Quantum Simulation of Open Quantum Systems

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Abstract

Over the last two decades the field of quantum simulations has experienced incredible growth, which, coupled with progress in the development of controllable quantum platforms, has recently begun to allow for the realisation of quantum simulations of a plethora of quantum phenomena in a variety of controllable quantum platforms. Within the context of these developments, we investigate within this thesis methods for the quantum simulation of open quantum systems.

More specifically, in the first part of the thesis we consider the simulation of Markovian open quantum systems, and begin by leveraging previously constructed universal sets of single-qubit Markovian processes, as well as techniques from Hamiltonian simulation, for the construction of an efficient algorithm for the digital quantum simulation of arbitrary single-qubit Markovian open quantum systems. The algorithm we provide, which requires only a single ancillary qubit, scales slightly superlinearly with respect to time, which given a recently proven "no fast-forwarding theorem" for Markovian dynamics, is therefore close to optimal. Building on these results, we then proceed to explicitly construct a universal set of Markovian processes for quantum systems of any dimension. Specifically, we prove that any Markovian open quantum system, described by a one-parameter semigroup of quantum channels, can be simulated through coherent operations and sequential simulations of processes from the universal set. Under the assumption that these universal Markovian processes can be efficiently implemented, this allows us to propose an efficient algorithm for a wide class of Markovian open quantum systems, while simultaneously providing a tool for combining and exploiting existing simulation methods.

In the second part of this thesis we then consider the simulation of many-body non-Markovian open quantum systems. In particular, we develop an algorithmic procedure for the quantum simulation of system propagators which are not completely positive maps, which allows us to provide an explicit algorithm for the digital quantum simulation of many-body locally-indivisible non-Markovian open quantum systems described by time-dependent master equations. Finally we construct generalised Suzuki-Lie-Trotter theorems which allow us to analyse the efficiency of our method, which is expected to be experimentally achievable for a variety of interesting cases.

Preface

The research contained in this thesis was completed by the candidate while based in the School of Chemistry and Physics of the College of Agriculture, Engineering and Science, University of KwaZulu-Natal, Westville Campus, South Africa. The research was financially supported by the National Research Foundation of South Africa.

The contents of this work have not been submitted in any form to another university and, except where the work of others is acknowledged in the text, the results reported are due to investigations by the candidate.

Signed:

Prof. Francesco Petruccione (Supervisor)
November 23, 2016

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November 23, 2016

Declaration 1: Plagiarism

I, Ryan Sweke, declare that

1. The research reported in this thesis, except where otherwise indicated, is my original research.
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Declaration 2: Publications

The results of this thesis appear in the publications listed below. In all publications I conceptualised the research, performed all the calculations following discussions with co-authors, and was both the lead and corresponding author of the manuscript.

Chapter 2:

R. Sweke, I. Sinayskiy and F. Petruccione, Simulation of single-qubit open quantum systems, Phys. Rev. A **90**, 022331 (2014) .

Chapter 3:

R. Sweke, I. Sinayskiy, D. Bernard and F. Petruccione, Universal simulation of Markovian open quantum systems, Phys. Rev. A **91**, 062308 (2015).

Chapter 4:

R. Sweke, M. Sanz, I. Sinayskiy, F. Petruccione and E. Solano, Digital quantum simulation of many-body non-Markovian dynamics, Phys. Rev. A **94**, 022317 (2016).

In addition to the publications above, I have been involved as lead author in research leading to the following publications, whose results are not included in this thesis.

1. R. Sweke, I. Sinayskiy and F. Petruccione, Dissipative Preparation of Large W states in Optical Cavities, Phys. Rev. A **87**, 042323 (2013).
2. R. Sweke, I. Sinayskiy and F. Petruccione, Dissipative Preparation of generalised Bell States, J. Phys. B: At. Mol. Opt. Phys. **46** 104004 (2013).

Signed:

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Chapter 1

Introduction

1.1 Physics today: The role of simulations

Since the advent of digital computers as a practical tool for physicists, it has been clear that many-body quantum mechanical systems of even a moderate size are exceptionally hard to simulate [1, 2]. As is now well known, the root of this difficulty is the so called *exponential explosion* - the fact that the number of complex numbers necessary to fully specify the state of a quantum many-body system is an exponential function of the number of particles within the system itself. A direct consequence of this fundamental property of quantum mechanics is that the number of *computational resources* required for the simulation of such systems on classical computers, at least by any naive strategy, scales exponentially with the size of the system. Adding one more spin-1/2 particle to a simulation requires doubling the amount of memory, and long before 50 particles are reached any straightforward strategy becomes totally infeasible.

However, meaningful progress in physics relies crucially not only on conceptual advances and the development of more sophisticated mathematical tools and techniques, but also on our ability to perform experiments, of which simulations can be considered an important special case. Simulations, and experiments more generally, allow us to both verify our intuition and proposed physical models, as well as develop our intuition and subsequently gain the inspiration for new conceptual frameworks. In particular, despite the fact that the fundamental framework of quantum mechanics was established almost 100 years ago, there are now as many open questions, prospective new directions and deep paradoxes in quantum many-body physics and its related fields as there ever have been. In light of this exciting state of quantum many-body physics, the fundamental

obstacles inherent in simulating quantum mechanical systems on classical computers, and the critical role played by simulations in the maturation of any physical theory, the development of novel and creative methods for the practically feasible simulation of many-body quantum systems is crucial.

The subject of this thesis is situated within the field of *quantum simulations*, which is by now a broad and mature field [2–4]. In particular, research within this field is concerned with both exploiting and motivating progress in the experimental control of individual quantum mechanical systems for the development and implementation of methods for the simulation of many-body quantum physics, which are not hampered by the same fundamental obstacles as traditional numerical methods [2–4]. Although this thesis is primarily concerned with the development of quantum simulation methods directly applicable to the simulation of *open quantum systems*, as introduced in Section 1.4, it is hoped that the methods and techniques introduced in this work will contribute to both the broader conceptual foundation and growing toolbox of theoretical techniques for quantum simulation. As alluded to above, there are currently a wealth of both novel ideas and big open questions in quantum many-body physics and its related fields, all of which may be directly explored and developed through the use of quantum simulations. In particular, the following is a (brief and non-exhaustive[1]) selection of some of the fundamental ideas and questions of interest at this moment in time, to which quantum simulations have already provided, or promise to provide, new insights:

Condensed matter physics: In the late 1970's it appeared as if Landau's Fermi liquid theory and symmetry-breaking paradigm provided all the tools necessary to understand all possible phases of matter and their associated phase transitions [5]. However, the discovery in the 1980's of fractional quantum Hall systems [6, 7], which exhibit many distinct zero-temperature phases with the same symmetries, and exotic materials such as high T_c cuprate superconductors [8], which admit no description as a Fermi liquid, has ushered in a new and exciting era of so called *modern* condensed matter physics [9, 10]. In particular, from a fundamental perspective, it is now clear that new models and frameworks, such as that of topological order[2], are necessary for obtaining a full understanding of novel and exotic phases of matter, such as quantum magnetism and high T_c superconductivity, amongst many others. Furthermore, from a technological perspec-

[1] See the review [2] for a more comprehensive and detailed list of the potential applications of quantum simulation.

[2] It is exciting to be able to note that the 2016 Nobel prize in Physics was awarded jointly to David Thouless, Duncan Haldane and Michael Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter".

tive, there are a multitude of suggestions for how such exotic materials may be exploited - fault tolerant topological quantum computation with Majorana fermions is one such example [11] - and it remains to be seen how and to what extent this might be achieved.

Non-equilibrium dynamics and quantum statistical mechanics: The majority of fundamental principles of statistical mechanics were laid down by the early 1900's [12,13]. However, we are as of yet to obtain a comprehensive understanding of how these now familiar macroscopic notions, such as thermalisation and equilibration, arise from the underlying microscopic unitary dynamics of closed many-body quantum systems. In particular, amongst other things, we would like to understand what exactly it means for a quantum mechanical system to either equilibrate or thermalise, under what conditions this occurs, how typical are these conditions, and on what time scales such processes occur [14–17]. In addition, it is now clear that there is an extremely interesting class of systems which *fail* to thermalise in any conventional sense, retaining locally and indefinitely information about their initial conditions, and exhibiting a wealth of fascinating phenomenology, which has now been collected under the banner of many-body localisation. Such systems present a variety of interesting open questions, which are just beginning to be explored, both theoretically and experimentally [14–18].

Quantum gravity and emergent space-time: Developing a proper understanding of quantum gravity is one of the most pressing outstanding physical questions of our time. Although a variety of approaches exist, in the late 1990's an interesting and powerful conceptual tool, known now as the AdS/CFT correspondence, was introduced [19]. This *holographic* correspondence provides a relation between the physics of strongly correlated many-body quantum systems and the classical dynamics of a gravitational theory in one dimension higher [20]. Although it is worth pointing out that the model of classical gravity within the original AdS/CFT correspondence, a five-dimensional anti-de Sitter space, *does not* describe the universe that we live in, generalised holographic correspondences hold the potential for elucidating a mechanism via which the geometry of space-time might arise naturally from the physics of an underlying many-body quantum system [21]. Tensor Networks, which provide efficient "entanglement representations" of many-body quantum states, developed originally as a tool for the efficient *classical* simulation of many-body quantum systems [22,23], are of particular current interest as a tool for the development of holographic approaches to quantum gravity, as they provide a natural and elegant mechanism for the construction of bulk gravitational geometries from the entanglement properties of boundary critical many-body systems [24–27]. In addi-

tion, very recently the first proposals for the quantum simulation of minimal AdS/CFT models have appeared, ushering in the prospect of finally exploring notions of quantum gravity within the laboratory [28].

Quantum chemistry: The field of quantum chemistry provides many difficult and foundational open questions, with strong economic and technological motivations in a broad range of contexts [29]. First and foremost, we would like to be able to calculate the static electronic structure of complicated atoms and molecules - a problem which in principle requires only a solution to the Schrödinger equation, but in practice runs directly into an exponential explosion [30]. Secondly, it is of great interest to develop methods for the elucidation of chemical reaction dynamics in a variety of contexts, an effort which, as in the case of biological nitrogen fixation, promises important industrial applications [31–33].

Quantum biology: Despite being predominantly "wet and warm", there is currently a large body of evidence which strongly suggests that quantum mechanical phenomena may lie at the root of certain paradoxically efficient, or hitherto unexplained, biological processes [34, 35]. More specifically, there are now a variety of biological processes for which it has been suggested that a full quantum mechanical description of the system may be necessary in order to obtain a complete understanding of the process. Of particular interest is the role that quantum mechanical effects may play in facilitating efficient energy transport within light harvesting mechanisms of photosynthetic systems [36–41]. Again, despite being of fundamental interest, obtaining a full understanding of the mechanisms via which the observed efficiencies are achieved in such systems promises a variety of high impact technological applications. In addition to processes related to photosynthesis, there are also suggestions for the role quantum mechanics may play in avian magnetoreceptive navigation, as well as more speculative suggestions concerning olfaction, vision and enzyme catalysis. [34, 35].

1.2 Quantum simulations

At this point we have established that investigating and developing efficient methods for the simulation of quantum many-body systems is certainly a worthwhile endeavour, with a multitude of established and potential applications in a wide variety of contemporary contexts. While it is certainly true that naive or straightforward approaches to the classical simulation of quantum mechanical systems are often substantially restricted,

it is definitely worth noting that the importance of simulations for making progress in any of the directions mentioned in Section 1.1 has motivated the development of a variety of more sophisticated classical numerical techniques, all of which make attempts to circumvent the inevitable exponential explosion in some way. Of these techniques, the broad class of so called Quantum Monte Carlo methods [42–44], based on random sampling techniques, and the tensor network approaches, such as the Density Matrix Renormalisation Group and Time Evolving Block Decimation [22, 23], have been particularly successful in a variety of contexts and deserve special mention as widely utilised practical tools. However, all such classical techniques rely on approximation methods of some form, and while they often perform excellently within the contexts for which they are tailored, they are often completely unsuitable for others. As an example, it is by now well known that Monte Carlo methods suffer from the infamous *sign problem* when applied to large systems of strongly interacting fermions, while tensor network approaches are generically constrained to systems with a low entanglement content, and are therefore often unsuitable for the simulation of such systems where this property cannot be guaranteed. As a result of these inevitable limitations, even within the most sophisticated currently available classical numerical techniques, quantum simulation methods, as will be introduced in more detail in this section, are an exciting and important tool.

So, what *exactly* is a quantum simulation? In order to answer this question in a precise way, and to provide the foundational context for this thesis, it is worthwhile briefly exploring the history and development of quantum simulations as both a concept and a set of techniques. Any such discussion should begin with Richard Feynman, who, confronted in the early 1980's with the difficulty of simulating quantum physics on conventional computers, was the first to articulate a vision of quantum simulation [1]. In essence, Feynman envisaged having access to a *controllable* many-body quantum system - one in which the parameters of the Hamiltonian, such as coupling strengths, external fields and lattice geometry/connectivity amongst others, could be tuned at will by the experimentalist inside the laboratory. The idea was then that one would tune the parameters of the Hamiltonian describing the system in the lab until there was a clear correspondence between the Hamiltonian of the controllable quantum platform in the lab and the conjectured Hamiltonian of the inaccessible system you would like to study. To be more precise, the two systems were said to be *in correspondence*, if by observing the dynamics of the laboratory system you could extrapolate desired properties of the inaccessible system. In modern language, as discussed in Section 1.2.2, we recognise Feynman's vision as that of *analog* quantum simulation - constructing an analog of the system you wish to study in order to mimic aspects of its behaviour and observe its

properties - the quantum equivalent of using a rubber band and a stone to predict where a cannonball might land.

At this point there are two observations to make. Firstly, it must be noted that the notion of analog simulations is indeed an ancient concept - see for example the Greek Antikythera mechanism for making astronomical predictions [45] - and although hindsight is 20/20, it is perhaps surprising that this idea was only first suggested in the 1980's, more than half a century into the age of quantum mechanics. The most plausible reason for this delay is the considerable difficulty inherent in building truly controllable quantum mechanical systems of the type Feynman envisaged. In fact, at the time this was a completely implausible suggestion, and it is only relatively recently, after a significant amount of effort that we have begun to obtain the necessary control over individual quantum mechanical systems in a variety of platforms. Such control is the foundation of all quantum simulation methodologies discussed here, and we refer to the excellent review [2] for an overview of the state of the art, covering trapped ions, cold gases, optical cavities, superconducting-circuits, photonic systems, NMR systems and many others.

The second necessary observation concerns the properties of inaccessible systems that we would like to have access to, in order to make meaningful progress on problems such as the ones listed in the previous section. In particular, it is important to interrogate the extent to which our systems need to be "in correspondence" to allow us to extract the required information. For example, in the context of condensed matter and the study of materials we are most often interested in *linear responses*, such as conductivity, modelled mathematically by time-ordered correlation functions [9]. As a result, having an analogue of the state we wish to study, prepared for example by mimicking the system's dynamics up to some point in time, may not be sufficient. This may be the case if the experimental system does not respond to subsequent perturbations in an analogous way to the system we are trying to study, or if time-ordered correlation functions cannot be extracted easily by some other readily available experimental method. Another example can be found in the high-energy context, where studying the scrambling of information in black holes via the holographic dual theory requires obtaining out-of-time order correlation functions, which are certainly not experimentally accessible in a straightforward way [28,46]. Although the point is subtle, the crux is that in general we can only ever expect our controllable quantum system to mimic *certain aspects* of the system we would like to study, and ensuring the ability to extract the required information is an important prerequisite of any quantum simulation scheme.

At this stage, building on the foundations laid by Feynman, and taking into account

the subtleties and concerns mentioned above, we can put forward our own working definition of quantum simulation.

Definition 1.1 (Quantum simulation)**.** *A quantum simulation of a system S, is any procedure during which control over some quantum mechanical system S', is exploited for the calculation of pre-specificied properties of S.*

This definition is deliberately broad, and we will see in the subsequent sections that it allows us to take a much more nuanced view of quantum simulations than the conventional digital/analog divide which is often discussed. In particular, such a definition, which places a strong emphasis on the ability to extract information, allows for the construction of hybrid simulation methods, with which this thesis will often be concerned.

Before continuing, we note that the definition of quantum simulation put forward above makes no mention of *efficiency*. Of course, the original motivation for developing quantum simulations is rooted in the inefficiency of classical simulation methods, and as such we would like to gain at least a heuristic understanding of when an alternative strategy can be considered efficient. We will postpone a rigorous definition of efficiency (see Section 3.2), and note here that very loosely a simulation can be considered efficient when the number of *standard computational resources* required to obtain the desired pre-specified properties of S' - to within some specified accuracy and with some specified probability of success - scales *polynomially* with respect to the size of S', typically specified by the number of particles S' contains.

The first aspect of this notion of efficiency which requires interrogation is that of "standard computational resources". On a conventional computer we can think of both space resources, such as the amount of memory required, and time resources, such as the amount of clock time or number of fundamental operations required. Similarly, in any controllable quantum platform, there will be both space and time resources, however as we will discuss in detail below, the *standard* resources might vary widely between both the controllable quantum platform and the quantum simulation strategy. The second aspect which requires comment is the use of a polynomial function of the size of S'. While a rigorous discussion of such a requirement can be found in any book on computational complexity [47], the motivation behind such a definition is that asymptotically we would like the number of resources required to grow in a slow manner as the size of the systems we are trying to simulate grows. Although there are many subtleties to this definition, in most senses polynomial functions capture well this behaviour, as opposed to exponential growth functions typical of asymptotic behaviour one would like to avoid.

Given this setting, we can proceed to briefly survey the distinct approaches to quan-

tum simulation which now exist, in order to properly locate the context and setting of this thesis.

1.2.1 Digital quantum simulation

One way to interpret Feynman's proposal for quantum simulators, is as a proposal to build special purpose analog computers in which the information is encoded in the states of the individual quantum mechanical systems comprising the simulator. In this sense, "special purpose" should be understood as meaning that the quantum simulator is only capable of implementing the dynamics of a restricted set of Hamiltonians (determined by the experimental set-up and accessible range of tunable parameters), and subsequently only capable of implementing a subset of all possible physical/unitary transformations. However, a few years after Feynman's original suggestion, inspired by the underlying notion of encoding information into the quantum mechanical states of individual quantum particles, and challenged by a physical reformulation of the Church-Turing thesis, David Deutsch considered the possible structure and potential capabilities of a *universal* quantum computer, capable in principle of implementing *all* unitary transformations [48].

Although Deutsch originally constructed the framework for such a universal quantum computer through a quantum generalisation of a universal Turing machine, it is often now more convenient to consider such a device within the computationally equivalent circuit-model [49]. In this model, a universal quantum computer is typically considered to be any device consisting of the following elements [50]: Firstly, such a device should contain a collection of stable/long lived (typically) two-level quantum mechanical subsystems, now known as qubits, in which information can be encoded[3]. Secondly, the device should be capable of implementing a universal set of fundamental *quantum gates*, which is a subset of unitary operations, such as CNOT's and single qubit gates, with the property that *any* unitary transformation of the global quantum mechanical state can be implemented through sequential implementations of elements of the universal set. Finally, the device should be able to implement arbitrary measurements on any subset of qubits. This model allows us to move beyond just quantum simulations, and consider constructing algorithms, specified via sequences of quantum gates, for more general computational problems. Within this context, the space resources of such a *quantum algorithm* are the required number of qubits, and the time resources can be taken as the

[3]To be *truly* universal the device should really consist of an infinite number of qubits. However, just as the infinite number of tape cells of a classical universal Turing machine can never be realised in practice, we understand that physically realisable approximations of such devices will always be confined to finite numbers of qubits.

