta}\right\} d\delta\left(E_\beta - E_\lambda - \epsilon\right). \tag{2.7}$$

Thus each component of the Ω operator induces an integral transformation, with respect to the Dirac measure. Its output is the intergrand valued at the Bohr-frequency, corresponding to that component. We shall use upper indices to denote an operator valued at a given frequency.

$$\int D(\epsilon) A(\epsilon)_{\alpha\lambda} \left\{\mathcal{R}[\rho(t)]_{\lambda\beta} - \mathcal{S}[\rho(t)]_{\lambda\beta}\right\} d\delta\left(E_\beta - E_\lambda - \epsilon\right) = D^{\beta\lambda} A^{\beta\lambda}_{\alpha\lambda} \left\{\mathcal{R}[\rho(t)]^{\beta\lambda}_{\lambda\beta} - \mathcal{S}[\rho(t)]^{\beta\lambda}_{\lambda\beta}\right\}.$$

This is as far as we need to go but for the sake of argument, we shall show where the component representation leads us.

Let $\mathcal{R}[\rho] = \rho R$ and $\mathcal{S}[\rho] = S\rho$. Then for component α, β of the functional from eq. 1.18 we have by the above results

$$\hbar^2\Lambda = D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}\rho_{\lambda\sigma}R^{\beta\lambda}_{\sigma\beta} - D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}S^{\beta\lambda}_{\lambda\sigma}\rho_{\sigma\beta} - D^{\lambda\alpha}\rho_{\alpha\sigma}R^{\lambda\alpha}_{\sigma\lambda}\tau^{\lambda\alpha}_{\lambda\beta} + D^{\lambda\alpha}S^{\lambda\alpha}_{\alpha\sigma}\rho_{\sigma\lambda}\tau^{\lambda\alpha}_{\lambda\beta} + h.c.. \tag{2.8}$$

For simplification we shall only look at the first two terms. We can express them as,

$$D_{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}\left\{S^{\beta\lambda}_{\lambda\sigma}\rho_{\sigma\beta} - \rho_{\lambda\sigma}R^{\beta\lambda}_{\sigma\beta}\right\} = D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}S^{\beta\lambda}_{\lambda\sigma}\rho_{\sigma\beta} - D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}\rho_{\lambda\sigma}R^{\beta\lambda}_{\sigma\beta} \tag{2.9}$$

From this expression, obtaining a component of the Density matrix, requires a meticulous collection of terms related to it. E.g. the terms associated with component $(1,1)$ in the expression above are

$$\sum_{\alpha\lambda}\left(D^{1\lambda}\tau^{1\lambda}_{\alpha\lambda}S^{1\lambda}_{\lambda 1}\rho_{11} - D^{1\lambda}\tau^{1\lambda}_{\alpha\lambda}\rho_{\lambda 1}R^{1\lambda}_{11}\right) \tag{2.10}$$

and

$$\sum_{\alpha\beta}\left(D^{\beta 1}\tau^{\beta 1}_{\alpha 1}S^{\beta 1}_{11}\rho_{1\beta} - D^{\beta 1}\tau^{\beta 1}_{\alpha 1}\rho_{11}R^{\beta 1}_{1\beta}\right). \tag{2.11}$$

And this becomes even more convoluted as we consider the other six terms. Thus it is clear that a more sophisticated approach is needed. In the following section we provide such an approach and show how to obtain exact expressions for each component of the density matrix from the results that we have in 2.2.

2.3 The Hadamard Product & The Dirac Delta Matrix

We have seen that the source of non-triviality in the equations is that the integral transformation the Markov approximation induces is related to the index of the Ω component. Our aim will be to express this relation while conserving the relation between the physical operators at stake.

Firstly, we define a matrix of Dirac Delta functionals such that,

$$\Delta_{\alpha\beta} = \delta(E_\alpha - E_\beta - \epsilon) = \delta^{\alpha\beta}. \tag{2.12}$$

We will call this "The Dirac Delta Matrix". We can wield this structure to unravel the threads of confusion via the Hadamard product ($\odot$), i.e. a component wise multiplication between two matrices.

$$(A \odot B)_{\alpha\beta} = A_{\alpha\beta} B_{\alpha\beta}. \tag{2.13}$$

The Hadamard product is commutative, associative and distributive over addition. However it is not distributive over matrix multiplication. For demonstration, let A and B be any operators in the Fock space and consider terms of the form $\int DA\Omega B$. As a shorthand notation we let $\mathcal{R}[\rho(t)] = \mathcal{R}$ and $\mathcal{S}[\rho(t)] = \mathcal{S}$.