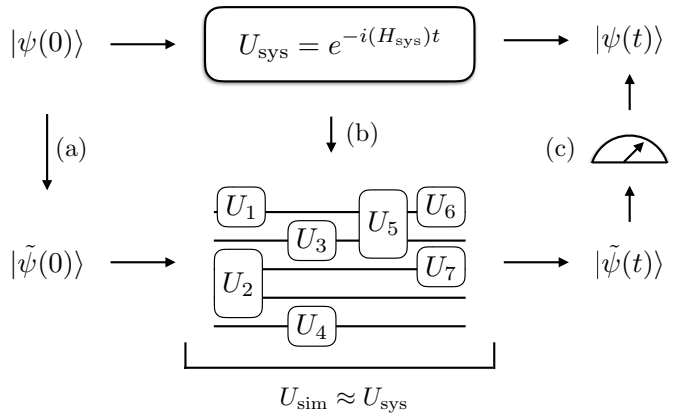

Figure 1.1: An example of a digital quantum simulation for obtaining an approximation to the time evolved state $|\psi(t)\rangle$ of a quantum system specified by a Hamiltonian H_{sys}. (a) An approximation $|\tilde{\psi}(0)\rangle$ to the desired intital state $|\psi(0)\rangle$ needs to be prepared in an array of qubits. (b) The unitary propagator $U_{\text{sys}} = e^{-i(H_{\text{sys}})t}$ needs to be decomposed into a sequence of gates from a universal set, such that $U_{\text{sim}} = \prod_{i=1}^{N} U_i$ approximates U_{sys} to within a desired tolerance. (c) The output state of the quantum circuit $|\tilde{\psi}(t)\rangle$, an approximation to $|\psi(t)\rangle$, needs to be measured to extract information about some pre-specified property of either H_{sys} or $|\psi(t)\rangle$.

number of required gates from the universal set [49]. The study of which problems admit efficient algorithms on a universal quantum computer, and how this set compares with the corresponding set for a classical computer (the physical approximation to a classical universal Turing machine), is now a mature field [51–53]. In particular, this field has provided the impetus (and hype) for the development of such devices by demonstrating the existence of problems, such as integer factorization and the searching of unsorted lists, which admit algorithms on universal quantum computers demonstrating substantial asymptotic speed-ups over the best known classical algorithms [53–55].

At this point, as illustrated in Fig. 1.1, it is possible to understand a *digital quantum simulation* as a quantum algorithm, executed on a universal quantum computer, which calculates some desired pre-specified properties of a given quantum mechanical system. This approach to quantum simulation naturally has a variety of both advantages and handicaps. Firstly, as a natural consequence of universality, digital quantum simulation methods hold the potential to be extremely flexible and versatile. Furthermore, because *any* controllable quantum platform which can realise the three conditions discussed above can be considered a universal quantum computer, such simulations are not restricted to a specific quantum technology. However, in order to achieve such versatility, we

require platforms which can reliably and accurately implement universal gate sets on large numbers of stable qubits - which is unfortunately a highly non-trivial task! Despite these challenges, small scale quantum computers have now been realised in a variety of technologies, and we once again point out the review [2] which offers an excellent overview.

As of yet we have not mentioned *how*, given a specified quantum mechanical system and a desired set of properties, one might go about designing an efficient quantum algorithm (digital quantum simulation) for the calculation of these properties - which is of course in itself a difficult task. As this thesis will be primarily concerned with the construction of methods for the digital quantum simulation of open quantum systems, we will present a technical and detailed discussion of existing digital quantum simulation methods and strategies in Section 1.3.

1.2.2 Analog quantum simulation

In contrast to digital quantum simulations, which are executed on platform nonspecific universal quantum computers, analog quantum simulations are designed to exploit the naturally occurring time-evolution of specific non-universal controllable quantum platforms. As illustrated in Fig. 1.2, and in line with Feynman's seminal vision [1], one aims to tune the parameters of a laboratory based controllable quantum mechanical system until a well defined correspondence exists between the Hamiltonian of the simulator, H_{sim}, and the Hamiltonian of the system to be simulated, H_{sys}. Using the details of this correspondence one could then study a variety of phenomena by observing the dynamics of the laboratory based system, possibly while the controllable parameters are being varied. For example, one might be able to prepare an approximation to the ground state of H_{sys}, or at least a state from which properties of the ground state of H_{sys} can be extrapolated, by cooling the laboratory based system into its ground state. As another example, one might study phase transitions within the inaccessible system by observing the dynamics of the laboratory system as relevant parameters of H_{sim} are varied, or one might study the time evolution via H_{sys} of an initial state $|\psi(0)\rangle$ by observing the time evolution of an approximation to $|\psi(0)\rangle$ under H_{sim}.

As with all simulation methodologies, analog quantum simulation has a variety of strengths and weaknesses. Once again we will briefly mention the most important of these points here, while pointing to the review [2] in which such issues are discussed in detail. Firstly, as a result of the fact that all that is required for an analog quantum simulation is a controllable laboratory based system whose Hamiltonian is in correspondence

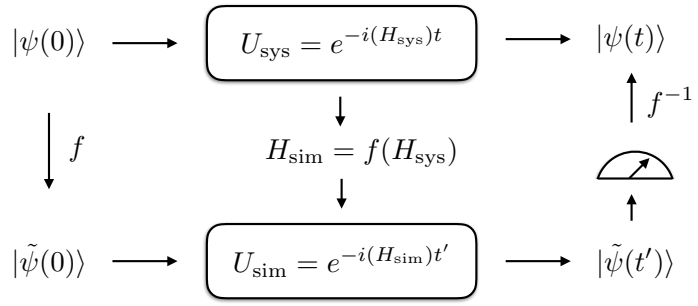

Figure 1.2: An example of a analog quantum simulation for obtaining an approximation to the time evolved state $|\psi(t)\rangle$ of a quantum system specified by a Hamiltonian H_{sys}. The starting point is developing a correspondence f between H_{sys} and the the Hamiltonian H_{sim} of some controllable quantum platform. Given this correspondence one then prepares the initial state $|\tilde{\psi}(0)\rangle$, which is chosen in such a way to ensure that after time evolution under H_{sim} for some period of time t', desired properties of $|\psi(t)\rangle$ can be obtained by applying details of the correspondence to measurement results obtained from $|\tilde{\psi}(t')\rangle$. We note that if the correspondence is truly one-to-one, then we may have $t = t'$, but that generically this is not the case.

with the system you would like to study - as opposed to a fully universal quantum device - the experimental obstacles one is required to overcome are typically far less than for digital quantum simulation, which requires both long lived stable qubits and the ability to accurately and efficiently implement a universal gate set. However, of course the price that you pay for such non-universality is often a confinement to a specific controllable quantum platform for the simulation of a specific class of quantum systems. Another strength however, as a result of the fact that analog quantum simulation typically exploits the naturally occurring continuous time evolution of the laboratory based system, is that analog quantum simulations have the potential to be far more robust than digital quantum simulations against errors and uncertainty within the experimental process, which in digital quantum simulations have the potential to accumulate both with the implementation of each fundamental gate and as the qubit coherence/stability lifetimes are reached. As a result of this inherent robustness, and lower technological/experimental barrier to entry, analog quantum simulations are by far the most advanced and widely utilised quantum simulation methodology, and by this point an incredible number of successful analog quantum simulations have been performed, of a plethora of phenomena, in a large variety of platforms. A detailed list of such successes can be found in [2].

Finally, before moving on it is interesting to briefly explore the notion of efficiency

within the context of analog quantum simulations, which is perhaps slightly more opaque than in the setting of digital quantum simulations, in which the number of qubits and fundamental gates provides a natural measure of space and time complexity. Within the context of analog simulation, it is often most practical to consider the actual time taken by the simulator to yield the desired state or result, and express this as a function of either the system size of the simulated system, or the evolution time one would like to simulate. There are some natural cases, as in the case of simulating time evolution with a system Hamiltonian that is in one to one correspondence with the simulator Hamiltonian, in which the time taken by the simulator will be identical to the time up until which you are trying to simulate. However in other cases, in which the system/simulator correspondence is perhaps more complex, or in which one is trying to perhaps prepare a thermal state or a ground state, the time taken by the simulator might be a more complicated function of either the number of particles in the system or the time which would be naturally taken by the system to be simulated.

Obstacles of this nature are routinely encountered in adiabatic quantum computation, which can be thought of as an analog simulation approach to quantum computation [56, 57]. Very roughly, in this approach to quantum computation, the solution to some computational problem is encoded in the ground state of some potentially complicated Hamiltonian H_{fin}, and the task is to prepare this state. To do this, one looks for a Hamiltonian H_{ini}, whose ground state can be easily realised in the laboratory, and which can be transformed into H_{fin} through a continuous variation of parameters over which the experimentalist has control. The adiabatic theorem then tells us that if one "slowly" varies the parameters in the Hamiltonian, starting from H_{ini} and ending in H_{fin}, then one can prepare the desired ground state of H_{fin} - i.e. one has to essentially perform an analog simulation with a computational interpretation. The crux is that the how "slowly" one must go depends on the properties of H_{fin} (the spectral gap, to be precise) and in some cases the amount of time required by this process can be an exponential function of the number of particles in the system [58].

1.2.3 Digital/Analog quantum simulation

Typical introductions to quantum simulation tend to separate all quantum simulations into either analog or digital simulations. However, recent years have witnessed the birth and evolution of a variety of hybrid approaches to quantum simulation, which aim to incorporate strengths of both digital and analog methodologies. As a result, these methods offer a particularly promising and appealing approach to quantum simulation. Of

these emerging strategies, the first hybrid approach that we shall discuss is (fittingly) referred to as digital/analog quantum simulation [59–61]. In particular, this approach aims to exploit the flexibility of digital quantum simulations while simultaneously leveraging the ability of analog simulation platforms to easily implement certain classes of complex quantum dynamics.

In order to understand this approach it is useful to undertake a sceptical re-examination of digital quantum simulation from a variety of perspectives. Firstly, what actually happens when one implements a gate U_j from a universal gate set? In essence, although at a risk of being over simplistic for illustrative purposes, typically the experimentalist is implementing the time evolution according to some corresponding Hamiltonian H_j, for a specific period of time t, such that $U_j = e^{-iH_j t}$. Building a universal quantum computer then, in a very loose sense, consists of building a controllable quantum platform which is capable of realising (or simulating) all the Hamiltonians required to implement a complete set of universal gates, which is a formidable task. However, as we have hinted at in our discussion of analog quantum simulation, there are a plethora of currently available quantum platforms, each of which can implement a specific class of interesting Hamiltonians [2]. Typically, in an analog quantum simulation as conventionally understood, as illustrated in Fig. 1.2, one selects a specific setting of the simulator Hamiltonian parameters, in correspondence with some desired system Hamiltonian, and then completes the simulation either slowly varying or keeping these parameters constant. However, if we interpret the implementation of a quantum gate U_j as an analog simulation of some Hamilton H_j for a specific period of time, then we see that in fact we could view a given analog quantum simulator as being to implement a *platform-specific, non-universal*, set of quantum gates - each one corresponding to the evolution of the simulator Hamiltonian with some specific parameter settings, for some specific amount of time. If one views the capabilities of an analog quantum simulator in this way, then one can extract more flexibility from the specific experimental platform by utilising the digital strategy of implementing a desired task via a sequence of quantum gates.

With this point of view, one can view digital/analog quantum simulations, illustrated in Fig. 1.3, as being simulations in which the desired properties of some system are calculated via quantum algorithms specified not in terms of sequences of gates from a universal set, but rather in terms of platform specific (possibly non-universal) quantum gates which exploit the naturally occurring physical properties of the quantum simulator at hand. As a result, such a strategy inherits some of the flexibility of digital quantum simulation (though not necessarily its universality), while retaining the practical advantages of analog quantum simulation. Of course, there is a reasonable argument to be

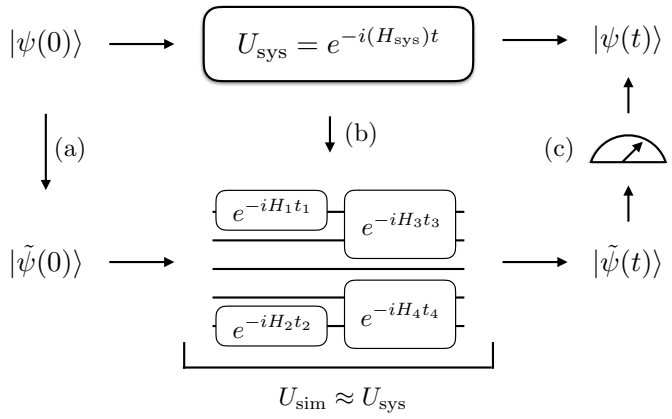

Figure 1.3: An example of a digital/analog quantum simulation for obtaining an approximation to the time evolved state $|\psi(t)\rangle$ of a quantum system specified by a Hamiltonian H_{sys}. The methodology is very similar to that of digital quantum simulation, as illustrated in Fig. 1.1, however in this case the unitary evolution to be approximated is decomposed into a sequence of possibly non-universal naturally occurring (or more readily available) platform specific quantum gates $e^{-iH_jt_j}$.

made that the strategy described above is really nothing but an analog quantum simulation, in which each subsequent "gate" just corresponds to a well timed changing of the simulator Hamiltonian parameters! However, there is another reasonable argument to be made that this is nothing but a digital quantum simulation with a restricted/natural gate set [4]! However persuasive these arguments, typical approaches to both analog and digital quantum simulation are not phrased in this manner, and we feel that one can gain both a particularly useful perspective and novel design toolbox by drawing a conceptual distinction between conventional analog simulations, conventional digital simulations and digital/analog simulations as discussed here. In addition, recent years have seen a variety of both proposals for, and realisations of, digital/analog simulations, for a plethora of physical models, and as such the distinction drawn here represents accurately the current state of the art [59–61].

Furthermore, another strong motivating factor for such an approach to quantum simulation is that certain desired operations may be much more easily achieved by utilising naturally occurring interactions/processes within the available quantum platform, as opposed to concatenations of gates from a conventional universal set. A first natural example of such a situation can be found within the context of trapped ions, where a particularly highly useful global entangling operation can be achieved extremely easily

through one application of a readily available operation known as the Mølmer-Sørensen (MS) gate, but would require multiple CNOT gates if decomposed into a conventional sequence of universal gates [62, 63]. Within the context of trapped ions, it therefore makes far more sense to express a given algorithm requiring such an entangling operation in terms of MS gates, as opposed to CNOT's [64]. A second example of such a situation, which is highly relevant to this thesis, is the simulation of open quantum systems. As will be explained in much more detail in Section 1.4, conventional digital approaches to the simulation of open quantum systems often involve the introduction of a significant number of additional ancilla qubits. However, *all* physical controllable quantum platforms have some type of environment induced naturally occurring dissipation and decoherence, and in many cases much more efficient simulation methods may be devised if one utilises these dissipative processes as "gates" within the simulation algorithm [65, 66].

These last two examples force us once again to interrogate the notions of efficiency and *standard computational resources* within the framework of digital/analog simulation. In particular, using the example of the MS gate, if performing a simulation within trapped ions it makes sense to view this gate as such a standard resource, and evaluate the complexity of the algorithm not necessarily in terms of the number of CNOT gates required, but rather in terms of the number of MS gates required. We therefore see that the evaluation of efficiency within a digital/analog context needs to be performed on a platform specific basis, given a reasonable evaluation of what can be considered standard computational resources within the given platform. It is also clear how this approach provides a more pragmatic strategy than the more abstract methodology of constructing an algorithm in terms of sequences of universal gates, which may not be physically realisable in a straightforward manner. In addition, as we will see in subsequent chapters, within the context of open quantum systems it allows us to shift our attitude towards dissipation and decoherence - instead of viewing these processes as obstacles to be overcome if one wants implement accurate fundamental gates or maintain long qubit lifetimes, one can potentially view dissipation and decoherence as a computational resource [65]!

1.2.4 Algorithmic quantum simulation

In all of the strategies that we have discussed so far, there has been an implicit suggestion that the entire simulation, or computational process, takes place within the controllable quantum system (the simulator). While such an approach is potentially feasible - and has definitely seen some success in the context of analog quantum simulations [2] - im-

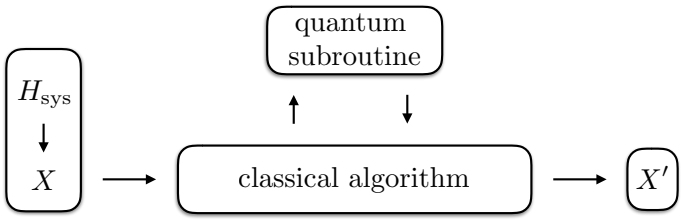

Figure 1.4: An illustration of the algorithmic quantum simulation methodology. The inputs to the simulation are a description of a system H_{sys}, as well as a specification of some property X of the system one would like to calculate (in the case of time evolution, the description of the system may include a particular desired initial state $|\psi(0)\rangle$). An algorithmic simulation is then a classical algorithm, which makes calls to a quantum subroutine executed either on a quantum simulator or universal quantum computer, and which outputs X', an approximation to X.

plementing digital or digital/analog simulations which are beyond the reach of current classical computers will require large scale quantum computational devices, capable of fault-tolerantly implementing thousands of quantum gates, on at least hundreds (but more realistically thousands) of stable qubits. Although rapid progress is being made in our ability to perform digital and digital/analog simulations, especially within superconducting circuit architectures [67–69], scalability of these devices is still a formidable challenge and it is unclear when the large scale quantum computational devices required to consistently outperform the best classical algorithms will be available.

In light of this, one natural approach, which is variously referred to as either algorithmic quantum simulation or hybrid quantum/classical simulation, seeks to outsource to a conventional classical computer all possible computation which can be done efficiently on such a platform [32, 70–73]. The hope is that many simulations of quantum many-body systems might be broken down into classical algorithms, possibly employing some approximation methods, which are inefficient because of the need to solve some smaller problem than the entire simulation, which might be done efficiently on a quantum computer. The entire process, as illustrated in Fig. 1.4, then involves a feedback loop between a classical computer and a quantum simulator (of any type), and in the ideal case will run efficiently while requiring a much smaller controllable quantum platform than would be required if the entire simulation was to be done in a quantum manner.

As in the case of digital/analog simulation, the adoption and formulation of such a strategy is clearly motivated by a realisation of the potential of quantum simulations,

but with a strong view towards pragmatism and ensuring that minimal amounts of expensive and complex quantum resources are required. Again, it is clear that one could argue that *all* quantum simulations are in fact hybrid quantum/classical simulations, as one inevitably has to use a classical computer to perform tasks such as processing of final measurement results, and that in fact such an approach is clearly the most natural strategy. However, while this is correct in some sense, it is clear that there is a conceptual distinction between the use of a classical computer to perform processing of data, and the use of a classical computer to perform a complex algorithm which calls a (potentially small-scale) quantum simulator to execute a specific subroutine. As with digital/analog quantum simulations, we believe that an advantage can be gained from referring to the latter case (though the line may admittedly be hard to draw) as algorithmic, or hybrid quantum/classical simulation, as this labelling may potentially prompt or inspire the development of novel algorithms and techniques.

Given that the notion of algorithmic quantum simulation is indeed very natural, it may not be surprising that there have recently been a number of proposals for algorithmic quantum simulation of a large variety of systems. As a first example, it has been realised that Dynamical Mean Field Theory, a widely utilised classical algorithm for calculating properties of strongly correlated fermion systems, can be greatly improved by solving the impurity problem at the root of the classical algorithm on a quantum simulator, which may only need to contain hundreds of qubits to outperform the entire algorithm running on a classical computer [70–72]. In the context of quantum chemistry, such an approach has also been used to develop algorithmic methods for the calculation of molecular energies, in which the quantum phase estimation algorithm is used as the critical subroutine within a larger classical algorithm [29]. Then, in the context of open quantum systems, it has been shown how simulations of memory effects in a specific system may be achieved via a classical algorithm which requires simulations of different open quantum systems exhibiting no memory effects [73], which is far easier to achieve (and for which, in fact, a variety of methods are presented in this thesis). Finally, as will be discussed in more detail in Section 1.5, in Chapter 4 we provide a method for how one might implement non-completely positive maps, describing the evolution of open quantum systems initially correlated with their environment, via an algorithmic procedure only requiring simulations of conventional quantum channels [74].

1.2.5 Embedded quantum simulation

Apart from algorithmic quantum simulations, another implicit assumption in the other simulation strategies presented in this section is that the simulations were *one-to-one*. By this, we mean that typically (though, not always) the size/number of particles in the simulator is the same as the number of particles in the system one is trying to simulate, and as illustrated in Figs 1.1, 1.2 and 1.3, one typically obtains from the simulator a state $|\tilde{\psi}(t)\rangle$ which is a direct approximation to some state $|\psi(t)\rangle$, about whose properties you are interested. In order to obtain these properties, such as the expectation value of some observable, one then has to prepare and appropriately measure the state multiple times, which is relatively straightforward.

However, as stressed earlier, in order to answer the physical questions with which one might be concerned, which motivate the simulation in the first place, it may very often be necessary to obtain properties of H_{sys} or $|\psi(t)\rangle$ which *cannot* be straightforwardly calculated from a one-to-one approximation $|\tilde{\psi}(t)\rangle$. Natural examples of such properties are multi-time and out-of-time order correlation functions, as well entanglement monotones, which require an expensive full quantum state tomography procedure [75]. In order to address this critical issue, a natural approach, illustrated in Fig. 1.5 and which has begun to be labelled as *embedding* quantum simulators, is to add additional ancillary particles, and then design the simulation in such a way that is not necessarily one-to-one, as is most intuitive, but that ensures that the properties one is interested in can be easily obtained from an *efficient* number of straightforward measurements of either just the ancillary particles, or the entire output state of the simulator [76]. Perhaps naturally, there now exist explicit proposals for how one might embed quantum simulators for the calculation of the properties discussed above, such as multi-time correlation functions [77] and entanglement monotones [76]. Surprisingly, there have also been proposals for the simulation of *unphysical* operations, such as charge conjugation, via embedded quantum simulators [78]. It is interesting to note that embedding a quantum simulator naturally involves optimising a trade-off between space and time complexity. An embedded quantum simulator may require more qubits, however the time cost (number of gates, real time or repetitions of the experiment required) may be drastically reduced by virtue of being easily able to extract the desired information from the output state of the simulator.

Once again it is clear, especially in light of the working definition of quantum simulation provided in this thesis (which prioritises the calculation of any pre-specified property), that one could strongly argue that the notions of simulation previously dis-

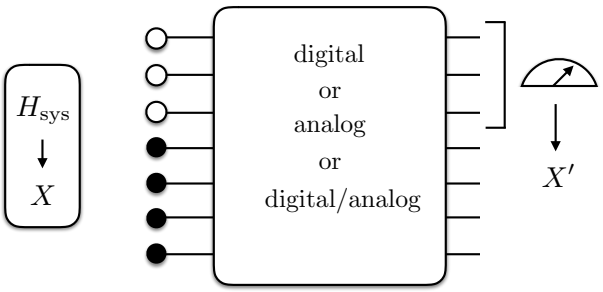

Figure 1.5: An illustration of the notion of an embedded quantum simulation. Again, one is given a description of a system H_{sys}, as well as a specification of some property X of the system one would like to calculate. On a quantum simulator with additional ancillary qubits, shown as empty circles, one then executes either a digital, analog or digital/analog quantum simulation, designed in such a way that an approximation to X' can be extracted via measurements of the ancillary qubits. This is in contrast to a one-to-one simulation which would typically mimic the dynamics of H_{sys} in a quantum simulator consisting only of system qubits, shown as filled circles.

cussed already include the possibility of adding additional particles as a computational device. Certainly, it is true that at no point in our discussion have we specified that any of the previous simulation strategies are confined to being one-to-one. However, the crux is that the vast majority of current simulation methods, both proposed and realised, *are* one-to-one simulations. As such there is potentially a lot to be gained by making explicit the distinction between one-to-one simulations and embedded simulations, as it not only provides a spotlight on the issue of providing efficient means for calculating specific non-trivial properties, but also suggests an avenue for how this might be achieved. Even so, it is certainly true that the notion of embedded quantum simulators is not quite a completely distinct quantum simulation strategy, but rather a complimentary or additional approach which could, and often should, be combined with another simulation strategy as a means to enhance the versatility and flexibility of the underlying method.

1.2.6 Verifying quantum simulations

As quantum technology develops, and large scale quantum simulations become a reality, an increasingly important question is: *how do we know that our simulation is correct?* After all, a quantum simulation by (our) definition exploits the dynamics of some quantum mechanical system, whose properties are often non-trivial to model in the first place and require a host of simplifying assumptions. This is especially true as quantum simu-

lators grow in size, and more and more complicated methodologies and interactions are exploited. While this is certainly an important question, in some sense, as we will briefly discuss now, the answer is as straightforward or as complicated as one prefers.

On the one hand, many will argue that the solution to this problem is both clear and straightforward. We gain confidence in the correctness or accuracy of a simulation if its results agree with both our analytical predictions and the results of alternative simulation methods, both in classical and quantum devices. If one adopts this natural approach, then the key to gaining confidence in the results of quantum simulations relies on progress in multiple fronts. Firstly, given a specific system to be simulated, it is essential to develop multiple methods for its simulation on alternative quantum and classical devices, in order to facilitate benchmarking of the results. Secondly, given a specific quantum platform or simulator, it is important to develop more accurate models for the simulators themselves, and benchmark these models via experiments in a variety of parameter regimes. Finally, it is important to invest effort in the development of improved mathematical and analytical models of the systems we are trying to simulate. This approach is certainly the most natural, and allows us to gain more and more confidence in the results of quantum simulations as progress is naturally made in all relevant fields, both experimental and theoretical.

However, often we would like to use a specific quantum simulation precisely because the system that we are interested in *cannot* be easily simulated on a classical computer. In addition, it might be true that the quantum simulation we have in mind relies on very specific properties of a specific controllable quantum platform, and alternative quantum simulation methods in different platforms *cannot* be easily derived. Furthermore, it may be possible that we can propose alternative simulation methods on different quantum technologies, but that these technologies are not currently well developed enough to implement such proposals. In all such cases, which at present are certainly plausible, it is necessary to develop intrinsic methods which allow us to trust the results of a single computational process or simulation, which is a significantly more complicated approach.

At present there are a variety of strategies for achieving such methods. Firstly, within the context of digital quantum simulations, there is a massive effort to develop quantum error-correction methods. These methods allow for the implementation of quantum algorithms in a manner which is fault-tolerant and robust against certain classes of noise and errors, provided that these errors occur with a frequency less than some threshold dictated by the error correction scheme. In this approach, provided the error rate is low enough, and that the source of the errors is well understood, we can trust the result of our simulation as long as our underlying algorithm is correct. This is an important and

rapidly growing approach, incorporating a vast number of techniques, and we refer to the excellent books and reviews [79–81] for an overview.

Another interesting and more recent approach is that of verification based on interactive proofs. In this strategy, which incorporates methods from complexity theory which we will only very briefly sketch here, one can design the simulation in such a way that requires interaction with a "sceptical prover", who is able to make a final decision regarding the correctness of the computation [82–84]. These emerging methods certainly hold both considerable conceptual appeal and potential, and it will be interesting to follow the extent to which they can be generalised away from the highly specific contexts in which they are being developed (such as measurement based quantum computing, or provers with access to a quantum computer), towards more natural frameworks such as analog quantum simulations and provers with purely classical resources [85–87].

1.3 Strategies for digital quantum simulation

So far our discussions of quantum simulation have been primarily conceptual, and perhaps even partly philosophical. However, as this thesis will be uniquely concerned with the presentation of novel digital and digital/analog techniques for the simulation of open quantum systems, in this section we will provide a slightly more technical introduction to digital quantum simulation methodologies, within the context of closed quantum systems for simplicity, with the aim of providing the formal foundations for the new results presented in this work. Once again we note that a thorough and complete overview of contemporary digital quantum simulation strategies is not necessary to provide the background and context that we require, and so we refer to the reviews [2–4] for a survey of additional techniques not covered in this section.

Firstly, in this thesis we will be uniquely concerned with digital or digital/analog quantum simulation strategies for simulating *time evolution*, as opposed to for instance finding ground states or preparing thermal states, and as such we restrict ourselves to this setting here. Within the context of closed quantum systems this problem can be formulated as follows:

Problem 1.1. *Given a description of a time-independent Hamiltonian H, an initial state $|\psi(t_0)\rangle$, a desired final time t and an acceptable error tolerance ϵ, construct an algorithm which yields a state $|\tilde{\psi}(t)\rangle$ such that*

$$\big|\big||\tilde{\psi}(t)\rangle - |\psi(t)\rangle\big|\big| \leq \epsilon, \tag{1.1}$$

where $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle = e^{-iH(t-t_0)}|\psi(t_0)\rangle$.

In other words, more colloquially, we want an algorithm which provides an approximation to the time-evolved state of a system described by some Hamiltonian H, at some given time t, having started from some well defined initial state $|\psi(0)\rangle$. At this point, a few comments are in order. Firstly, the above problem can obviously be straightforwardly generalised to the context of time-*dependent* Hamiltonians, which would just require specifying that

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle = \mathcal{T}e^{-i\int_{t_0}^{t} H(\tau)d\tau}|\psi(t_0)\rangle, \tag{1.2}$$

i.e. the system propagator $U(t,t_0)$ is just given in this case by the time-ordered exponential of the Hamiltonian [88]. With this straightforward generalisation in mind, we will from now restrict ourself in this section to the simpler case of time-dependent Hamiltonians. Secondly, we have not specified the norm in Eq. (1.1). There are a variety of ways to measure the distance between quantum states, and in principle any of these measures might suffice within this problem definition, depending on the context and the desired properties of $|\psi(t)\rangle$ one would like to calculate [49]. However, typically one would use the so called trace or 1-norm, which provides a measure of how well two states can be distinguished if one is allowed to perform arbitrary measurements on either state [49]. In later chapters we will provide a more thorough definition and motivations of the utilised norms, but for now we choose to leave this unspecified, and note that one may refer to [49, 89] for a detailed discussion of such issues. Finally, we assume that the desired initial state $|\psi(0)\rangle$ can be easily prepared, and is available as an input to our algorithm at no cost. Although this assumption is often highly problematic in practice, and constructing methods for the efficient preparation of physically relevant classes of quantum states is an active and important research topic [2], with this simplifying assumption the problem above is equivalent to constructing a circuit/algorithm U such that

$$||U - U(t,t_0)|| \leq \epsilon', \tag{1.3}$$

with the norm and the value of ϵ' chosen in such a way so as to ensure that condition (1.3) implies condition (1.1).

Now, given an algorithm which provides a solution to the problem specified above, with the caveats concerning initial state preparation, how do we determine whether or not our algorithm is *efficient*. Firstly, lets specify that the Hamiltonian H acts on n qubits. Then, in line with our earlier discussions, we say that the algorithm, specified

by a quantum circuit U of standard gates, is efficient if U consists of $\text{poly}(n, t, 1/\epsilon)$ gates, where poly just denotes any polynomial function [2–4]. Once again, as per our examination of the subtle difference between digital and digital/analog simulations, we explicitly point out that the notion of "standard gates" may depend on the experimental context. Given this definition of efficiency, we now say that a Hamiltonian H can be efficiently simulated if there exists an efficient algorithm solving Problem 1.1 for all $t > 0$.

So, within this setting, given a description of a Hamiltonian H acting on n qubits, when and how can we come up with an efficient algorithm for the digital quantum simulation of the time evolution of the system described by H? Although by no means complete, "Childs' rules" provide a list of Hamiltonians for which straightforward techniques exist [57]. As generalisations of these techniques will form the foundation for our efforts to provide methods for the digital(/analog) simulation of open quantum systems, it is of value to reproduce here those rules which are of relevance to us, along with some brief comments foreshadowing issues concerning their generalisation to the open quantum systems context. The complete list of rules, from which the following are extracted, can be found in the Ph.D. thesis of Andrew Childs [57].

Rule 1.1 (Strictly Local Hamiltonians)**.** *If H acts non-trivially on only a constant ($\mathcal{O}(1)$) number of qubits, then it can be efficiently simulated.*

Any such Hamiltonian, which acts non-trivially on only a constant number of qubits, as the size n of the system is possibly increased (as indicated by the Bachmann-Landau "big-O" notation [47]), will be referred to as a *strictly local* Hamiltonian. In other words, strictly local Hamiltonians can be thought of as Hamiltonians acting non-trivially on a number of qubits which does not depend on the total system size. The fact that such Hamiltonians can be efficiently simulated follows from the Solovay-Kitaev theorem [90], a foundational result in the theory of quantum computing, which we will not present here.

Rule 1.2 (Rescaling)**.** *If H can be efficiently simulated, then cH can be efficiently simulated for $c = \text{poly}(n)$.*

Interestingly, for Hamiltonian simulation, this rule is *not* restricted to $c > 0$, as a result of the reversibility of quantum computation. However, it is important to note that the analogous rule will not hold for negative c in the context of digital/analog simulation of open quantum systems, as discussed in detail in Chapter 4, as a result of both the irreversibility of analog dissipative gates and additional subtleties concerning completely-positive maps, as will be introduced in Section 1.4.

Rule 1.3 (Unitary Conjugation)**.** *If H can be efficiently simulated, and the unitary transformation U can be efficiently implemented, then $UHU^\dagger$ can be efficiently simulated.*

Essentially this rule, which follows straightforwardly from the identity

$$e^{-iUHU^\dagger} = Ue^{-iH}U^\dagger, \tag{1.4}$$

tells us that the Hamiltonian H can be efficiently simulated in any basis, as long as the basis transformation itself can be efficiently implemented. This rule provides an extremely useful tool for algorithm construction, and in Chapters 2 and 3 we will provide a generalisation of this rule to a particular class of open quantum systems, as first presented in [91].

Rule 1.4 (Sums of Hamiltonians)**.** *If H_1 and H_2 can be efficiently simulated, then $H_1 + H_2$ can be efficiently simulated.*

In the simple case when H_1 and H_2 commute, this is easy to see, as

$$[H_1, H_2] = 0 \implies e^{-i(H_1+H_2)t} = e^{-iH_1t}e^{-iH_2t}. \tag{1.5}$$

In the case when $[H_1, H_2] \neq 0$, the starting point for demonstrating the truth of Rule 1.4 is the Lie-Trotter product formula [92],

$$e^{-i(H_1+H_2)t} = \lim_{m\to\infty} \left(e^{-iH_1t/m}e^{-iH_2t/m}\right)^m. \tag{1.6}$$

In particular, given some $\epsilon > 0$, one can show that if one wants to truncate the right hand side of eq. 1.6 such that

$$\left|\left|\left(e^{-iH_1t/m}e^{-iH_2t/m}\right)^m - e^{-i(H_1+H_2)t}\right|\right| \leq \epsilon, \tag{1.7}$$

then it suffices to take $m = \mathcal{O}((\nu t)^2/\epsilon)$, where $\nu \equiv \max\{||H_1||, ||H_2||\}$ [57]. If H_1 and H_2 can be efficiently simulated, this then implies that $\nu = \text{poly}(n)$, and therefore that $H = H_1 + H_2$ can be efficiently simulated (as a result of the fact that compositions of polynomials are again polynomials).

Now, either using compositions of Rule 1.4, or by using the same strategy as utilised to prove Rule 1.4, one can in fact show that given $k = \text{poly}(n)$ Hamiltonians $\{H_i\}|_{i=1}^k$, each of which can be efficiently simulated, then $H = \sum_{i=1}^k H_i$ can be efficiently simulated.

This follows from the observation that

$$\Big|\Big|\Big(\prod_{i=1}^{k} e^{-iH_i t/m}\Big)^m - e^{-i(\sum_{i=1}^{k} H_i)t}\Big|\Big| \leq \epsilon, \tag{1.8}$$

provided $m = \mathcal{O}(k(\tilde{\nu}t)^2/\epsilon)$, where $\tilde{\nu} \equiv \max_i\{||H_i||\}$ [57].

At this stage, by combining Rules 1.1, 1.2 and 1.4, we see that in fact any linear combination of $k = \text{poly}(n)$ strictly local Hamiltonians can be efficiently simulated! This was first pointed out by Lloyd in his seminal 1996 paper [93], and has extremely powerful implications for the simulation of *physical* Hamiltonians. In particular, particles in generic many-body quantum mechanical systems typically interact directly only with a small number of their closest nearest neighbours, and as a result Hamiltonians describing such realistic physical systems can naturally be written as a sum of strictly local Hamiltonians. Furthermore, in physical systems with such geometrically local interactions, a simple counting argument shows that the number of strictly local terms in the Hamiltonian is generically proportional to the number of particles in the system [4], and as such the system can be efficiently simulated. As an example, this is clearly illustrated by the one-dimensional Ising model for a spin chain of length n with periodic boundary conditions,

$$H = \sum_{j=1}^{n} \big(- J(\sigma_j^z \sigma_{j+1}^z) - \mu\ \sigma_j^x \big) \tag{1.9}$$

$$= \sum_{j=1}^{n} H_{(j,j+1)}, \tag{1.10}$$

which is the sum of n nearest-neighbour, or strictly 2-local, Hamiltonians.

Since Lloyd's landmark result in 1996, which (along with Peter Shor's 1995 quantum algorithm for efficient integer factorisation [54]) provided a massive motivation for the development of digital quantum computers, there has been a gigantic effort to both improve upon the efficiency of Lloyd's fundamental result, and extend the class of Hamiltonians which can be efficiently simulated [3, 4]. While we will not survey these efforts in detail, it will be worthwhile to present a few key tools and directions, with the goal of extracting the dominant strategies and approaches, which will later be adopted in this thesis for the simulation of open quantum systems.

Firstly, given $H = \sum_{i=1}^{k} H_i$, lets define N_{exp} as the number of short-time simulations of individual Hamiltonians H_i required to simulate H to within an accuracy of some given ϵ. From Eq. 1.8 we see that in Lloyd's original method, which involves simulating

each Hamiltonian H_i sequentially for a time period of t/m, and repeating this process m times, we have that

$$N_{\text{exp}} = km = \mathcal{O}(k^2(\tilde{\nu}t)^2/\epsilon). \tag{1.11}$$

A natural question to ask is whether we might be able to improve the scaling of N_{exp} with respect to parameters such as t and ϵ? It turns out that this is indeed the case, and while many results have been achieved with respect to the scaling in ϵ (see [3]) for a detailed discussion), we will focus here on the scaling with respect to t, which can be improved through a more sophisticated approach to approximating the exponential of sums of non-commuting operators, and will be of interest to us in the remainder of the thesis. In particular, through the use of Suzuki's higher order integrators [94, 95], which will be presented here, one can achieve scaling in t which is arbitrarily close to linear [96]. To do this, one defines a simple variant of the basic Lie-Trotter formula as the first order Suzuki integrator,

$$S_2(\lambda) = \prod_{j=1}^{k} e^{H_j\lambda} \prod_{j'=k}^{1} e^{H_{j'}\lambda}, \tag{1.12}$$

from which the δ'th higher order integrator can be defined via the recursion relation

$$S_{2\delta}(\lambda) = [S_{2\delta-2}(p_\delta\lambda)]^2 S_{2\delta-2}((1-4p_\delta)\lambda)[S_{2\delta-2}(p_\delta\lambda)]^2, \tag{1.13}$$

with $p_\delta = (4 - 4^{1/(2\delta-1)})^{-1}$ for $\delta > 1$. Given this formalism, analogously to eqs. (1.7) and (1.8), we would now like to understand the efficiency of approximating e^{-iHt} with expressions of the form $[S_{2\delta}(-it/m)]^m$ for various values of m and δ. Such an understanding is provided by the following theorem, summarising results originally proven in [96]:

Theorem 1.1. *Given any ϵ such that $0 < \epsilon \leq 1 \leq 2k5^{\delta-1}||H||t$, where δ is an arbitrary positive integer, taking*

$$m = \frac{2^{1/2\delta}(2k5^{\delta-1}||H||t)^{1+1/2\delta}}{\epsilon^{1/2\delta}}, \tag{1.14}$$

guarantees that

$$\left|\left|[S_{2\delta}(-it/m)]^m - e^{-i(\sum_{i=1}^{k} H_i)t}\right|\right| \leq \epsilon, \tag{1.15}$$

and that

$$N_{\text{exp}} \leq k5^{2\delta}(k||H||t)^{1+1/2\delta}/\epsilon^{1/2\delta}. \tag{1.16}$$

In particular, it is now clear from Theorem 1.1 that by taking δ arbitrarily large we

can achieve scaling in t which is arbitrarily close to linear. However, as noted in [96], the right hand side of eq. (1.16) is minimized for

$$\delta = \text{round}\Big[\frac{1}{2}\sqrt{\log_5(k||H||t/\epsilon)+1}\Big], \tag{1.17}$$

which when substituted into eq. (1.16) yields

$$N_{\text{exp}} \leq 2k^2||H||te^{2\sqrt{\ln(5)\ln(k||H||t/\epsilon)}}. \tag{1.18}$$

As we set out to achieve, the scaling in (1.18), which is now independent of δ, is close to linear in t for large values of $k||H||t$. Interestingly, as discussed in [89, 96], this scaling is close to optimal, as one can show that sublinear scaling in t is not possible for generic Hamiltonians, a result known as the "no fast-forwarding" theorem. However, despite being very close to optimal, these results can in fact be slightly improved by taking into account the norms of individual constituent Hamiltonians [97], and such improved Suzuki-Lie-Trotter (SLT) results will be of use to us in Chapters 2 and 3, where they will be presented in detail. Furthermore, it is also possible to generalise such SLT constructions for the simulation of time-dependent Hamiltonians [98, 99], and such results will be extensively utilised in Chapter 4, where they will be presented in detail.