Let $\mathcal{Z}$ be the matrix which corresponds to the general form of terms which we have encountered. It is a measure over the density of states. Its component representation is given by:

$$\mathcal{Z}_{\alpha\beta} = D^{\sigma\lambda} A^{\sigma\lambda}_{\alpha\lambda} \left\{ \mathcal{R}^{\sigma\lambda}_{\lambda\sigma} - \mathcal{S}^{\sigma\lambda}_{\lambda\sigma} \right\} B^{\sigma\lambda}_{\sigma\beta}, \tag{2.14}$$

and its matrix representation is given by:

$$\mathcal{Z} = \int DA \left\{ \left(\mathcal{R} - \mathcal{S} \right) \odot d\Delta^T \right\} B. \tag{2.15}$$

Proof. We have,

$$\Delta^T = \begin{bmatrix} \delta^{11} & \delta^{21} & \cdots & \delta^{n1} \\ \delta^{12} & \delta^{22} & \cdots & \delta^{n2} \\ \vdots & \vdots & \ddots & \vdots \\ \delta^{1n} & \delta^{2n} & \cdots & \delta^{nn} \end{bmatrix} \tag{2.16}$$

Then,

$$\left(\mathcal{R} - \mathcal{S} \right) \odot \Delta^T = \begin{bmatrix} \left(\mathcal{R}_{11} - \mathcal{S}_{11} \right) \delta^{11} & \left(\mathcal{R}_{12} - \mathcal{S}_{12} \right) \delta^{21} & \cdots & \left(\mathcal{R}_{1n} - \mathcal{S}_{1n} \right) \delta^{n1} \\ \left(\mathcal{R}_{21} - \mathcal{S}_{21} \right) \delta^{12} & \left(\mathcal{R}_{22} - \mathcal{S}_{22} \right) \delta^{22} & \cdots & \left(\mathcal{R}_{2n} - \mathcal{S}_{2n} \right) \delta^{n2} \\ \vdots & \vdots & \ddots & \vdots \\ \left(\mathcal{R}_{n1} - \mathcal{S}_{n1} \right) \delta^{1n} & \left(\mathcal{R}_{n2} - \mathcal{S}_{n2} \right) \delta^{2n} & \cdots & \left(\mathcal{R}_{nn} - \mathcal{S}_{nn} \right) \delta^{nn} \end{bmatrix}. \tag{2.17}$$

By multiplying this matrix with the matrices associated with the operators A and B (from left and right respectively), we get

$$\mathcal{Z} = \begin{bmatrix} \int DA_{1\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 1} d\delta^{\sigma\lambda} & \int DA_{1\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 2} d\delta^{\sigma\lambda} & \cdots & \int DA_{1\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma n} d\delta^{\sigma\lambda} \\ \int DA_{2\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 1} d\delta^{\sigma\lambda} & \int DA_{2\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 2} d\delta^{\sigma\lambda} & \cdots & \int DA_{2\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma n} d\delta^{\sigma\lambda} \\ \vdots & \vdots & \ddots & \vdots \\ \int DA_{n\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 1} d\delta^{\sigma\lambda} & \int DA_{n\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma 2} d\delta^{\sigma\lambda} & \cdots & \int DA_{n\lambda} \left(\mathcal{R}_{\lambda\sigma} - \mathcal{S}_{\lambda\sigma} \right) B_{\sigma n} d\delta^{\sigma\lambda} \end{bmatrix}.$$

So component (α, β) can be written as:

$$\mathcal{Z}_{\alpha\beta} = sD^{\sigma\lambda} A^{\sigma\lambda}_{\alpha\lambda} \left\{ \mathcal{R}^{\sigma\lambda}_{\lambda\sigma} - \mathcal{S}^{\sigma\lambda}_{\lambda\sigma} \right\} B^{\sigma\lambda}_{\sigma\beta} \tag{2.18}$$

□

Now for the case of $A = \tau$ and $B = Id$, where Id is the identity operator, we have:

$$\mathcal{Z} = D\tau \left\{ \left(\mathcal{R} - \mathcal{S} \right) \odot \Delta^T \right\} \tag{2.19}$$

It is easy to show that the Hadamard product of two matrices cannot be represented by a linear transformation in the Liouville space, however this turns out not to be the case when one considers the Liouville tensor space. In the next section we will make use of this structure and show how this can be done. Consequently it will become attainable to invent a computational scheme using the parallel Intel BLAS in Fortran.