So far we have considered only the simulation of local Hamiltonians, which are naturally specified as the sum of strictly-local Hamiltonians. In this case, we have seen that through *stroboscopic* implementation of the (rescaled) constituent strictly-local Hamiltonians, formalised via some flavour of SLT decomposition, we can efficiently simulate the total Hamiltonian. While such a setting is definitely the most natural for *physical* Hamiltonians, it is also of interest, both for the simulation of certain physical systems and for the construction of algorithms which rely on the simulation of some Hamiltonian, to consider methods for the efficient simulation of more general Hamiltonians. In this regard, we begin by noting that if we have a system of n qubits, then a generic Hamiltonian for such a system will be a $2^n \times 2^n$ Hermitian matrix, and as such storing or reading every matrix element is clearly not possible in an efficient manner. As such, a natural setting for considering the simulation of more general Hamiltonians is to assume the existence of an oracle, which when provided with a row and column number, can provide the matrix entry at that location [57, 89]. Within this setting, a large amount of effort has been invested into developing methods for the simulation of *sparse* Hamiltonians [3, 89, 100–106], while various fundamental limitations concerning the efficient simulation of non-sparse Hamiltonians have been formulated [89, 107].

While a variety of methods are now known for the simulation of sparse Hamiltonians [100–106], with recent methods achieving scaling which is nearly optimal in almost all relevant parameters [105,106], it is of interest to us to very briefly discuss the strategy behind early approaches for the simulation of such Hamiltonians, as such strategies will be heavily utilised in the remainder of this thesis. In particular, from our discussion of Childs' rules we have seen that there is a class of Hamiltonians which can be efficiently simulated. From our discussion of SLT decompositions we then saw that any linear combination of Hamiltonians which can be efficiently simulated, can again be efficiently simulated. The natural idea behind early approaches to the simulation of sparse Hamiltonians, is then to come up with an *efficient* method for decomposing the given sparse Hamiltonian into the linear combination of constituent Hamiltonians, which one can prove can be efficiently simulated. As long as this decomposition results in a polynomial number of constituent Hamiltonians, then SLT methods, as presented above, can be utilised to efficiently recombine these Hamiltonians into an acceptable approximation of the original Hamiltonian [89]. We will call such a strategy a *decomposition/recombination* approach. As mentioned above, such an approach, largely exploiting graph-theoretic decompositions of the given sparse Hamiltonian, provided many of the first algorithms for the simulation of sparse Hamiltonians [89]. Such a decomposition/recombination approach will also play a crucial role in the methods for the simulation of open quantum systems presented in Chapters 2 and 3.

1.4 Open quantum systems

As of yet, to allow for both illustration and clarity, we have restricted ourselves to discussions concerning closed, or isolated, quantum mechanical systems. However, most realistic quantum systems are in contact with some environment to some extent, at least over realistically accessible time scales, and as such developing an understanding of so called *open quantum systems* is a crucial task. As this thesis is concerned with the construction of methods for the digital, digital/analog and algorithmic quantum simulation of certain classes of open quantum systems, we will now proceed to shift our attention to such systems. In particular, we aim in this section to provide a motivation for the study of open quantum systems, an introduction to the formalism of such systems, and a brief overview of previous work regarding the quantum simulation of open quantum systems. This will allow us to situate the novel contributions of this thesis within the context of current research.

1.4.1 Motivation

As discussed in Section 1.1, contemporary physics offers a wealth of fascinating directions, unanswered questions and important paradoxes to explore, and this is just as true for the field of open quantum systems as it is for many-body quantum physics in general. While a complete and thorough overview of contemporary research directions is beyond the scope of this work, we will aim in this section to provide a (very) brief sketch of a selection of current fields of interest, towards which it is hoped that the simulation methods presented in this thesis may make some direct contribution.

Phase transitions and criticality in driven-dissipative many-body open quantum systems: In recent years, largely resulting from developments in quantum technologies which have enabled the prospect of experimental preparation and observation of driven-dissipative many-body quantum systems [66, 108–110], there has been an incredible interest in obtaining a foundational understanding of the non-equilibrium phases and phase transitions in such systems. In particular, it is now appreciated that the competition between coherent and dissipative dynamics in the non-thermal and non-equilibrium steady states of such systems gives rise to an incredibly rich phenomenology, such as new universality classes, often with no immediate analogue in conventional isolated many-body systems [111–128]. Additionally, it is interesting to point out that developments in quantum technologies have spurred the study not only of dissipative generalisations of conventional many-body models from the condensed matter context, but also of novel open many-body quantum systems, such as Jaynes-Cummings lattices in superconducting circuit QED systems [110], with no natural coherent condensed matter analogue. Furthermore, many of the tools and techniques utilised for the study of isolated many-body quantum systems are not applicable within this context, and as a result there is a clear need for new analytical techniques [129], as well as both classical and quantum simulation methods.

Thermalisation: Just as in the context of isolated many-body quantum systems, as discussed in Section 1.1, there are a variety of open questions concerning the manner in which open quantum systems thermalise to the thermal state of the underlying Hamiltonian. In particular, it is of great interest to understand the conditions under which thermalisation occurs in many-body quantum systems in contact with some type of environment/bath, and the time scales on which such a process occurs under different constraints [130–136]. As in the context of isolated quantum systems, it is also

of foundational interest to explore the manner in which correlations spread in different classes of open quantum systems, and the insights that such correlation dynamics can provide into thermalisation [137]. Finally, it is of interest to explore the robustness of phenomena explored within the context of isolated many-body quantum systems, such as many-body localisation, in order to understand the extent to which such phenomena might be studied in the laboratory [138, 139].

Dissipation as a resource: Typical approaches to quantum computation and quantum information processing treat dissipation and decoherence as a fundamental obstacle which needs to be overcome in order to implement robust information processing protocols and algorithms [49]. However, relatively recently a paradigm shift has occurred through which it has become clear that dissipation and decoherence might in fact be utilised as a computational *resource* [65]. Instead of designing ingenious methods for suppressing or correcting the effects of dissipation and decoherence, this revised perspective suggests that one might rather focus on designing methods to exploit either naturally occurring or engineered dissipation as the driver of some desired computational process. A very natural first application of such a strategy would of course be the preparation of non-equilibrium steady states of driven-dissipative many-body models, whose phenomenology is currently of great interest, as discussed above. This application has shown vast potential, with many experimental proposals and successes [140–145]. However, it has also been shown, both experimentally and theoretically, that a dissipatively driven state-preparation strategy can be utilised for the preparation of alternative states of interest, such as topologically ordered ground states of certain Hamiltonians [66, 146], and various large-scale entangled states [147–150], which may then be exploited as a computational or communication resource. In addition to state preparation driven by dissipation, there have been various proposals for dissipatively driven quantum computation [65, 151, 152]. Although it has recently been proven that dissipative quantum computing and conventional quantum computing are equivalent from a computational complexity perspective, a result known as the "Dissipative Church-Turing Thesis" [153], this approach to quantum computing still holds considerable conceptual appeal as a result of the potential inherent robustness such an approach might demonstrate. Within this vein, there have also very recently been suggestions for how one might exploit dissipation and decoherence for the construction of robust decoders within topological quantum error correction schemes [154–156].

In light of all these results, both experimental and theoretical, it is of both fundamental and practical interest to investigate and develop novel computational applications

of dissipation and decoherence. Crucially however, all applications of "dissipation as a resource" rely fundamentally on the ability to engineer and implement controlled dissipation and decoherence, as the protocols are effectively implemented through the *simulation* of some specified open quantum system. While there has been a rapid amount of development in this direction, enabling the successful experimental demonstrations mentioned above, new techniques for the implementation of a wider variety of open quantum systems, as will be discussed in this thesis, offer the potential to enable a wider class of protocols. In particular, it is especially interesting to consider the manner in which creative simulation strategies, such as digital/analog simulations, might be leveraged to allow for full exploitation of naturally occurring dissipation and decoherence, or rather "standard resources" in the complexity theoretic language previously utilised.

Memory effects in open quantum systems: As a result of the interaction between an open quantum system and its possibly complex or highly structured environment, there is the possibility of non-trivial "memory" effects in open quantum systems, and there is currently a wide and growing interest in exploring this (currently very broad) notion of memory in such systems. In particular, it is of interest to explore when and how non-trivial "memory" effects might arise within open quantum systems, to rigorously catalogue this broad phenomenology of memory, and to understand how such effects relate to the plethora of competing definitions for quantum non-Markovianity [157–159]. Given the notion of dissipation as a resource discussed above, it will also be exceedingly interesting to understand the extent to which non-trivial memory effects in open quantum systems might be used as either a computational or communication resource [160, 161]. Once again, in addition to the foundational motivation, this resource-theoretic perspective provides a potential practical motivation for the development of methods for the implementation of various open quantum systems exhibiting memory effects.

Quantum Biology: Despite being "wet and warm", biological systems, such as photosynthetic reaction centres for example, are most certainly complex open quantum systems! As a result, progress in multiple directions in quantum biology, as discussed in Section 1.1, relies heavily on gaining a more sophisticated understanding of the dynamics and properties of various biologically inspired models for many-body open quantum systems, often with highly complex structured environments [34, 35]. As an example, within the context of photosynthesis, various proposals have already been suggested for the role decoherence may play in efficient energy transfer [36–41], and it is currently of interest to investigate alternative, possibly more biologically plausible, models.

1.4.2 Formalism

From the working definition for a quantum simulation given in Section 1.1, it is clear that the first key step in any quantum simulation is a description of the system one would like to simulate! In the context of closed quantum systems, one typically provides the system Hamiltonian H, either time-dependent or time-independent, and possibly specified via some oracle for the matrix elements, or one provides the unitary time evolution system propagator $U(t, t_0)$ for some specified initial and final times t_0 and t respectively. In the context of open quantum systems however, the situation is slightly more complicated, as there is a selection of ways to specify an open quantum system depending on a variety of factors, such as the number and type of approximations one is able to make. As a result, in this section we will provide a brief introduction to the formalism of open quantum systems, with a strong emphasis on providing the various descriptions possible as starting points for meaningful simulations. As this discussion will be approached with this specific goal in mind, we will omit many technical details and proofs, which can easily be found in standard texts [162–166].

In order to facilitate this presentation, we will from now on adopt the following notation: Given a finite-dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^d$, we denote the space of all bounded linear operators $A : \mathcal{H} \to \mathcal{H}$ as $\mathcal{B}(\mathcal{H})$. Furthermore, we will denote the set of all positive semi-definite operators with unit trace (i.e. the set of density matrices) as $\mathcal{D}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$. Given this notation, we will be fundamentally concerned with bipartite systems $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$, where $\mathcal{H}_S$ is the Hilbert space of the subsystem whose dynamics or properties we are interested in (referred to as the open quantum system), and $\mathcal{H}_E$ is the Hilbert space of the environment with which the system is in contact.

As a starting point for our discussion, as illustrated in Fig. 1.6, we note that if we are given an initially uncorrelated system/environment state $\rho(t_0) = \rho_S(t_0) \otimes \rho_E(t_0)$, then the state of the system at some time $t > t_0$, after some unitary evolution of the global system/environment combination under $U(t, t_0)$, can be obtained via

$$\rho_S(t) = \mathrm{tr}_E\Big[U(t, t_0)\big(\rho_S(t_0) \otimes \rho_E(t_0)\big)U(t, t_0)^\dagger\Big]. \tag{1.19}$$

In the above expression tr_E is the *partial trace* operation over the environment, which

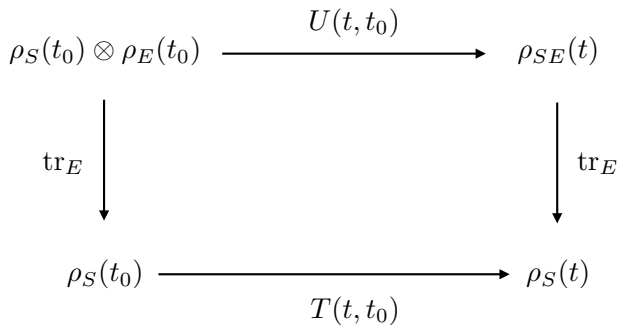

Figure 1.6: The state of an open quantum system at some time $t \geq 0$ can either be obtained through the unitary evolution of the global system/environment combination, or through the action of an intrinsic system propagator which acts directly on the initial state of the open quantum system.

satisfies the relationship

$$\langle O_S \otimes \mathbb{1}_E \rangle_\rho = \mathrm{tr}\Big[\big(O_S \otimes \mathbb{1}_E\big)\rho\Big] \tag{1.20}$$

$$= \mathrm{tr}\Big[O_S\big(\mathrm{tr}_E[\rho]\big)\Big] \tag{1.21}$$

$$= \mathrm{tr}\Big[O_S \rho_S\Big] \tag{1.22}$$

$$= \langle O_S \rangle_{\rho_S}, \tag{1.23}$$

for any observable $O_S \in \mathcal{B}(\mathcal{H}_S)$ and any state $\rho \in \mathcal{D}(\mathcal{H}_S \otimes \mathcal{H}_E)$, where $\rho_S \equiv \mathrm{tr}_E[\rho] \in \mathcal{D}(\mathcal{H}_\mathcal{S})$ is the reduced state of the open quantum system. However, it is also possible to obtain the final state of the system through the action of an *intrinsic* system propagator $T(t, t_0) : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$, a linear superoperator (i.e. an operator that acts on operators) with the property that

$$T(t, t_0)(\rho_S(t_0)) = \mathrm{tr}_E\Big[U(t, t_0)\big(\rho_S(t_0) \otimes \rho_E(t_0)\big)U(t, t_0)^\dagger\Big], \tag{1.24}$$

for all $\rho_S(t_0) \in \mathcal{D}(\mathcal{H}_S)$ and for all $\rho_E(t_0) \in \mathcal{D}(\mathcal{H}_E)$. More specifically, *with the assumption of an initially uncorrelated system/environment state*, one can show that the system propagator $T(t, t_0)$ will be a *quantum channel*, a map which is both trace-preserving and completely positive (CPTP) [166]. In this context, a map $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is trace-preserving if

$$\mathrm{tr}\big[T(\rho)\big] = \mathrm{tr}[\rho], \tag{1.25}$$

for all $\rho \in \mathcal{B}(\mathcal{H})$, and completely-positive if it is both positivity-preserving, i.e. $T(\rho) \geq 0$ for all $\rho \geq 0$, and satisfies

$$\big[T \otimes \mathbb{1}_d\big](\rho) \geq 0, \tag{1.26}$$

for all $\rho \geq 0 \in \mathcal{B}(\mathcal{H} \otimes \mathbb{C}^d)$, for all $d > 0$. From these properties it is clear that quantum channels map density operators to density operators[4]. At this stage, as a result of Eq. 1.24, we see that in order to perform a simulation of the dynamics of an open quantum system, which should yield the state $\rho_S(t)$ for some $t > t_0$, any of the following descriptions of the open quantum system, in addition to the initial state of the system $\rho_S(t_0)$, will suffice as a reasonable starting point:

1. A description of the global system/environment Hamiltonian H and the initial state of the environment $\rho_E(t_0)$.

2. A description of the global unitary propagator $U(t, t_0)$ and the initial state of the environment $\rho_E(t_0)$.

3. A description of the CPTP system propagator $T(t, t_0)$.

While it is now clear that one could obtain an approximation to the desired state $\rho_S(t)$ through a Hamiltonian simulation of the global system/environment combination, we will focus in this thesis on the development of methods for the simulation of open quantum systems specified through some intrinsic means, such as a time-evolution propagator, or family of propagators. In particular, this will allow for the construction of algorithms which scale efficiently with respect to the size of the open quantum system, as opposed to the size of the global system/environment combination. Furthermore, as will be discussed below, this will also allow for the simulation of a broad range of open quantum systems phenomenology, without necessarily requiring an understanding of the underlying microscopic dynamics of the system/environment combination.

Because of the crucial role played by both linear superoperators and quantum channels in the dynamics of open quantum systems, we will now provide a brief summary of the properties of, and relationships between, different methods for representing linear superoperators and quantum channels. These fundamentals will then allow us to discuss how one might specify different families of quantum channels, and the relation of these families to corresponding classes of underlying microscopic dynamics. In order to keep

[4]Clearly maps which are merely linear, trace-preserving and positivity preserving would also maps density matrices to density matrices, however there are examples of such maps, like the transposition map, which then do not preserve positivity when acting on only part of a larger system [49, 166].

the presentation concise we will omit proofs of the relevant theorems, which can be found in [166, 167].

The first representation that we will introduce is often called the *natural* representation. In order to introduce this representation we first define the linear mapping $\text{vec} : \mathcal{B}(\mathcal{H}) \to \mathcal{H} \otimes \mathcal{H}$, which is defined via its action on basis elements for $\mathcal{B}(\mathcal{H})$,

$$\text{vec}(|i\rangle\langle j|) = |i\rangle|j\rangle, \tag{1.27}$$

where $\{|k\rangle\}|_{k=1}^{d}$ is any orthonormal basis for $\mathcal{H} \approx \mathbb{C}^d$. In terms of this mapping we then provide the following definition.

Definition 1.2. *The natural representation of a linear superoperator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is the unique linear operator $\hat{T} \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$ satisfying*

$$T(\rho) = \text{vec}^{-1}\big(\hat{T}(\text{vec}(\rho))\big), \tag{1.28}$$

for all $\rho \in \mathcal{B}(\mathcal{H})$.

The second representation that we will introduce is most typically known as the *Choi-Jamiolkowski* representation, and is defined as follows:

Definition 1.3. *Given a linear superoperator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, the corresponding Choi-Jamiolkowski state is the linear operator*

$$\tau(T) = \big(T \otimes \mathbb{1}_{\mathcal{B}(\mathcal{H})}\big)(\text{vec}(\mathbb{1}_{\mathcal{H}})\text{vec}(\mathbb{1}_{\mathcal{H}})^{\dagger}), \tag{1.29}$$

where $\mathbb{1}_{\mathcal{B}(\mathcal{H})} \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is the identity superoperator, and $\mathbb{1}_{\mathcal{H}} \in \mathcal{B}(\mathcal{H})$ is the identity operator.

Given such a representation for T, we call the rank of $\tau(T)$ the *Kraus* rank of T, denoted as $\text{Kr}(T) = \text{rank}(\tau(T))$. As we will see in Theorem 1.2, this name comes from the close relationship between the Choi-Jamiolkowski representation of a quantum channel, and the next representation we will introduce, known as the *Kraus* representation.

Definition 1.4. *Given a linear superoperator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, a Kraus representation of T is any collection of linear operators $\{A_i \in \mathcal{B}(\mathcal{H})\}|_{i=1}^{r}$ and $\{B_i \in \mathcal{B}(\mathcal{H})\}|_{i=1}^{r}$, with $r \geq 1$, such that*

$$T(\rho) = \sum_{i=1}^{r} A_i \rho B_i^{\dagger}, \tag{1.30}$$

for all $\rho \in \mathcal{B}(\mathcal{H})$.

Notice that the Kraus representation of a linear superoperator is *not* unique - however in Theorem 1.2 we will show the existence of a minimal representation for quantum channels. Finally, the last representation that we will introduce is the so called *Stinespring* representation, another representation which is not unique, and is defined as follows:

Definition 1.5. *Given a linear superoperator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, a Stinespring representation of T is any pair of linear operators $A, B : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_E$, for any ancillary Hilbert space $\mathcal{H}_E$, such that*

$$T(\rho) = \mathrm{tr}_E\big[A\rho B^\dagger\big], \tag{1.31}$$

for all $\rho \in \mathcal{B}(\mathcal{H})$.

We will refer to the smallest Hilbert space H_E from which it is possible to construct a Stinespring dilation as the *minimal dilation space*. Given all these representations for linear superoperators, the following theorem now provides a complete summary of both their properties, and the relationships between them, in the case of quantum channels. We refer to [166, 167] for detailed proofs of these fundamental results.

Theorem 1.2. *Given a linear superoperator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, with $\mathcal{H} \simeq \mathbb{C}^d$, the following are equivalent:*

1. *T is a quantum channel.*
2. *$\tau(T) \geq 0$, i.e the Choi-Jamiolkowski state is positive semidefinite, and $\mathrm{tr}_{\mathcal{H}_1}[\tau] = \mathbb{1}_{\mathcal{H}}$ if we consider $\tau \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ with $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$.*
3. *There exists a collection of operators $\{A_i \in \mathcal{B}(\mathcal{H})\}|_{i=1}^r$, such that $\sum_{i=1}^r A_i^\dagger A_i = \mathbb{1}$ and*
$$T(\rho) = \sum_{i=1}^r A_i \rho A_i^\dagger \tag{1.32}$$
for all $\rho \in \mathcal{B}(\mathcal{H})$.
4. *Statement 3 holds for $r = \mathrm{Kr}(T)$, and is the smallest possible r for which this statement holds.*
5. *There exists a dilation Hilbert space $\mathcal{H}_E$ and a linear isometry $A : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_E$ such that*
$$T(\rho) = \mathrm{tr}_E\big[A\rho A^\dagger\big], \tag{1.33}$$
for all $\rho \in \mathcal{B}(\mathcal{H})$.

6. Statement 5 holds for $\mathcal{H}_E \simeq \mathbb{C}^{\mathrm{Kr}(T)}$, and this is the minimal dilation space.

Before moving on it is of interest to make some brief observations concerning the results contained in Theorem 1.2, without necessarily providing the full proof. Firstly, it is of course no coincidence that the Kraus rank provides both the size of the minimal Kraus representation and the minimal dilation space. This is because the minimal set of Kraus operators can in fact be obtained directly from the eigenvalues and "unvectorised" eigenvectors of the Choi-Jamiolkowski state, while the minimal Stinespring linear isometry can be constructed through "stacking" the Kraus operators (see [166, 167] for details). In addition, as a result of this close relationship between the Kraus representation, the Stinespring dilation and the Kraus rank, we see that if $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ with $\mathcal{H} \simeq \mathbb{C}^d$, then in the worst case scenario, when $\tau(T)$ is full rank, we will require d^2 Kraus operators and subsequently a dilation space $\mathrm{H}_E \simeq \mathbb{C}^{d^2}$. Furthermore, we note that as a result of the normalisation property in Statement 3, a quantum channel T has $\mathrm{Kr}(T) = 1$ if and only if the single Kraus operator is a unitary operator. Therefore a quantum channel describes unitary evolution if and only if the Kraus rank is equal to one, and in this case the Stinespring dilation is clearly trivial (it is the unique Kraus operator). Finally, as shown in [166], one can easily extend the linear isometry A in Statement 5 of Theorem 1.2 into a unitary operator $U \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H}_E)$, such that

$$T(\rho) = \mathrm{tr}_E\big[U(\rho \otimes |0\rangle\langle 0|)U^\dagger\big], \tag{1.34}$$

for all $\rho \in \mathcal{B}(\mathcal{H})$, where $|0\rangle$ is some basis state of $\mathcal{H}_E$.

As a result, at this stage we see from both the definitions above and Theorem 1.2, that one can specify a quantum channel, describing the possibly non-unitary evolution of some system in an initially uncorrelated state with some environment, in a variety of closely related ways. As we will see in the rest of the thesis, different representations will provide different advantages in different contexts, however we note that the Stinespring dilation is particularly suggestive of a natural method for the implementation of a quantum channel through the unitary evolution of a minimally dilated space.

So far we have focused on methods for the description of quantum channels, the time-evolution system propagators for open quantum system dynamics starting from an initially uncorrelated system environment state. However, in the case of closed quantum systems, one does not typically specify the unitary system propagator $U(t, t_0)$ as the starting point of a simulation, but rather some Hamiltonian $H(t)$, which then provides

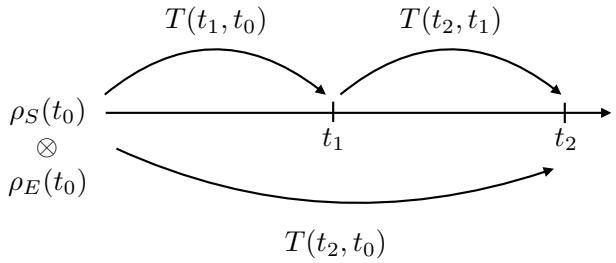

Figure 1.7: Given an open quantum system initially uncorrelated with the environment, the system propagators $T(t_1, t_0)$ and $T(t_2, t_0)$ will be quantum channels for all $t_1, t_2 \geq 0$. However, if the global system/environment unitary evolution leads to correlations between the system and the environment at time t_1, then the propagator $T(t_2, t_1)$ will not be a quantum channel.

a family of unitary system propagators via

$$U(t, t_0) = \mathcal{T} e^{-i \int_{t_0}^{t} H(\tau) d\tau}, \tag{1.35}$$

for all pairs of final and initial times $t \geq t_0$. Similarly, in the open quantum systems context, we will be interested in the simulation of different classes of families of system propagators, each with some relationship to an underlying category of microscopic global system/environment dyamics. In order to introduce these classes and the manner in which they are specified, let's consider the evolution of a generic open quantum system, depicted in Fig. 1.7. Clearly, as a result of the continuity of time evolution, we require that the system propagators fulfil

$$T(t_2, t_0) = T(t_2, t_1) T(t_1, t_0), \tag{1.36}$$

$$T(t_0, t_0) = \mathbb{1}, \tag{1.37}$$

for all $t_2 \geq t_1 \geq t_0 \geq 0$. We will refer to any *two-parameter* family of operators satisfying conditions (1.36) and (1.37) as an evolution family (EF), and clearly any physical family of system propagators is an evolution family. However, there are two very important special cases of which we need to take note. Firstly, if we assume that the initial state of the system is part of an uncorrelated global system environment state, i.e. $\rho_{SE}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0)$, then we know that both $T(t_2, t_0)$ and $T(t_1, t_0)$ will be quantum channels. However, it may be the case that the time evolution from t_0 to t_1 induced correlations between the system and the environment which are present at t_1, in which

case $T(t_2, t_1)$ will *not* be a quantum channel! In light of this we define an evolution family *of quantum channels* as a family of two-parameter propagators satisfying conditions (1.36) and (1.37), and for which $T(t_f, t_i)$ is a quantum channel for all $t_f \geq t_i \geq 0$. At this stage we therefore see that there are already two distinct possible classes of families of system propagators in which one might be interested. At this stage it may seem that the conditions required to obtain an evolution family of quantum channels are extremely stringent. However as will be discussed in more detail shortly, we briefly note that, among other requirements, if the coupling between the system and the environment is extremely weak, or if any correlations between the system and the environment decay on a time scale which is much faster then the time scale with which it is possible to probe the open quantum system, than an evolution family of quantum channels may indeed provide a good approximation to the dynamics of the open quantum system [162, 165].

The next special case of which we need to take note is best illustrated through the analogue of coherent unitary evolution. In this case, if the Hamiltonian of the system is time dependent we clearly have that $U(t, t_0)$, given by (1.35), depends explicitly on both t and t_0. However, in the case when the Hamiltonian of the system is time independent, we have that

$$U(t, t_0) = e^{-iH(t-t_0)} \tag{1.38}$$
$$= e^{-iH(\Delta t)} \tag{1.39}$$
$$= U(\Delta t), \tag{1.40}$$

and we see that the system propagator in fact depends explicitly not on the two parameters t and t_0, but only on the single parameter Δt, the time difference. Analogously, in the case of open system dynamics, we will call an evolution family of system propagators a *one-parameter semigroup* (OPSG) if every propagator $T(t_f, t_i)$ in fact depends only on the time difference $\Delta t = t_f - t_i$, i.e. $T(t_f, t_i) = T(\Delta t)$, and the family of propagators satisfies the conditions

$$T(r)T(s) = T(r + s), \tag{1.41}$$
$$T(0) = \mathbb{1} \tag{1.42}$$

for all $r, s \geq 0$. As per the previous discussion, we will call an OPSG of system propagators an OPSG *of quantum channels* if conditions (1.41) and (1.42) are satisfied and $T(s)$ is a quantum channel for all $s \geq 0$.

Given these fundamental classes of families of system propagators, the following

theorems, originally stated in [165] where the proofs can be found, formalise the existence of a *generator* for each class, which plays a role analogous to that of the Hamiltonian in the closed quantum systems context. Before stating the theorems we note that an OPSG is called uniformly continuous if the map

$$t \to T(t) \tag{1.43}$$

is continuous [165]. With this in hand, we can now state the theorems.

Theorem 1.3. *Any uniformly continuous OPSG can be written in the form* $T(t) = e^{\mathcal{L}t}$*, where* $\mathcal{L}$ *is the time-independent generator of the semigroup and is the only solution to the differential problem*

$$\frac{dT(t)}{dt} = \mathcal{L}T(t), \qquad t \in \mathbb{R}^+ \tag{1.44}$$

$$T(0) = \mathbb{1}. \tag{1.45}$$

Theorem 1.4. *A differentiable evolution family* $\{T(t,s)\}$ *is the only solution to the differential problems*

$$\frac{dT(ts)}{dt} = \mathcal{L}(t)T(t,s), \qquad t \geq s \tag{1.46}$$

$$T(s,s) = \mathbb{1}, \tag{1.47}$$

and

$$\frac{dT(ts)}{ds} = -T(t,s)\mathcal{L}(t) \qquad t \geq s \tag{1.48}$$

$$T(s,s) = \mathbb{1}, \tag{1.49}$$

for some time-dependent generator $\mathcal{L}(t)$

Theorem 1.5. *If the generator* $\mathcal{L}(t')$ *of a differentiable evolution family* $\{T(t,s)\}$ *is bounded in the interval* $[t,s]$ *then the evolution family can be written in the form*

$$T(t,s) = \mathcal{T}e^{-i\int_s^t \mathcal{L}(t')dt'}. \tag{1.50}$$

As one can now see, it is possible to specify either an evolution family or one-parameter semigroup of propagators, describing intrinsically the time-evolution of an open quantum system, through the specification of a generator for the family of propagators, analogous to the Hamiltonian of a closed quantum system. However, we have not

as of yet provided any insight into how one might go about specifying these generators. As we will see from the following theorems (whose proofs can be found in [165]), for the case of EF's and OPSG's *of quantum channels* this question admits an elegant and straightforward answer. Firstly, in the case of OPSG's, the following landmark theorem due to Gorini, Kossakowski, Sudarshan and Lindblad (GKSL) [162] provides the characterisation we are looking for:

Theorem 1.6. *A time-independent superoperator $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is the generator of a OPSG of quantum channels if and only if it can be written in the form*

$$\mathcal{L}(\cdot) = -i[H, \cdot] + \sum_k \gamma_k \Big[L_k \cdot L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \cdot\}_+ \Big], \tag{1.51}$$

for some time-independent Hermitian operator $H \in \mathcal{B}(\mathcal{H})$, some set of $k \geq 0$ time-independent operators $\{L_k \in \mathcal{B}(\mathcal{H})\}$, known as Lindblad operators, and some set of k positive numbers $\{\gamma_k \in \mathbb{R}^+\}$.

Furthermore, from the definition of the system propagator, as well as both Theorem 1.3 and Theorem 1.6, we now see the state $\rho_S(t)$ of any open quantum system undergoing time evolution described by a one-parameter semigroup of quantum channels, can be obtained by solving the differential equation

$$\frac{d\rho(t)}{dt} = \mathcal{L}\big(\rho(t)\big) \tag{1.52}$$

$$= -i[H, \rho(t)] + \sum_k \gamma_k \Big[L_k \rho(t) L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho(t)\}_+ \Big]. \tag{1.53}$$

for some H, $\{L_k\}$ and $\{\gamma_k\}$ which satisfy the same conditions as in Theorem 1.6. We call an equation in the form of (1.53) a *master equation* in the GKSL form, and the time evolution of an open quantum system according to such an equation is often known as Markovian semi-group dynamics [162]. While we have arrived at this equation of motion through primarily abstract considerations, we note that, as alluded to before, such intrinsic Markovian master equations for the dynamics of an open quantum system can in fact be derived from a microscopic model for the global/system environment combination which satisfies certain assumptions. To be more precise, if we are given a time-independent microscopic Hamiltonian $H_{SE} \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_E)$, with

$$H_{SE} = H_S \otimes \mathbb{1}_{\mathcal{H}_E} + \mathbb{1}_{\mathcal{H}_S} \otimes H_E + \omega H_I, \tag{1.54}$$

then a master equation in the GKSL form for the subsystem dynamics can be derived if

the Hamiltonian H_{SE} satisfies the weak-coupling, Born-Markov and rotating-wave approximations [162,165], which place restraints on the time scales of correlation dynamics in the global system/environment combination. We will not discuss these approximations in detail here, as a full derivation and discussion of these approximations can be found in [162,165]. We will however note that if the Hamiltonian H_{SE} does satisfy these approximations, we will be able to derive a master equation in the GKSL form in which the Hermitian operator H in eq. (1.51) is the Lamb-shifted system Hamiltonian H_S, and the Lindblad operators represent physical dissipation processes, summarising the effects of the interaction between the system and the environment.

Now, given this result for OPSG's of quantum channels, we can move on to EF's of quantum channels. In this case the following Theorem, a proof of which can be found in [165], generalises the seminal GKSL result:

Theorem 1.7. *A time-dependent superoperator $\mathcal{L}(t) \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is the generator of an EF of quantum channels if and only if it can be written in the form*

$$\mathcal{L}(t)(\cdot) = -i[H(t), \cdot] + \sum_k \gamma_k(t)\Big[L_k(t) \cdot L_k(t)^\dagger - \frac{1}{2}\{L_k(t)^\dagger L_k(t), \cdot\}_+\Big], \tag{1.55}$$

where $H(t)$ and $L_k(t)$ are time-dependent operators, with $H(t)$ Hermitian and $\gamma_k(t) \geq 0$ for all k and for all t.

Once again, the definition of the system-propagator, along with the results of the previous theorems, then allows us to see that the state $\rho_S(t)$ of any open quantum system undergoing time evolution described by an evolution family of quantum channels, can be obtained by solving the differential equation

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t)\big(\rho(t)\big), \tag{1.56}$$

for some time-dependent generator in the form (1.55). An equation in the form of (1.56) is known as a time-dependent master equation in the GKSL form, and can be derived from a (possibly time-dependent) microscopic model for the system/environment combination under similar approximations to those required for Markovian semigroup dynamics [165].

So, what have we achieved so far? Up until now we have seen that the following are all legitimate *intrinsic* ways to specify the dynamics of an open quantum system:

1. One can specify a quantum channel, via any of the representations given in Definitions 1.2-1.5, which provides a description of the time evolution of some open

quantum system up to a particular point in time, under the assumption that the system was initially uncorrelated with the environment.

2. One can provide a time-independent superoperator of the form given in Theorem 1.6, which provides a description of the evolution of an open quantum system via a one-parameter semigroup of quantum channels.

3. One can provide a time-dependent superoperator of the form given in Theorem 1.7, which provides a description of the evolution of an open quantum system via an evolution family of quantum channels.

As of yet we have not however discussed a method to specify the dynamics of an open quantum system evolving via an evolution family which is not necessarily an evolution family of quantum channels. This class of dynamics is particularly interesting for a variety of reasons. Firstly, while there are physical systems (especially for instance in quantum optics [163]) which do satisfy the microscopic assumptions necessary to derive the *time-local* master equations given in eqs. (1.52) and (1.56), for many realistic physical systems, in a wide variety of contexts, these assumptions are *not* satisfied. Secondly, it is often within this class of systems that a plethora of interesting "memory effects" may be observed [159]. In order to facilitate the discussion around such systems, we will from now on refer to such evolution families as *indivisible*, and we provide the following definition to make this notion precise:

Definition 1.6. *An evolution family of linear superoperators* $\{T(t,s)\}|_{t\geq s\geq 0}$ *is called indivisible if there exists some* $t_f \geq t_i \geq 0$ *for which* $T(t_f, t_i)$ *is not a quantum channel.*

Before we can continue, it is also necessary to define the slightly refined notion of a *completely positive* indivisible evolution family:

Definition 1.7. *An indivisible evolution family of linear superoperators* $\{T(t,s)\}|_{t\geq s\geq 0}$ *is called completely positive if* $T(t,0)$ *is a quantum channel for all* $t \geq 0$.

As quantum channels are the most general class of linear superoperators which preserve density matrices (physical states), we therefore see that being completely positive is actually a necessary requirement for an indivisible evolution family to describe the evolution of a physically plausible open quantum system. If an evolution family is not completely positive, it means that there exists some time t for which $T(t,0)$ is not a quantum channel, and therefore there exists some initial state $\rho(0)$ for which $\rho(t) = T(t,0)\big(\rho(0)\big)$ is not a density matrix, and therefore does not represent a physical state. With this in

mind we would therefore now like to present potential methods for specifying completely positive evolution families. Unfortunately however, this case is significantly more complex than the cases previously discussed, and is in fact still an open and active research direction. As a result we will not attempt to present all current approaches and results, and will rather briefly mention just two specific methods. For a more complete overview, we refer to the reviews [159, 165].

The first potential approach is through time-local time-dependent master equations in the GKSL form, as shown in eq. (1.56), but with dissipation rates $\gamma_k(t)$ which may be negative for some periods of time. While the corresponding time-dependent generator will certainly generate an indivisible evolution family, a concise and general statement of the conditions which need to be satisfied by the dissipation rates in order for the evolution family to be completely positive is currently not known. Despite the lack of a general criterion, there are some simpler cases in which conditions are known, and which are useful for exploring a variety of phenomena. As an example, if we consider time-dependent generators of the form

$$\mathcal{L}(t)(\cdot) = \sum_{j=1}^{m} \tilde{\gamma}_j(t)\mathcal{L}_j(\cdot), \tag{1.57}$$

where each $\mathcal{L}_j$ is the time-independent generator of an OPSG of quantum channels, and $[\mathcal{L}_i, \mathcal{L}_j] = 0$ for all i, j, then via the GKSL theorem and the properties of time-ordered exponentials it is possible to show that $\mathcal{L}(t)$ will generate a completely positive indivisible evolution family provided

$$F_j(t) = \int_0^t \tilde{\gamma}_j(s)ds \geq 0, \tag{1.58}$$

for all j and for all t [168].