The reason we use the parallel Intel BLAS in Fortran is because of its speed and our existing codebase. Using Python we can use QuTiP [17] which allows one to investigate the dynamics of an open quantum system. QuTiP has been used to look for iterative solutions to the steady-state of an optomechanical system [18]. Although the eigenvalue routine that we use is iterative, we use it as a black box without any particular conditioning which could speed up the calculations.

2.4 The Liouville Tensor Space

To obtain an expression for each component of the density matrix we introduce algebraic operators in the Kronecker product space of the Liouville space. We have seen at the end of section 2 in this chapter, that obtaining such an expression in the component representation required meticulous book keeping of an overwhelming number of indices. The insight gained in the previous section however, offers a new path around this problem.

The elements of the Kronecker product of any vector space are blockmatrices given by the tensor product

$$A \otimes B = \begin{bmatrix} A_{1,1}B & A_{1,2}B & \cdots & A_{1,n}B \\ A_{2,1}B & A_{2,2}B & \cdots & A_{2,n}B \\ \vdots & \ddots & \ddots & \vdots \\ A_{n,1}B & A_{n,2}B & \cdots & A_{n,n}B \end{bmatrix} \tag{2.20}$$

Where we assume that A and B are operators in the Fock many-body space represented by $n \times n$ matrices.

There are a couple of algebraic operators that we will consider with regards to the elements of this space. These operators will allow us to obtain the solutions in a convenient form.
Definition 2.4.1. Let A be an $n \times n$ matrix. The vectorization of a A is the linear operator which converts the matrix A into an n^2 dimensional column vector given by,

$$\mathrm{vec}\,(A) = [A_{1,1}, \ldots, A_{n,1}, A_{1,2}, \ldots, A_{1,n}, \ldots, A_{n,n}]^T \tag{2.21}$$

The diagonalization operator is a linear operator which gives an $n^2 \times n^2$ matrix defined by,

$$\mathrm{Diag}(A) = \begin{bmatrix} A_{1,1} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & A_{2,1} & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \vdots & 0 & A_{2,n} & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & 0 & A_{1,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \cdots & 0 & A_{n,n} \end{bmatrix} \tag{2.22}$$

i.e. an operator that takes the column vectors, stacks them up and puts them on the main

diagonal. For the Dirac Delta matrix we shall let,

$$\Delta_\beta^T = \begin{bmatrix} \delta^{\beta 1} & 0 & \cdots & 0 \\ 0 & \delta^{\beta 2} & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \delta^{\beta n} \end{bmatrix} \tag{2.23}$$

Thus we can see that,

$$\mathrm{Diag}(\Delta^T) = \begin{bmatrix} \Delta_1^T & 0 & \cdots & 0 \\ 0 & \Delta_2^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Delta_n^T \end{bmatrix} \tag{2.24}$$

Theorem 2.4.1. *Let A, ρ and B be matrices representing elements in an $n \times n$ vector space. The following identities hold true:*

$$\begin{aligned} i) \quad & \mathrm{vec}(A\rho B) = \left(B^T \otimes A\right) \mathrm{vec}(\rho) \\ ii) \quad & \mathrm{vec}(A \odot B) = \mathrm{Diag}(B)\, \mathrm{vec}(A) \\ iii) \quad & \mathrm{vec}(A \odot B) = \mathrm{vec}(A) \odot \mathrm{vec}(B) \end{aligned}$$

We omit the proof. One can be found in [19] for example.

By the first identity we can see that any equation such as

$$\mathcal{Z} = A\rho B \tag{2.25}$$

can be put on the form:

$$\mathrm{vec}(\mathcal{Z}) = \left(B^T \otimes A\right) \mathrm{vec}(\rho) \tag{2.26}$$

Thus enabling a way to find values of ρ that fulfill the equation.

Furthermore, we can use these identities to help us unravel the mysteries concerning our integral. The integral takes the form,

$$\mathcal{Z}_{AB} = \int DA \left\{ (\mathcal{R} - \mathcal{S}) \odot d\Delta^T \right\} B, \tag{2.27}$$

where the subscript denotes the operators on each side of the factor containing the measure.