The second approach that we will briefly mention is that of time non-local memory kernel master equations [165, 168, 169]. In this approach, one specifies a *memory kernel* $K(t_f, t_i) \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, and the dynamics of the system are then described by an integro-differential equation of the form

$$\frac{d}{dt}\rho_S(t) = \int_0^t K(t,\tau)\big(\rho(\tau)\big)d\tau. \tag{1.59}$$

In this phenomenologically motivated approach, which attempts to explicitly take into account the memory effects in such systems, the state of the system at some time $t \geq 0$ clearly depends on the history of the state for all times $0 \leq \tau \leq t$. While sufficient conditions on the memory kernel, for eq. (1.59) to describe time evolution via a com-

pletely positive evolution family, have been known for some time [169], very recently necessary and sufficient conditions have been formulated [170]. These conditions enable both the analysis of previously suggested classes of memory kernels [159, 165], as well provide a framework for the formulation of new classes of completely positive memory kernel equations. Before moving on, we quickly mention one particular class of memory kernels, which provides a clear connection with Markovian semigroup dynamics and provides some physical intuition towards the "memory" interpretation of such integro-differential equations. In particular, if we consider homogenous memory kernels of the form

$$K(t,s)(\cdot) = \tilde{K}(t-s)\mathcal{L}(\cdot), \tag{1.60}$$

where $\mathcal{L}$ is the generator of an OPSG of quantum channels, then we see that (1.59) reduces to a time-independent master equation in GKSL form in the limit that $\tilde{K}(t-s)$ tends to a delta function [165].

At this stage we have managed to obtain a broad, if not entirely complete, overview of the methods and approaches for intrinsically specifying the dynamics of an open quantum system. As will be detailed in Section 1.5, a selection of these methods will be of interest to us in the remainder of this thesis as the fundamental starting point for the design of digital and digital/analog simulation methods. Before continuing however, we note for completeness that while intrinsic descriptions are of interest to us in this work, there are definitely physical scenarios in which a description of the global system is both more convenient and physically relevant. This is especially true in the case of open quantum system dynamics via indivisible evolution families, where, as we have seen, explicitly completely positive intrinsic descriptions may be hard to obtain. In this case, a particularly convenient description is often obtained by assuming that the environment can be modelled by a (potentially infinite) ensemble of harmonic oscillators, after which the global microscopic dynamics can be specified by providing the system Hamiltonian and the *spectral density* of the environment, which specifies the coupling strength of the system to each mode of the environment. We refer to [162] for more details, as well as discussion of which spectral densities result in equations of motion in the GKSL form.

1.4.3 Previous work

Given the above formalism for specifying the dynamics of open quantum systems, we will now proceed to survey a selection of previously suggested methods for the simulation of a variety of open quantum systems. As this survey will primarily serve as a vehicle to provide the context for the contributions of this thesis, which will be detailed in Section

1.5, we will focus on digital, digital/analog and algorithmic methods. Despite this focus here, it is essential to briefly acknowledge that an analog approach to the simulation of open quantum systems has in fact also been widely successful, particularly as a tool for the preparation of non-equilibrium steady states of many-body driven-dissipative systems. For details, we refer to the general reviews of quantum simulations in trapped ions [64,171], ultracold quantum gases [172], superconducting circuits [110] and photonic systems [173], all of which make mention of the current platform-specific state of the art regarding analog simulation of open quantum systems, sometimes known as "reservoir engineering".

As in Section 1.4.2 we will start with methods for the simulation of quantum channels, describing discrete time-evolution up to a specific point in time, under the assumption of an initially uncorrelated system/environment state. In this direction, the first proposal for the simulation of quantum channels was in fact made by Lloyd in his seminal 1996 paper on the simulation of local Hamiltonian systems [93]. In this paper, in a brief section foreshadowing the importance and physical relevance of constructing methods for the simulation of open quantum systems, Lloyd essentially recognises that the Stinespring dilation, in the form detailed in Eq. (1.34), provides a natural method for the simulation of quantum channels through unitary evolution of a dilated space. In particular, as discussed in Section 1.4.2, Lloyd recognised that any quantum channel $T \in \mathcal{B}((\mathcal{B}(\mathcal{H}_S \simeq \mathbb{C}^d)))$ could be implemented on a universal quantum computer through the evolution of the corresponding Stinespring unitary $U \in \mathcal{B}(\mathcal{H} \otimes \mathbb{C}^{d^2})$, requiring only a dilation space with dimension the square of the original system dimension, and the ability to initialise the environment in a specified pure state. This natural strategy provided the fundamental foundation for all subsequent quantum channel simulation methodologies, and prompted the following questions: Firstly, might it be possible to design methods which require smaller dilation spaces? Then secondly, can one construct upper and lower bounds on the number of "difficult" fundamental gates, like CNOTs for example, required for the simulation via dilation of different classes of quantum channels? With regards to the first question, Lloyd conjectured that a dilation space of equal dimension to the system may suffice if one is able to exploit initially mixed environment states, setting the direction for future research.

Unfortunately it was very quickly realised that Lloyd's conjecture was false. To be more precise, it was shown that there exist single qubit quantum channels for which a two qubit environment is necessary for the construction of a Stinespring dilation, even if one allows initially mixed states of the environment [174]. This result dashed hopes that straighforward *digital* Stinespring dilation strategies with optimally sized

environments would be universally applicable, however it prompted research into more sophisticated *algorithmic* methods. In particular, in 2002 Lloyd showed that if one allowed for measurement of the system, computation on a classical device, and feedback to the quantum simulator, then *any* quantum channel, acting on an arbitrarily sized system, could be implemented via a procedure requiring only a single resettable ancilla qubit [175].

Almost simultaneously, it was demonstrated how any *single-qubit* quantum channel could be decomposed into the convex sum of so called "generalised extreme channels", which require only the minimal dilation space of a single qubit for implementation via the Stinespring dilation [176]. Although this result was achieved primarily within the context of investigations into the fundamental geometric properties of quantum channels, it suggested a natural algorithmic simulation methodology for the simulation of an arbitrary quantum channel through classical random sampling of the generalised extreme channels in its convex decomposition. Precisely this methodology was later formalised by Wang and Sanders, through the construction of a "Solovay-Kitaev" type algorithm for single-qubit channels [177]. To be more precise, directly inspired by the fundamental Solovay-Kitaev algorithm in the context of closed quantum systems [90], they constructed an algorithm which was able to provide an explicit quantum circuit, consisting only of gates from any specified universal gate set, for the implementation of an arbitrary single qubit quantum channel. In particular, through the construction of their algorithm, which relied fundamentally on the geometric properties of quantum channels, they were able to show that classical randomness, one ancilla qubit, one CNOT gate and four single qubit operations suffice for the simulation of an arbitrary single qubit quantum channel. Furthermore, this CNOT count was shown to be independent of the universal gate set one chose.

Despite the fundamental difficulties inherent in gaining analytic insight into the geometric structure of the set of arbitrary quantum channels, Lloyd and Wang were later able to generalise their single qubit result to the case of qudit channels on arbitrarily sized Hilbert spaces [178]. In particular, through sophisticated methods for the *approximate* convex decomposition of qudit channels into the convex sum of generalised extreme channels, they were able to construct a classical algorithm which yields a quantum circuit (requiring classical randomness for the reconstruction of convex sums through classical random sampling) for the simulation of any quantum channel. In particular, the circuits generated by their algorithm required only a single ancillary qudit, and exhibited a time complexity (number of fundamental gates) which was logarithmic with respect to the allowed error tolerance and quadratic with respect to the Hilbert space dimension of the

states on which the qudit channel acts (i.e. the dimension of the qudit).

Very recently Iten et al. have formalised the models in which all of the previous work discussed here has taken place, and simultaneously constructed explicit upper and lower bounds on the CNOT counts required within each model [179]. In particular, they define the "Quantum Circuit Model" (QCM), in which only dilations and unitary operations are allowed (as studied initially by Lloyd and Terhal [93, 174]), the "Random Quantum Circuit Model" (RQCM), in which dilations, unitary operations and classical randomness is allowed (as studied by Wang and Sanders [177, 178]) and finally the "Measured Quantum Circuit model" (MQCM), in which dilations, unitary operations, measurement and classical feedback is allowed (as initially studied by Lloyd [175]). In all of these models, building on the previous work discussed here, they provide near optimal schemes, with a focus on an algorithm within MQCM which improves upon Lloyd's initial results for channels from m to n qubits. This recent work has provided a rigorous formalism for further research, and provided concrete lower bounds as a goal for future efforts.

Given this description of the state of the art concerning the simulation of individual quantum channels, we now turn our attention to the simulation of Markovian semigroup (MSG) dynamics, specified by a time-independent generator in the GKSL form, as shown in eq. (1.51). Before we begin a discussion of the methods currently available, it is essential to briefly discuss why such methods are even necessary! After all, a Markovian semigroup is nothing but a one-parameter semigroup of quantum channels, and therefore in principle any of the previously discussed methods for the simulation of quantum channels could be used for the simulation of MSG dynamics up to a specific point in time (i.e. for the simulation of any channel from the semigroup). The crux of the matter however is that we are not provided with a conventional description of the quantum channels (as discussed in Section 1.4.2) in the semigroup, but rather with a description of the generator of the semigroup, and for an arbitrary generator there is no *efficient* way to go directly from the generator to a useful description of the quantum channel describing time evolution up to a specific point in time. This is completely analogous to the situation in closed quantum systems discussed in Section 1.3, in which direct exponentiation of the Hamiltonian to obtain the unitary propagator is not feasible, and as a result one requires methods to efficiently decompose the Hamiltonian into constituents which can be easily exponentiated, and from which the total unitary evolution can be efficiently reconstructed. Similarly, in the open quantum systems context, in order to obtain efficient algorithms we need methods for simulating the time evolution up to a specific point in time directly from a description of the generator of the semigroup of quantum channels.

Once again, the first suggestion in this direction was by Lloyd in his seminal 1996 paper [93]. Although extremely vague and devoid of details, Lloyd suggested that it might be possible to utilise the naturally occurring dissipation within a universal quantum computer to facilitate the simulation of a master equation in the GKSL form through an "open" simulation of the system Hamiltonian, in which dissipative effects are deliberately not suppressed. In light of our previous discussions, we recognise in this idea the seeds of the notion of "dissipation as a resource" [65]. Although it would take some time for this notion to be satisfactorily formalised, once again this original paper set the general direction for future research.

The first formal contribution in this direction was made by Bacon et al. in 2001, in which they explicitly constructed a universal set of generators for the simulation of arbitrary Markovian dynamics of a *single qubit* [180]. To be more precise, they provided a set of MSG generators, parameterised by three continuous parameters, which, in the spirit of the decomposition/recombination approach discussed in Sec 1.3, they showed was universal in the sense that *any* MSG could be simulated provided one could simulate the MSG's specified by generators within the universal set, and perform arbitrary unitary basis transformations. This work, very much a first attempt at developing a set of rules analogous to "Childs' rules" for open quantum systems (Andrew Childs was in fact a co-author of the work), left open a plethora of interesting open questions. In particular, the first open question was whether the simulations of channels from semigroups generated by elements of the universal set could be *efficiently* recombined - i.e. the issue of generalising the SLT results for closed quantum systems into the superoperator context, and thereby rigorously proving the efficiency of recombination, was left open. The next set of open questions concerned the construction of methods for the simulation of semigroups generated by elements of the universal set, as efficient methods for the simulation of these systems is clearly a necessary precondition for this decomposition/recombination strategy to yield an efficient algorithm. This is directly analogous to how the availability of methods for the efficient simulation of strictly-local Hamiltonians is a keystone of Lloyd's decomposition/recombination algorithm for the simulation of local Hamiltonians [93]. Finally, the question as to the structure and dimension of the universal set for arbitrary MSG's was left open, although the authors conjectured that for a quantum system with Hilbert space $\mathcal{H} \simeq \mathbb{C}^d$ a set of generators parameterised by $d^2 - 3$ parameters would be necessary. As will be discussed in Section 1.5, the questions arising from this work provide the foundations for the new results provided in Chapters 2 and 3 of this thesis, which serve to provide explicit answers to these questions.

Roughly concurrently to the work by Bacon et al., but in a completely different di-

rection, there were a variety of proposals for the simulation of MSG dynamics inspired by collision models [181]. In this approach, the dynamics of the open quantum system, evolving via a master equation in the GKSL form, is modelled through the conceptual framework of an isolated system which constantly undergoes a series of discrete "collisions" with a stream of "environment particles". This collision model framework naturally suggests a methods for the simulation of MSG dynamics via discretised coherent simulations exploiting a continually refreshed ancilla system, and certainly exhibits conceptual appeal. Unfortunately however suggestions for moving beyond the original proposals for simulation of single qubit systems have not yet been developed.

The next major event in the development of methods for the simulation of open quantum systems came in 2011, from the Innsbruck groups of P. Zolller and R. Blatt. In particular, building on two decades of progress in the experimental control over atomic and trapped ion systems, they were able to propose and realise a variety of methods for the digital/analog simulation of a plethora of Markovian dissipative spin models [66, 109, 146, 171, 182, 183]. In particular, in both Rydberg atom based and trapped ion systems, it was demonstrated how platform specific global entangling operations, such as the MS gate in trapped ions [62,63], could be used to digitally implement complex many-body spin interactions, which when augmented with controlled dissipation, realised for example by optical pumping, allowed for the simulation of specific classes of dissipative spin models. This theoretical work, and the accompanying small scale experimental implementations, demonstrated for the first time the true practical potential of both digital/analog methodologies, and dissipation as a resource. In effect, this work has layed the foundation for *non-universal* approaches to quantum simulation of physically relevant models, which, as demonstrated in these works, often do not require the full power of universal quantum computers, and benefit strongly from a deep understanding of the physics of the simulator itself.

Given the foundation provided by the groundbreaking work of the Innsbruck groups, a relatively large number of proposals have emerged in the last few years which seek to either improve the efficiency of previous methods, extend the applicability of the approach, or provide conceptual frameworks which are platform agnostic. In particular, there have been a variety of proposals for how one might formalise experimentally plausible fundamental "dissipative gadgets", or "dissipative modules", through which the simulation of arbitrary Markovian open quantum systems could be achieved [152,184,185] - a goal and strategy which is in line with the vision of the original work by Bacon et al. [180], but informed by the recent experimental successes of the Innsbruck groups. In the language of quantum simulations utilised here, these dissipative modules are essentially dissipative

analog building blocks, motivated by experimental plausibility, but through which some measure of universality can be obtained. Though the details of all these proposals differ, and will not be fully discussed here, a common idea underlying all of the proposals is to assume the existence and availability of a set of qubits, each of which is undergoing some simple dissipation process, such as amplitude damping, and over which the experimentalist has some measure of control. Given some type of fundamental analog dissipative resource of this type, each of the proposals then puts forward different methods for combining these fundamental resources with conventional coherent resources, in order to achieve the simulation of arbitrary Markovian generators. As mentioned above, this work is clearly inspired by the practical success and pragmatic approach of the digital/analog methods introduced by the Innsbruck groups, but with a view to achieving greater flexibility. However, as we have seen, universality and flexibility typically comes at the price of experimental plausibility, and the future of this line of research will depend strongly on the experimental feasibility of the required dissipative modules. Before continuing, we mention briefly a recent proposal in the same vein as the works on dissipative modules discussed here, but with the goal of simulating arbitrary *purely* dissipative Markovian systems [186].

In addition to the methods already discussed, we mention two recent innovative and distinct conceptual approaches to the simulation of arbitrary Markovian open quantum systems. The first approach, proposed by Dive et al., can be thought of as an extension of the Stinespring dilation methodology for individual quantum channels to families of quantum channels [187]. To be more precise, as we have discussed at length, the Stinespring dilation provides a correspondence between a single quantum channel and a unitary operation on a dilated space. In Ref. [187] the authors consider the possibility of extending this approach to a correspondence between a family of quantum channels and a (controlled time-dependent) Hamiltonian on a finite minimally sized dilated space, constructed in such a way so as to ensure that the time evolution of the open quantum system, via the family of channels, can be simulated up to any point in time through a simulation of the corresponding Hamiltonian on the dilated space. This approach is both natural and conceptually extremely elegant, and allows for the exploitation of the by now well developed toolbox for coherent quantum control. In particular, the authors show that such a Hamiltonian (at least approximately) can be constructed for any Markovian semigroup, and as such the extent to which this idea can be realised now depends on our ability to implement the required controlled Hamitonians.

The second method we will mention for the simulation of Markovian semigroup dynamics is an algorithmic approach proposed by Di Candia et al. [188]. In particular,

using perturbation series techniques and leveraging previously proposed methods for the calculation of multi-time correlation functions on a quantum computer, they show how the expectation value of any physical observable can be obtained through a simulation of the coherent part of the dynamics, and the calculation of perturbative corrections extracted from the value of specific multi-time correlation functions. Once again, this approach has considerable conceptual appeal, and adds to the toolbox of algorithmic techniques with which it is hoped that the quantum resources required for the simulation of open quantum systems can be drastically reduced.

Finally, very recently Childs. et al. have proposed a digital quantum simulation method for the efficient simulation of Markovian quantum dynamics which is not necessarily local, and which is specified by a *sparse* generator of a Markovian semigroup of quantum channels [189]. In addition, they prove a "no fast-forwarding" theorem for Markovian semi-group simulation, providing a fundamental limitations on the time complexity of what may be achieved in this regard. This work provides a very natural extension of the large body of work on simulation of sparse Hamiltonians into the open quantum systems context [100–106] . In particular, as in the case of sparse Hamiltonian simulation, this work opens up the potential of algorithmic applications of open quantum system simulation.

At this stage we are now in a position to discuss various proposals for the simulation of both divisible and indivisible evolution families. Firstly, in the case of evolution families of quantum channels (divisible evolution families), M. Kliesch et al. have shown how to efficiently simulate on a universal quantum computer the evolution of an open quantum system via any *local* generator in the time-dependent GKSL form [153]. Essentially their method is a straightforward extension of Lloyd's seminal method for the simulation of local Hamiltonians. To be more precise, they first observe that any *strictly-local* time-independent generator in GKSL form can be simulated efficiently on a universal quantum computer, via a straightforward implementation of the Stinespring dilation. Given this, they then extend time-dependent SLT decompositions, developed for the simulation of time-dependent local Hamiltonians, into the superoperator setting. These generalised results prove rigorously that one can efficiently simulate any time-dependent local generator through the stroboscopic simulation of time-independent strictly-local generators, which are obtained by averaging the time-dependent strictly-local generator within the stroboscopic time interval. Interestingly, this archetypal decomposition/recombination result was published as the "Dissipative Quantum Church-Turing Theorem", as it effectively provides a polynomial time reduction between any dissipative quantum computing algorithm and a corresponding algorithm on a conventional universal quantum

computer. As a result, this work proves that coherent quantum dynamics and the dynamics of open-quantum systems via divisible evolution families are equivalent from a complexity-theoretic point of view, settling an open question asking whether dissipative quantum computing might be a more powerful computational model. As discussed in the following section, in Chapter 4 we extend the applicability of these results to a class of *indivisible* evolution families of quantum channels.

The next algorithm we mention, proposed by Alvarez-Rodriguez et al., suggests an algorithmic approach to the simulation of indivisible evolution families of quantum channels specified via a specific class of time non-local memory kernel master equations [73]. In a very similar spirit to the work in Ref. [188], the authors use perturbation theory techniques to show how any such system can in fact be efficiently simulated through the algorithmic recombination of simulations of Markovian semigroups, specified by time-independent generators in the GKSL form. This approach has considerable conceptual appeal, as it allows for one to leverage all the previously mentioned techniques for the simulation of OPSG's of quantum channels, for the simulation of specific phenomenologically motivated indivisible evolution families. Once again, this algorithm demonstrates the considerable potential algorithmic approaches hold for leveraging currently available or simpler to implement technologies. Finally, we mention a very recent simulation method proposed by Chenu et al., which proposes to implement the evolution of (possibly indivisible) evolution families of quantum channels, specified via *strictly-local* generators in the GKSL form (but with possible negative rates), through the simulation of suitable stochastic Hamiltonians, in which the strength of the coherent many-body interactions are modulated via a stochastic process [190]. Once again, this proposal leverages a hybrid methodology, in this case exploiting the availability of classical randomness, to perform a simulation of a complicated system with significantly reduced experimental resource requirements.

1.5 Structure and contributions

From the discussion in the previous section it is clear that there are currently a plethora of different approaches to the simulation of open quantum systems, all of which exhibit context dependent advantages and weaknesses, and therefore suggest natural open questions and directions for new research. Given this context, and the strong motivations already discussed, in the following chapters we will explicitly address a selection of these natural questions, as detailed below. Finally, we will conclude this thesis in Chapter 5 with some perspectives on the consequences of the work presented here, perspectives for

new research directions, and some pressing remaining open questions.

1.5.1 Chapter 2

In this chapter we resolve a selection of the open questions remaining from the foundational work of Bacon et al. [180], using tools and techniques from both digital Hamiltonian simulation methods and methods for the simulation of individual quantum channels. In resolving these questions we provide a complete algorithm for the efficient digital quantum simulation of arbitrary single qubit Markovian open quantum systems. To be more precise, as discussed in the previous section, Bacon et al. have explicitly constructed a set of generators for the Markovian dynamics of a single qubit, which is *universal* in the sense that *any* MSG of single qubit channels can be simulated provided one can simulate the MSG's specified by generators within the universal set, and perform arbitrary single qubit unitary basis transformations. In Chapter 3 we extend this result by making two distinct contributions. Firstly, by generalising the most recent SLT results from Hamiltonian simulation [97] into the super operator context, we rigorously and constructively prove that *efficient* simulation of arbitrary single-qubit MSG dynamics can be achieved through stroboscopic simulations of semigroups generated by elements of the universal set. Secondly, exploiting the methodology introduced by Wang and Sanders for the simulation of abitrary qubit quantum channels [177], we provide an explicit quantum circuit (requiring classical randomness) for the efficient digital quantum simulation of any MSG generated by an element of the previously constructed universal set, which requires only a single ancilla qubit and a single CNOT gate. Together these two contributions allow us to construct an efficient digital quantum algorithm for simulation of any Markovian dynamics of a qubit, described by a semigroup of single qubit quantum channels $\{T_t\}$ specified by a generator $\mathcal{L}$. This algorithm requires only single qubit and CNOT gates and approximates the channel $T_t = e^{t\mathcal{L}}$ up to chosen accuracy ϵ, with slightly super-linear cost $\mathcal{O}\big((||\mathcal{L}||_{(1\to 1)}t)^{1+1/2k}/\epsilon^{1/2k}\big)$ for any integer k, which given a recently proven "no fast-forwarding" theorem analogous to the Hamiltonian context [189], is close to optimal.

1.5.2 Chapter 3

From both a foundational perspective and the results presented in Chapter 2, building on the groundbreaking work of Ref. [180], it is clear that the existence and specification of a universal set of MSG generators is a powerful tool for the construction of algorithms for the efficient simulation of Markovian open quantum systems. As such,

in this chapter, using the recombination framework introduced in [180], we explicitly construct a universal set of MSG generators for quantum systems of any finite Hilbert space dimension. To be more precise, for quantum systems of Hilbert space dimension d, we explicitly construct a universal set of semigroup generators, parametrised by d^2-3 continuous parameters, and prove that within this particular recombination framework a necessary and sufficient condition for the dynamical simulation of a d dimensional Markovian quantum system is the ability to implement a) quantum channels from the semigroups generated by elements of the universal set of generators, and b) unitary operations on the system. This result effectively resolves a long standing open question originally posed in Ref. [180]. Furthermore, utilising superoperator SLT decompositions developed in Chapter 2, we provide an explicit algorithm for simulating the dynamics of an arbitrary Markovian open quantum system through simulations of MSG's generated by elements of the universal set. In particular, we prove that this algorithm is efficient when the number of distinct Lindblad operators (representing physical dissipation processes) in the GKSL form of the generator scales polynomially with respect to the number of particles in the open quantum system. As done in Chapter 2, this result clearly allows one to focus both theoretical and experimental effort on designing methods for the simulation of MSG's generated by elements of the universal set, and in principle any of the currently existing methods discussed in Section 1.4.3 may be utilised for this task, depending on the context and the experimental constraints. As such, this result provides a powerful practical tool for the simulation of arbitrary Markovian open quantum systems, which is able to leverage the advantages of any other method for the simulation of Markovian semigroups. From an alternative perspective, under the assumption that the dynamics of MSG's generated by elements of the universal set can be considered "standard resources", this algorithm provides an efficient digital/analog methodology for the simulation of a large class of physically relevant Markovian open quantum systems.

1.5.3 Chapter 4

In this chapter we focus our attention on the simulation of *indivisible* evolution families of quantum channels, specified by generators in the GKSL form but with possibly negative rates. In particular, we concern ourselves with *many-body* open quantum systems of this type, which as discussed earlier promise a wealth of fascinating phenomenology for which we currently lack a rigorous understanding. To be more precise, we provide in Chapter 4 the following results: Firstly, we prove rigorous SLT type results for sys-

tems of this type, which allows us to bound the error made when simulating the time evolution of an indivisible evolution family generated by a *local* time-dependent generator through the stroboscopic implementation of its *indivisible* strictly local constituents. These results extend into the indivisible setting the time-dependent superoperator SLT decompositions introduced in Ref. [153], and through the introduction of the concept of *local indivisibility*, a new tool for the study of non-Markovianity in many-body open quantum systems, we are able to prove a natural correspondence with the results of Ref. [153] in the limit of local generators which are the sum of divisible strictly-local constituents. Secondly, using the notion of quantum instruments [167], we provide an algorithmic method for the simulation of system propagators which are *not* quantum channels. This method then allows us to propose a complete algorithmic decomposition/recombination type algorithm for the simulation of indivisible evolution families of quantum channels specified by time-dependent local generators in the GKSL form, but with possibly negative dissipation rates. In particular, this algorithm exploits the proposed algorithmic simulation method for non-completely positive propagators as a subroutine for the implementation of the short-time stroboscopic dynamics required by the SLT decomposition. Finally, we analyse in detail the complexity of the proposed algorithm with respect to all relevant physical parameters, which allows us to show that for weakly locally indivisible systems this algorithm provides an experimentally feasible approach to the simulation of systems of this type.

Bibliography

[1] R. P. Feynman. Simulating physics with computers. *Int. J. Theoret. Phys.*, 21:467, 1982.

[2] I. M. Georgescu, S. Ashhab, and F. Nori. Quantum simulation. *Rev. Mod. Phys.*, 86:153, 2014.

[3] B. C. Sanders. Efficient Algorithms for Universal Quantum Simulation. In G. W. Dueck and D. M. Miller, editors, *Reversible Computation: 5th International Conference, RC 2013, Victoria, BC, Canada, July 4-5, 2013. Proceedings*, pages 1–10. Springer, 2013.

[4] K. L. Brown, W. J. Munro, and V. M. Kendon. Using quantum computers for quantum simulation. *Entropy*, 12:2268, 2010.

[5] E. M. Lifshitz and L. P. Pitaevskii. *Statistical Physics, Part 2: Theory of the Condensed State.*, volume 9 of *Landau and Lifshitz: Course of Theoretical Physics.* Butterworth-Heinemann, 1980.

[6] R. B. Laughlin. Anomalous quantum hall effect: An incompressible quantum fluid with fractionally charged excitations. *Phys. Rev. Lett.*, 50:1395, 1983.

[7] D. C. Tsui, H. L. Stormer, and A. C. Gossard. Two-dimensional magnetotransport in the extreme quantum limit. *Phys. Rev. Lett.*, 48:1559, 1982.

[8] E. W. Carlson, V. J. Emery, S. A. Kivelson, and D. Orgad. *Concepts in High Temperature Superconductivity*, pages 1225–1348. Springer, Berlin, Heidelberg, 2008.

[9] X.-G. Wen. *Quantum Field Theory of Many-Body Systems.* Oxford University Press, 2007.

[10] B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen. Quantum information meets quantum matter - from quantum entanglement to topological phase in many-body systems. arXiv:1508.02595 [cond-mat.str-el], 2015.

[11] A. Y. Kitaev. Fault-tolerant quantum computation by anyons. *Ann. Phys.*, 303:20, 2003.

[12] J. W. Gibbs. *Elementary principles in statistical mechanics.* C. Scribner: New York, 1902.

[13] L. D. Landau and E. M. Lifshitz. *Statistical Physics*, volume 3 of *Landau and Lifshitz: Course of Theoretical Physics*. Butterworth-Heinemann, 3rd edition, 1980.

[14] C. Gogolin and J. Eisert. Equilibration, thermalisation, and the emergence of statistical mechanics in closed quantum systems. arXiv:1503.07538 [quant-ph], 2015.

[15] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore. *Colloquium* : Nonequilibrium dynamics of closed interacting quantum systems. *Rev. Mod. Phys.*, 83:863, 2011.

[16] L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol. From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics. *Adv. in Phys.*, 65(3):239, 2016.

[17] J. Eisert, M. Friesdorf, and C. Gogolin. Quantum many-body systems out of equilibrium. *Nature Physics*, 11:124, 2015.

[18] R. Nandkishore and D. A. Huse. Many-Body Localization and Thermalization in Quantum Statistical Mechanics. *Ann. Rev. Cond. Mat. Phys.*, 6:15, 2015.

[19] J. M. Maldacena. The large N limit of superconformal field theories and supergravity. *Adv. Theor. Math. Phys.*, 2:231, 1998.

[20] H. Nastase. Introduction to AdS/CFT. arXiv:0712.0689 [hep-th], 2007.

[21] M. Van Raamsdonk. Lectures on Gravity and Entanglement. arXiv:1609.00026 [hep-th], 2016.

[22] R. Orús. A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States. *Ann. Phys.*, 349:117, 2014.

[23] U. Schollwöck. The density-matrix renormalization group in the age of matrix product states. *Ann. Phys.*, 326:96, 2011.

[24] R. Orús. Advances on tensor network theory: symmetries, fermions, entanglement, and holography. *The European Physical Journal B*, 87:280, 2014.

[25] B. Swingle. Constructing holographic space-times using entanglement renormalization. arXiv:1209.3304 [hep-th], 2012.

[26] B. Swingle. Entanglement Renormalization and Holography. *Phys. Rev. D*, 86:065007, 2012.

[27] M. Miyaji, T. Takayanagi, and K. Watanabe. From Path Integrals to Tensor Networks for AdS/CFT. arXiv:1609.04645 [hep-th], 2016.

[28] L. García-Álvarez, I. L. Egusquiza, L. Lamata, A. del Campo, J. Sonner, and E. Solano. Digital Quantum Simulation of Minimal AdS/CFT. arXiv:1607.08560 [quant-ph].

[29] B. P. Lanyon, J. D. Whitfield, G. G. Gillett, M. E. Goggin, M. P. Almeida, I. Kassal, J. D. Biamonte, M. Mohseni, B. J. Powell, M. Barbieri, A. Aspuru-Guzik, and A. G. White. Towards quantum chemistry on a quantum computer. *Nature Chemistry*, 2:106, 2010.

[30] I. Kassal, J. D. Whitfield, A. Perdomo-Ortiz, M.-H. Yung, and A. Aspuru-Guzik. Simulating chemistry using quantum computers. *Ann. Rev. Phys. Chem.*, 62:185, 2011.

[31] I. Kassal, S. P. Jordan, P. J. Love, M. Mohseni, and A. Aspuru-Guzik. Polynomial-time quantum algorithm for the simulation of chemical dynamics. *Proc. Natl. Acad. Sci. U. S. A.*, 105(48):18681, 2008.

[32] M. Reiher, N. Wiebe, K. M. Svore, D. Wecker, and M. Troyer. Elucidating reaction mechanisms on quantum computers. arXiv:1605.03590 [quant-ph], 2016.

[33] L. García-Álvarez, U. Las Heras, A. Mezzacapo, M. Sanz, E. Solano, and L. Lamata. Quantum chemistry and charge transport in biomolecules with superconducting circuits. *Sci. Rep.*, 6:27836, 2016.

[34] N. Lambert, Y.-N. Chen, Y.-C. Cheng, C.-M. Li, G.-Y. Chen, and F. Nori. Quantum biology. *Nature Physics*, 9:10, 2013.

[35] S. F. Huelga and M. B. Plenio. Vibrations, quanta and biology. *Contemp. Phys.*, 54:181, 2013.

[36] M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik. Environment-assisted quantum walks in photosynthetic energy transfer. *J. Chem. Phys.*, 129:174106, 2008.

[37] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, and A. Aspuru-Guzik. Environment-assisted quantum transport. *New J. Phys.*, 11:033003, 2009.

[38] M. B. Plenio and S. F. Huelga. Dephasing-assisted transport: quantum networks and biomolecules. *New J. Phys.*, 10:113019, 2008.

[39] A. Marais, I. Sinayskiy, A. Kay, F. Petruccione, and A. Ekert. Decoherence-assisted transport in quantum networks. *New J. Phys.*, 15:013038, 2013.

[40] I. Sinayskiy, A. Marais, F. Petruccione, and A. Ekert. Decoherence-assisted transport in a dimer system. *Phys. Rev. Lett.*, 108:020602, 2012.

[41] R. Dorner, J. Goold, and V. Vedral. Towards quantum simulations of biological information flow. *Interface Focus*, 2:522, 2012.

[42] B. M. Austin, D. Y. Zubarev, and W. A. Lester. Quantum Monte Carlo and related approaches. *Chem. Rev.*, 112:263, 2012.

[43] W. M. C. Foulkes, L. Mitas, R. J. Needs, and G. Rajagopal. Quantum Monte Carlo simulations of solids. *Rev. Mod. Phys.*, 73:33–, 2001.

[44] J. Kolorenč and L. Mitas. Applications of quantum Monte Carlo methods in condensed systems. *Rep. Prog. Phys.*, 74:026502, 2011.

[45] F. Charette. Archaeology: High tech from ancient greece. *Nature*, 444:551, 2006.

[46] B. Swingle, G. Bentsen, M. Schleier-Smith, and P. Hayden. Measuring the scrambling of quantum information. arXiv:1602.06271 [quant-ph], 2016.

[47] C. H. Papadimitrou. *Computational Complexity.* Pearson, 1993.

[48] D. Deutsch. Quantum theory, the Church-Turing principle and the universal quantum computer. *Proc. Roy. Soc. Lon.*, 400:97, 1985.

[49] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information.* Cambridge University Press, 2000.

[50] D. P. DiVincenzo. The physical implementation of quantum computation. arXiv:quant-ph/0002077, 2000.

[51] J. Watrous. Quantum computational complexity. arXiv:0804.3401 [quant-ph], 2008.

[52] E. Bernstein and U. Vazirani. Quantum complexity theory. *SIAM Journal on Computing*, 26:1411, 1997.

[53] A. Montanaro. Quantum algorithms: an overview. *npj Quant Inf.*, 2:15023, 2016.

[54] P. W. Shor. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. *SIAM J.Sci.Statist.Comput.*, 26:1484, 1997.

[55] L. K. Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*, pages 212–219. ACM, 1996.

[56] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser. Quantum computation by adiabatic evolution. arXiv:quant-ph/0001106, 2000.

[57] A. M. Childs. *Quantum information processing in continuous time*. PhD thesis, Massachusetts Institute of Technology, 2004.

[58] W. van Dam, M. Mosca, and U. Vazirani. How powerful is adiabatic quantum computation? arXiv:quant-ph/0206003, 2002.

[59] I. Arrazola, J. S. Pedernales, L. Lamata, and E. Solano. Digital-analog quantum simulation of spin models in trapped ions. *Scientific Reports*, 6:30534, 2016.

[60] L. Lamata. Digital-analog quantum simulation of generalized Dicke models with superconducting circuits. arXiv:1608.08025 [quant-ph], 2016.

[61] A. Mezzacapo, U. Las Heras, J. S. Pedernales, L. DiCarlo, E. Solano, and L. Lamata. Digital quantum Rabi and Dicke models in superconducting circuits. *Sci. Rep.*, 4:7482, 2014.

[62] Anders Sørensen and Klaus Mølmer. Quantum computation with ions in thermal motion. *Phys. Rev. Lett.*, 82:1971, 1999.

[63] A. Sørensen and K. Mølmer. Entanglement and quantum computation with ions in thermal motion. *Phys. Rev. A*, 62:022311, 2000.

[64] R. Blatt and C. F. Roos. Quantum simulations with trapped ions. *Nature Physics*, 8:277, 2012.

[65] F. Verstraete, M. M. Wolf, and J. I. Cirac. Quantum computation and quantum-state engineering driven by dissipation. *Nature Physics*, 5:633, 2009.

[66] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C.F. Roos, P. Zoller, and R. Blatt. An open-system quantum simulator with trapped ions. *Nature*, 470:486, 2011.

[67] R. Barends, L. Lamata, J. Kelly, L. García-Álvarez, A. G. Fowler, A. Migrant, E. Jeffrey, T. C. White, D. Sank, J. Y. Mutus, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, I. C. Hoi, C. Neill, P. J. J. O Malley, C. Quintana, P. Roushan, A. Vainsencher, J. Wenner, E. Solano, and J. M. Martinis. Digital quantum simulation of fermionic models with a superconducting circuit. *Nature Comm.*, 6:7654, 2015.

[68] R. Barends, A. Shabani, L. Lamata, J. Kelly, A. Mezzacapo, U. Las Heras, R. Babbush, A. G. Fowler, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, E. Jeffrey, E. Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, P. J. J. OMalley, C. Quintana, P. Roushan, D. Sank, A. Vainsencher, J. Wenner, T. C. White, E. Solano, H. Neven, and J. M. Martinis. Digitized adiabatic quantum computing with a superconducting circuit. *Nature*, 534:222, 2016.

[69] Y. Salathé, M. Mondal, M. Oppliger, J. Heinsoo, P. Kurpiers, A. Potočnik, A. Mezzacapo, U. Las Heras, L. Lamata, E. Solano, S. Filipp, and A. Wallraff. Digital quantum simulation of spin models with circuit quantum electrodynamics. *Phys. Rev. X*, 5:021027, 2015.

[70] J. M. Kreula, L. García-Álvarez, L. Lamata, S. R. Clark, E. Solano, and D. Jaksch. Few-qubit quantum-classical simulation of strongly correlated lattice fermions. *EPJ Quantum Technol.*, 3:11, 2016.

[71] J. M Kreula, S. R. Clark, and D. Jaksch. Non-linear quantum-classical scheme to simulate non-equilibrium strongly correlated fermionic many-body dynamics. *Sci. Rep.*, 6:32940, 2016.

[72] B. Bauer, D. Wecker, A. J. Millis, M. B. Hastings, and M. Troyer. Hybrid quantum-classical approach to correlated materials. *Phys. Rev. X*, 6:031045, 2016.

[73] U. Alvarez-Rodriguez, R. Di Candia, J. Casanova, M. Sanz, and E. Solano. Algorithmic quantum simulation of memory effects. arXiv:1604.02992 [quant-ph], 2016.

[74] R. Sweke, M. Sanz, I. Sinayskiy, F. Petruccione, and E. Solano. Digital quantum simulation of many-body non-Markovian dynamics. *Phys. Rev. A*, 94:022317, 2014.

[75] R. Di Candia, B. Mejia, H. Castillo, J. S. Pedernales, J. Casanova, and E. Solano. Embedding quantum simulators for quantum computation of entanglement. *Phys. Rev. Lett.*, 111:240502, 2013.

[76] R. Di Candia. *Embedding Quantum Simulators*. PhD thesis, University of the Basque Country, 2015.

[77] J. S. Pedernales, R. Di Candia, I. L. Egusquiza, J. Casanova, and E. Solano. Efficient quantum algorithm for computing n-time correlation functions. *Phys. Rev. Lett.*, 113:020505, 2014.