By applying the vectorization operator we get by identity i),

$$\mathrm{vec}(\mathcal{Z}_{AB}) = \int \left(B^T \otimes DA\right) \mathrm{vec}\left(\{\mathcal{R} - \mathcal{S}\} \odot d\Delta^T\right) \tag{2.28}$$

We note that the Hadamard product is distributive over addition, and the vec operator is linear in the Kronecker product space. Therefore by definition of $\mathcal{R}$ and $\mathcal{S}$ we have,

$$\mathrm{vec}(\mathcal{Z}_{AB}) = \int \left(B^T \otimes DA\right) \mathrm{vec}\left(\mathcal{S}\rho \odot d\Delta^T\right) - \int \left(B^T \otimes DA\right) \mathrm{vec}\left(\rho\mathcal{R} \odot d\Delta^T\right) \tag{2.29}$$

We denote the former integral by $\mathfrak{I}_{AB}$ and the latter by $\widetilde{\mathfrak{I}}_{AB}$ with the subscript referencing the operators multiplied by from left and right.

By theorem 2.4.1,

$$\mathfrak{I}_{AB} = \int \left(B^T \otimes DA\right) \mathrm{Diag}(d\Delta^T)\, (\mathcal{I} \otimes \mathcal{S})\, \mathrm{vec}\,(\rho) \tag{2.30}$$

Where $\mathcal{I}$ is the identity operator in the Liouville space. Notice that the Dirac matrix must escape the vectorization operator in precedence of $\mathcal{S}$ as the Hadamard product is not distributive over matrix multiplication.

An important observation is that the density operator has escaped the integral as it does not depend the measures, $\mathrm{Diag}(d\Delta^T)$.

$$\mathfrak{I}_{AB} = \left(\int \left(B^T \otimes DA \right) \mathrm{Diag}(d\Delta^T) \right) \left(\int \mathrm{Diag}(d\Delta^T) \left(\mathcal{I} \otimes \mathcal{S} \right) \right) \mathrm{vec}(\rho) \tag{2.31}$$

This result will prove convenient when we build the corresponding computational model.

Proceeding with the latter integral as we did with the former, results in

$$\widetilde{\mathfrak{I}}_{AB} = \left(\int \left(B^T \otimes DA \right) \mathrm{Diag}(d\Delta^T) \right) \left(\int \mathrm{Diag}(d\Delta^T) \left(\mathcal{R}^T \otimes \mathcal{I} \right) \right) \mathrm{vec}\left(\rho \right) \tag{2.32}$$

And thus we have reached our objective. The kernel of the dissipator Λ in equation 1.18 can now be written as,

$$\mathrm{vec}(\Lambda) = \frac{1}{\hbar^2} \left(\mathfrak{I}_{\mathcal{I}\tau} - \widetilde{\mathfrak{I}}_{\mathcal{I}\tau} + \mathfrak{I}_{\tau\mathcal{I}} - \widetilde{\mathfrak{I}}_{\tau\mathcal{I}} + h.c. \right) \mathrm{vec}(\rho). \tag{2.33}$$

3 The Composition of the Liouville Operator

In this chapter we will show how the results we've obtained in the previous chapter can aid in constructing a computational model. Based on those results, in the Liouville tensor space the Nakajima-Zwanzig equation takes the form,

$$\partial_t \operatorname{vec}(\rho) = \frac{-i}{\hbar}(I \otimes H - H^T \otimes I) \operatorname{vec}(\rho) + \int d\epsilon \operatorname{vec}(\Lambda). \tag{3.1}$$

The only non-trivial feature of this equation is how $\operatorname{vec}(\Lambda)$ is built. Nontheless, upon closer scrutiny it turns out that its structure is rather simple in terms of block matrices. In what follows we will prove a simple algorithm that constructs one of the factors from equation 2.33.

$$\mathfrak{I}_{\tau\mathcal{I}} = \left(\int d\epsilon \, (\mathcal{I} \otimes D\tau) \operatorname{Diag}\left(d\Delta^T\right) \right) \left(\int d\epsilon \operatorname{Diag}\left(d\Delta^T\right) (\mathcal{I} \otimes \mathcal{S}) \right) \tag{3.2}$$

By definition we have:

$$(\mathcal{I} \otimes D\tau) = \begin{bmatrix} D\tau & 0 & \cdots & 0 \\ 0 & D\tau & \cdots & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & D\tau \end{bmatrix} \tag{3.3}$$

thus,

$$(\mathcal{I} \otimes D\tau) \operatorname{Diag}(\Delta^T) = \begin{bmatrix} D\tau & 0 & \cdots & 0 \\ 0 & D\tau & \cdots & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & D\tau \end{bmatrix} \begin{bmatrix} \Delta_1^T & 0 & \cdots & 0 \\ 0 & \Delta_2^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Delta_n^T \end{bmatrix} \tag{3.4}$$

which yields a block diagonal matrix,

$$(\mathcal{I} \otimes D\tau) \operatorname{Diag}(\Delta^T) = \begin{bmatrix} D\tau\Delta_1^T & 0 & \cdots & 0 \\ 0 & D\tau\Delta_2^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D\tau\Delta_n^T \end{bmatrix} \tag{3.5}$$

where block β corresponds to

$$D\tau\Delta_\beta^T = \begin{bmatrix} D\tau_{11}\delta^{\beta 1} & D\tau_{12}\delta^{\beta 2} & \cdots & D\tau_{1n}\delta^{\beta n} \\ D\tau_{21}\delta^{\beta 1} & D\tau_{22}\delta^{\beta 2} & \cdots & D\tau_{2n}\delta^{\beta n} \\ \vdots & \vdots & \ddots & \vdots \\ D\tau_{n1}\delta^{\beta 1} & D\tau_{n2}\delta^{\beta 2} & \cdots & D\tau_{nn}\delta^{\beta n} \end{bmatrix} \tag{3.6}$$

And one can see that $\left(D\tau\Delta_\beta^T\right)_{\alpha\lambda} = D\tau_{\alpha\lambda}\delta^{\beta\lambda} = D^{\beta\lambda}\tau_{\alpha\lambda}^{\beta\lambda}$.

Now the objective is to use this to construct the matrix that corresponds to the Kronecker product

$$\int d\epsilon \, (\mathcal{I} \otimes D\tau) \operatorname{Diag}(\Delta^T) \tag{3.7}$$

By keeping in mind that β corresponds to the number of the block diagonal matrix and using the corresponding results that we've just obtained we conclude:

$$D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda} = \left((\mathcal{I}\otimes D\tau)\,\mathrm{Diag}(\Delta^T)\right)_{n(\beta-1)+\alpha,n(\beta-1)+\lambda} \tag{3.8}$$

That is, element (α,λ) in block matrix β is element $(n(\beta-1)+\alpha, n(\beta-1)+\lambda)$. in the Tensor product matrix $\int d\epsilon\,(\mathcal{I}\otimes D\tau)\,\mathrm{Diag}(\Delta^T)$

To construct this matrix we implement the following pseudo-code:

```
! We reset the matrix that we're about to construct as the zero matrix.
∫(I ⊗ Dτ) Diag(Δ^T) = Czero
! This is the number of the block matrix on the diagonal
! The Dirac delta function that acts on block matrix β is δ(ϵ − (E_β − E_λ))
DO β = 1, n
   DO λ = 1, n
      ! Reference a 4 dimensional array that contains Dτ at all energies
      D^{βλ}τ^{βλ} = Dτ_REG(β, λ, :, :)
      DO α = 1,n
         ∫ (I ⊗ Dτ) Diag(Δ^T)_{n(β−1)+α,n(β−1)+λ} = (D^{βλ}τ^{βλ})_{αλ}
      END DO
   END DO
END DO
```

Moving onto the latter factor, $\int d\epsilon\,\mathrm{Diag}\left(\Delta^T\right)(\mathcal{I}\otimes\mathcal{S})$, by a similar argument as before we get the block diagonal matrix,

$$\mathrm{Diag}(\Delta^T)\,(\mathcal{I}\otimes\mathcal{S}) = \begin{bmatrix} \Delta_1^T\mathcal{S} & 0 & \cdots & 0 \\ 0 & \Delta_2^T\mathcal{S} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Delta_n^T\mathcal{S} \end{bmatrix} \tag{3.9}$$

where block β corresponds to

$$\Delta_\beta^T\mathcal{S} = \begin{bmatrix} \delta^{\beta 1} & 0 & \cdots & 0 \\ 0 & \delta^{\beta 2} & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \delta^{\beta n} \end{bmatrix} \begin{bmatrix} \mathcal{S}_{1,1} & \mathcal{S}_{1,2} & \cdots & \mathcal{S}_{1,n} \\ \mathcal{S}_{2,1} & \mathcal{S}_{2,2} & \cdots & \mathcal{S}_{2,n} \\ \vdots & \ddots & \ddots & \vdots \\ \mathcal{S}_{n,1} & \mathcal{S}_{n,2} & \cdots & \mathcal{S}_{n,n} \end{bmatrix} \tag{3.10}$$

which gives:

$$\Delta_\beta^T\mathcal{S} = \begin{bmatrix} \mathcal{S}_{11}\delta^{\beta 1} & \mathcal{S}_{12}\delta^{\beta 1} & \cdots & \mathcal{S}_{1n}\delta^{\beta 1} \\ \mathcal{S}_{21}\delta^{\beta 2} & \mathcal{S}_{22}\delta^{\beta 2} & \cdots & \mathcal{S}_{2n}\delta^{\beta 2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{S}_{n1}\delta^{\beta n} & \mathcal{S}_{n2}\delta^{\beta n} & \cdots & \mathcal{S}_{nn}\delta^{\beta n} \end{bmatrix} \tag{3.11}$$

And one can see that $\left(\Delta_\beta^T\mathcal{S}\right)_{\lambda\sigma} = \mathcal{S}_{\lambda\sigma}\delta^{\beta\lambda} = \mathcal{S}^{\beta\lambda}_{\lambda\sigma}$.

As before we use this result to construct the program that corresponds to the factor

$$\int d\epsilon\,\mathrm{Diag}\left(\Delta^T\right)(\mathcal{I}\otimes\mathcal{S}) \tag{3.12}$$

Now β corresponds to the number of the block diagonal matrix and λ corresponds to the line number within that matrix and σ corresponds to the column number within that matrix.

$$\mathcal{S}^{\beta\lambda}_{\lambda\sigma} = \int d\epsilon\left(\mathrm{Diag}\left(\Delta^T\right)(\mathcal{I}\otimes\mathcal{S})\right)_{n(\beta-1)+\lambda,n(\beta-1)+\sigma} \tag{3.13}$$

That is, element (λ, σ) in block matrix β is element $(n(\beta-1)+\lambda, n(\beta-1)+\sigma)$.

We construct the matrix with the following pseudo-code.

```
! We reset the matrix that we're about to construct as the zero matrix.
∫ Diag(Δ^T)(I ⊗ S) = Czero
! This is the number of the block matrix on the diagonal
! The Dirac delta function that acts on block matrix β is δ(ϵ − (E_β − E_λ))
DO β = 1, n
   DO λ = 1, n
      ! Reference a 4 dimensional array that contains Dτ at all energies
      S^{βλ} = π(1 − F^{βλ})ConjugateTranspose(τ_REG(β, λ, :, :))
      DO σ = 1,n
         ∫ Diag(Δ^T) (I ⊗ S)_{n(β−1)+λ,n(β−1)+σ} = S^{βλ}_{λσ}
      END DO
   END DO
END DO
```

If we look at the multiplication of the two factors again with respect to what we've done,

$$\mathcal{Z} = \int d\epsilon \, (\mathcal{I} \otimes D\tau) \, \mathrm{Diag}\left(\Delta^T\right) \int d\epsilon \, \mathrm{Diag}\left(\Delta^T\right) (\mathcal{I} \otimes \mathcal{S}) \tag{3.14}$$

$$\Leftrightarrow$$

$$\mathcal{Z} = \begin{bmatrix} D\tau\Delta_1^T & 0 & \cdots & 0 \\ 0 & D\tau\Delta_2^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D\tau\Delta_n^T \end{bmatrix} \begin{bmatrix} \Delta_1^T\mathcal{S} & 0 & \cdots & 0 \\ 0 & \Delta_2^T\mathcal{S} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Delta_n^T\mathcal{S} \end{bmatrix} \tag{3.15}$$

$$\Leftrightarrow$$

$$\mathcal{Z}^{\beta\lambda}_{\alpha\sigma} = D^{\beta\lambda}\tau^{\beta\lambda}_{\alpha\lambda}\mathcal{S}^{\beta\lambda}_{\lambda\sigma} \tag{3.16}$$

Thereby proving that the algorithm produces the factors given in 2.8.

4 Conclusion

This thesis shows that under the Markov approximation the Nakajima-Zwanzig equation can be cast into an eigenvalue problem in the Liouville tensor space. This representation was obtained by considering the matrix form of the equation, which becomes attainable by introducing a Hadamard product of a matrix of Dirac measures. Building on these mathematical results, a simple algorithm constructing the eigenvalue problem was proved to be consistent with previous results. Experimental results show that the model can be effectively used to exploit the time evolution of a rather complex open quantum system.

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