[78] X. Zhang, Y. Shen, J. Zhang, J. Casanova, L. Lamata, E. Solano, M.-H. Yung, J.-N. Zhang, and K. Kim. Time reversal and charge conjugation in an embedding quantum simulator. *Nature comm.*, 6, 2015.

[79] D. A. Lidar and T. A. Brun. *Quantum Error Correction*. Cambridge University Press, 2013.

[80] B. M. Terhal. Quantum error correction for quantum memories. *Rev. Mod. Phys.*, 87:307, 2015.

[81] S. J. Devitt, W. J. Munro, and K. Nemoto. Quantum error correction for beginners. *Rep. Prog. Phys.*, 76:076001, 2013.

[82] S. Barz, J. F. Fitzsimons, E. Kashefi, and P. Walther. Experimental verification of quantum computation. *Nature Physics*, 9:727, 2013.

[83] A. Gheorghiu, E. Kashefi, and P. Wallden. Robustness and device independence of verifiable blind quantum computing. *New J. Phys.*, 17:083040, 2015.

[84] J. F. Fitzsimons and E. Kashefi. Unconditionally verifiable blind computation. arXiv:1512.04375 [quant-ph], 2015.

[85] J. F. Fitzsimons and M. Hajdušek. Post hoc verification of quantum computation. arXiv:1203.5217 [quant-ph], 2012.

[86] T. Morimae and J. F. Fitzsimons. Post hoc verification with a single prover. arXiv:1603.06046 [quant-ph], 2016.

[87] A. Mantri, T. F. Demarie, N. C. Menicucci, and J. F. Fitzsimons. Flow ambiguity: A path towards classically driven blind quantum computation. arXiv:1608.04633 [quant-ph], 2016.

[88] R. Shankar. *Principles of Quantum Mechanics*. Plenum press, 2nd edition, 1994.

[89] R. Kothari. Efficient simulation of Hamiltonians. Master's thesis, University of Waterloo, 2010.

[90] C. M. Dawson and M. A. Nielsen. The Solovay-Kitaev algorithm. *Quantum Information and Computation*, 6:81, 2006.

[91] D. Bacon, A. M. Childs, I. L. Chuang, J. Kempe, D. W. Leung, and X. Zhou. Universal simulation of Markovian quantum dynamics. *Phys. Rev. A*, 64:062302, 2001.

[92] H. F. Trotter. On the product of semi-groups of operators. *Proc. Amer. Math. Soc.*, 10:545, 1959.

[93] S. Lloyd. Universal quantum simulators. *Science*, 273:1073, 1996.

[94] M. Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Phys. Lett. A*, 146:319, 1990.

[95] M. Suzuki. General theory of fractal path integrals with applications to many body theories and statistical physics. *J. Math. Phys.*, 32:400, 1991.

[96] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders. Efficient quantum algorithms for simulating sparse Hamiltonians. *Comm. Math. Phys.*, 270:359, 2007.

[97] A. Papageorgiou and C. Zhang. On the efficiency of quantum algorithms for Hamiltonian simulation. *Quant. Inf. Proc.*, 11:541, 2012.

[98] N. Wiebe, D. Berry, P. Høyer, and B. C. Sanders. Higher order decompositions of ordered operator exponentials. *J. Phys. A: Math. Theor.*, 43:065203, 2010.

[99] D. Poulin, A. Qarry, R. Somma, and F. Verstraete. Quantum simulation of time-dependent Hamiltonians and the convenient illusion of hilbert space. *Phys. Rev. Lett.*, 106:170501, 2011.

[100] N. Wiebe, D. W. Berry, P. Høyer, and B. C. Sanders. Simulating quantum dynamics on a quantum computer. *J. Phys. A*, 44:445308, 2011.

[101] A. M. Childs. On the relationship between continuous- and discrete-time quantum walk. *Communications in Mathematical Physics*, 294:581, 2010.

[102] D. W. Berry and A. M. Childs. Black-box Hamiltonian simulation and unitary implementation. *Quantum Information and Computation*, 12:0029, 2012.

[103] A. M. Childs and N. Wiebe. Hamiltonian simulation using linear combinations of unitary operations. *Quantum Information and Computation*, 12:901, 2012.

[104] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma. Simulating Hamiltonian dynamics with a truncated Taylor series. *Phys. Rev. Lett.*, 114:090502, 2015.

[105] D. W. Berry, A. M. Childs, and R. Kothari. Hamiltonian simulation with nearly optimal dependence on all parameters. *Proceedings of the 56th IEEE Symposium on Foundations of Computer Science (FOCS 2015)*, pages 792–809, 2015.

[106] D. W. Berry and L. Novo. Corrected quantum walk for optimal Hamiltonian simulation. arXiv:1606.03443 [quant-ph], 2016.

[107] A. M. Childs and R. Kothari. Limitations on the simulation of non-sparse Hamiltonians. arXiv:0908.4398 [quant-ph], 2009.

[108] S. Diehl, A. Micheli, A. Kantian, B. Kraus, H. P. Büchler, and P. Zoller. Quantum states and phases in driven open quantum systems with cold atoms. *Nature Physics*, 4:878, 2008.

[109] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H. P. Büchler. A rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[110] A. A. Houck, H. E Türeci, and J. Koch. On-chip quantum simulation with superconducting circuits. *Nature Physics*, 8:292, 2012.

[111] K. Baumann, C. Guerlin, F. Brennecke, and T. Esslinger. Dicke quantum phase transition with a superfluid gas in an optical cavity. *Nature*, 464:1301, 2010.

[112] D. Nagy, G. Kónya, G. Szirmai, and P. Domokos. Dicke-model phase transition in the quantum motion of a Bose-Einstein condensate in an optical cavity. *Phys. Rev. Lett.*, 104:130401, 2010.

[113] S. Diehl, A. Tomadin, A. Micheli, R. Fazio, and P. Zoller. Dynamical phase transitions and instabilities in open atomic many-body systems. *Phys. Rev. Lett.*, 105:015702, 2010.

[114] A. Tomadin, S. Diehl, and P. Zoller. Nonequilibrium phase diagram of a driven and dissipative many-body system. *Phys. Rev. A*, 83:013611, 2011.

[115] T. E. Lee, H. Häffner, and M. C. Cross. Antiferromagnetic phase transition in a nonequilibrium lattice of rydberg atoms. *Phys. Rev. A*, 84:031402, 2011.

[116] E. M Kessler, G. Giedke, A. Imamoglu, S. F. Yelin, M. D. Lukin, and J. I. Cirac. Dissipative phase transition in a central spin system. *Phys. Rev. A*, 86:012116, 2012.

[117] M. Hoening, M. Moos, and M. Fleischhauer. Critical exponents of steady-state phase transitions in fermionic lattice models. *Phys. Rev. A*, 86:013606, 2012.

[118] B. Horstmann, J. I. Cirac, and G. Giedke. Noise-driven dynamics and phase transitions in fermionic systems. *Phys. Rev. A*, 87:012108, 2013.

[119] E. G. Dalla Torre, S. Diehl, M. D. Lukin, S. Sachdev, and P. Strack. Keldysh approach for non-equilibrium phase transitions in quantum optics: Beyond the Dicke model in optical cavities. *Phys. Rev. A*, 87:023831, 2013.

[120] L. M. Sieberer, S. D. Huber, E. Altman, and S. Diehl. Dynamical critical phenomena in driven-dissipative systems. *Phys. Rev. Lett.*, 110:195301, 2013.

[121] J. Qian, L. Zhou, and W. Zhang. Quantum phases of strongly interacting rydberg atoms in triangular lattices. *Phys. Rev. A*, 87:063421, 2013.

[122] C. Carr, R. Ritter, C. G. Wade, C. S. Adams, and K. J. Weatherill. Nonequilibrium phase transition in a dilute Rydberg ensemble. *Phys. Rev. Lett.*, 111:113901, 2013.

[123] N. Malossi, M. M. Valado, S. Scotto, P. Huillery, P. Pillet, D. Ciampini, E. Arimondo, and O. Morsch. Full counting statistics and phase diagram of a dissipative Rydberg gas. *Phys. Rev. Lett.*, 113:023006, 2014.

[124] M. Marcuzzi, E. Levi, S. Diehl, J. .P Garrahan, and I. Lesanovsky. Universal nonequilibrium properties of dissipative Rydberg gases. *Phys. Rev. Lett.*, 113:210401, 2014.

[125] N. Lang and H. P. Büchler. Exploring quantum phases by driven dissipation. *Phys. Rev. A*, 92:012128, 2015.

[126] J. Marino and S. Diehl. Driven Markovian quantum criticality. *Phys. Rev. Lett.*, 116:070407, 2016.

[127] J. Eisert and T. Prosen. Noise-driven quantum criticality. arXiv:1012.5013 [quant-ph], 2010.

[128] V. R. Overbeck, M. F. Maghrebi, A. V. Gorshkov, and H. Weimer. Multicritical behavior in dissipative Ising models. arXiv:1606.08863 [quant-ph], 2016.

[129] A. C. Y. Li, F. Petruccione, and J. Koch. Resummation for nonequilibrium perturbation theory and application to open quantum lattices. *Phys. Rev. X*, 6:021037, 2016.

[130] M. Žnidarič, G. Prosen, T.and Benenti, G. Casati, and D. Rossini. Thermalization and ergodicity in one-dimensional many-body open quantum systems. *Phys. Rev. E*, 81:051135, 2010.

[131] M. J. Kastoryano and F. G. S. L. Brandao. Quantum Gibbs samplers: the commuting case. *Comm. Math. Phys.*, page 1, 2014.

[132] K. Temme and M. J. Kastoryano. How fast do stabilizer Hamiltonians thermalize? arXiv:1505.07811 [quant-ph], 2015.

[133] K. Temme, F. Pastawski, and M. J. Kastoryano. Hypercontractivity of quasi-free quantum semigroups. *J. Phys. A: Math. and Theor.*, 47:405303, 2014.

[134] M. J. Kastoryano and K. Temme. Quantum logarithmic Sobolev inequalities and rapid mixing. *J. Math. Phys.*, 54:052202, 2013.

[135] F. G. S. L. Brandao and M. J. Kastoryano. Finite correlation length implies efficient preparation of quantum thermal states. arXiv:1609.07877 [quant-ph], 2016.

[136] M. Žnidarič. Relaxation times of dissipative many-body quantum systems. *Physi. Rev. E*, 92:042143, 2015.

[137] D. Poulin. Lieb-Robinson bound and locality for general Markovian quantum dynamics. *Phys. Rev. Lett.*, 104:190401, 2010.

[138] H. P. Lüschen, P. Bordia, S. S. Hodgman, M. Schreiber, S. Sarkar, A. J. Daley, M. H. Fischer, E. Altman, I. Bloch, and U. Schneider. Signatures of many-body localization in a controlled open quantum system. arXiv:1610.01613 [cond-mat.quant-gas], 2016.

[139] M. V. Medvedyeva, T. Prosen, and M. Žnidarič. Influence of dephasing on many-body localization. *Phys. Rev. B*, 93:094205, 2016.

[140] S. Diehl, W. Yi, A. J. Daley, and P. Zoller. Dissipation-induced d-wave pairing of fermionic atoms in an optical lattice. *Phys. Rev. Lett.*, 105:227001, 2010.

[141] C. Ates, B. Olmos, W. Li, and I. Lesanovsky. Dissipative binding of lattice bosons through distance-selective pair loss. *Phys. Rev. Lett.*, 109:233003, 2012.

[142] D. D. B. Rao and K. Mølmer. Dark entangled steady states of interacting Rydberg atoms. *Phys. Rev. Lett.*, 111:033606, 2013.

[143] A. W. Carr and M. Saffman. Preparation of entangled and antiferromagnetic states by dissipative Rydberg pumping. *Phys. Rev. Lett.*, 111:033607, 2013.

[144] M. Lemeshko and H. Weimer. Dissipative binding of atoms by non-conservative forces. *Nature communications*, 4, 2013.

[145] J. Otterbach and M. Lemeshko. Dissipative preparation of spatial order in Rydberg-dressed Bose-Einstein condensates. *Phys. Rev. Lett.*, 113:070401, 2014.

[146] M. Müller, K. Hammerer, Y. L. Zhou, C. F. Roos, and P. Zoller. Simulating open quantum systems: from many-body interactions to stabilizer pumping. *New J. Phys.*, 13:085007, 2011.

[147] R. Sweke, I. Sinayskiy, and F. Petruccione. Dissipative preparation of large W states in optical cavities. *Physical Review A*, 87:042323, 2013.

[148] M. J. Kastoryano, F. Reiter, and A. S. Sørensen. Dissipative preparation of entanglement in optical cavities. *Phys. Rev. Lett.*, 106:090502, 2011.

[149] F. Reiter, M. J. Kastoryano, and A. S. Sørensen. Driving two atoms in an optical cavity into an entangled steady state using engineered decay. *New J. Phys.*, 14:053022, 2012.

[150] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller. Preparation of entangled states by quantum Markov processes. *Phys. Rev. A*, 78:042307, 2008.

[151] I. Sinayskiy and F. Petruccione. Efficiency of open quantum walk implementation of dissipative quantum computing algorithms. *Quant. Inf. Proc.*, 11:1301, 2012.

[152] M. J. Kastoryano, M. M. Wolf, and J. Eisert. Precisely timing dissipative quantum information processing. *Physical review letters*, 110:110501, 2013.

[153] M. Kliesch, T. Barthel, C. Gogolin, M. J. Kastoryano, and J. Eisert. Dissipative Quantum Church-Turing Theorem. *Phys. Rev. Lett.*, 107:120501, 2011.

[154] F. Pastawski, L. Clemente, and J. I. Cirac. Quantum memories based on engineered dissipation. *Phys. Rev. A*, 83:012304, 2011.

[155] M. Herold, E. T. Campbell, J. Eisert, and M. J. Kastoryano. Cellular-automaton decoders for topological quantum memories. arXiv:1406.2338 [quant-ph], 2014.

[156] M. Herold, M. J. Kastoryano, E. T. Campbell, and J. Eisert. Fault tolerant dynamical decoders for topological quantum memories. arXiv:1511.05579 [quant-ph], 2015.

[157] H. P. Breuer, E. M. Laine, J. Piilo, and B. Vacchini. *Colloquium* : Non-Markovian dynamics in open quantum systems. *Rev. Mod. Phys.*, 88:021002, 2016.

[158] A. Rivas, S. F. Huelga, and M. B. Plenio. Quantum non-Markovianity: characterization, quantification and detection. *Rep. Prog. Phys.*, 77:094001, 2014.

[159] I. de Vega and D. Alonso. Dynamics of non-Markovian open quantum systems. arXiv:1511.06994 [quant-ph], 2015.

[160] B. Bylicka, D. Chruściński, and S. Maniscalco. Non-Markovianity as a resource for quantum technologies. arXiv:1301.2585 [quant-ph], 2013.

[161] D. M. Reich, N. Katz, and C. P. Koch. Exploiting non-Markovianity for quantum control. *Sci. Rep.*, 5, 2015.

[162] H.-P. Breuer and F. Petruccione. *The theory of open quantum systems*. Oxford University Press, 2002.

[163] H. Carmichael. *An open systems approach to quantum optics: lectures presented at the Université Libre de Bruxelles, October 28 to November 4, 1991*, volume 18. Springer Science & Business Media, 2009.

[164] C. Gardiner and P. Zoller. *Quantum noise: a handbook of Markovian and non-Markovian quantum stochastic methods with applications to quantum optics*, volume 56. Springer Science & Business Media, 2004.

[165] A. Rivas and S. F. Huelga. *Open Quantum Systems*. Springer, 2012.

[166] M. M. Wolf. Quantum channels & operations: Guided tour. Lecture notes available at http://www-m5.ma.tum.de/foswiki/pubM, 2012.

[167] J. Watrous. Theory of quantum information. Lecture notes available at https://cs.uwaterloo.ca/ watrous/CS766/LectureNotes/all.pdf, 2011.

[168] D. Chruściński and A. Kossakowski. Non-Markovian quantum dynamics: Local versus nonlocal. *Phys. Rev. Lett.*, 104:070406, 2010.

[169] D. Chruściński and A. Kossakowski. Sufficient conditions for a memory-kernel master equation. *Phys. Rev. A*, 94:020103, 2016.

[170] F. A. Wudarski and F. Petruccione. Who's afraid of non-local master equations? Private correspondence. Soon to be published, 2016.

[171] M. Müller, S. Diehl, G. Pupillo, and P. Zoller. Engineered open systems and quantum simulations with atoms and ions. *Adv. Atom. Mol. Opt. Phys*, 61:1, 2012.

[172] I. Bloch, J. Dalibard, and S. Nascimbene. Quantum simulations with ultracold quantum gases. *Nature Physics*, 8:267, 2012.

[173] A. Aspuru-Guzik and P. Walther. Photonic quantum simulators. *Nature Physics*, 8:285, 2012.

[174] B. M. Terhal, I. L. Chuang, D. P. DiVincenzo, M. Grassl, and J. A. Smolin. Simulating quantum operations with mixed environments. *Phys. Rev. A*, 60:881, 1999.

[175] S. Lloyd and L. Viola. Engineering quantum dynamics. *Phys. Rev. A*, 65:010101, 2001.

[176] M. B. Ruskai, S. Szarek, and E. Werner. An analysis of completely-positive trace-preserving maps on 2×2 matrices. *Linear Algebra and its Applications*, 347:159, 2002.

[177] D.-S. Wang, D. W. Berry, M. C. de Oliveira, and B. C. Sanders. Solovay-Kitaev decomposition strategy for single-qubit channels. *Phys. Rev. Lett.*, 111:130504, 2013.

[178] D.-S. Wang and B. C. Sanders. Quantum circuit design for accurate simulation of qudit channels. *New J. Phys.*, 17:043004, 2015.

[179] R. Iten, R. Colbeck, and M. Christandl. Quantum circuits for quantum channels. arXiv:1609.08103 [quant-ph], 2016.

[180] D. Bacon, A. M. Childs, I. L. Chuang, J. Kempe, D. W. Leung, and X. Zhou. Universal simulation of Markovian quantum dynamics. *Phys. Rev. A*, 64:062302, 2001.

[181] M. Ziman, P. Štelmachovič, and V. Bužek. Description of quantum dynamics of open systems based on collision-like models. *Open systems & information dynamics*, 12:81, 2005.

[182] P. Schindler, M Mueller, D Nigg, J. T. Barreiro, E. A. Martinez, M. Hennrich, T. Monz, S. Diehl, P. Zoller, and R. Blatt. Quantum simulation of open-system dynamical maps with trapped ions. In *APS Division of Atomic, Molecular and Optical Physics Meeting Abstracts*, volume 1, page 5005, 2013.

[183] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H.-P. Büchler. A Rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[184] P. Zanardi, J. Marshall, and L. C. Venuti. Dissipative universal Lindbladian simulation. *Phys. Rev. A*, 93:022312, 2016.

[185] J. Marshall, L. C. Venuti, and P. Zanardi. Modular quantum information processing by dissipation. arXiv:1607.03207 [quant-ph], 2016.

[186] H. Weimer. Tailored jump operators for purely dissipative quantum magnetism. arXiv:1608.02593 [quant-ph], 2016.

[187] B. Dive, F. Mintert, and D. Burgarth. Quantum simulations of dissipative dynamics: Time dependence instead of size. *Phys. Rev. A*, 92:032111, 2015.

[188] R. Di Candia, J. S. Pedernales, A. Del Campo, E. Solano, and J. Casanova. Quantum simulation of dissipative processes without reservoir engineering. *Sci. Rep.*, 5, 2015.

[189] A. M. Childs and T. Li. Efficient simulation of sparse Markovian quantum dynamics. arXiv:1611.05543 [quant-ph], 2016.

[190] A. Chenu, M. Beau, J. Cao, and A. del Campo. Quantum simulation of many-body decoherence: Noise as a resource. arXiv:1608.01317 [quant-ph], 2016.

Chapter 2

Simulation of single-qubit open quantum systems

A quantum algorithm is presented for the simulation of arbitrary Markovian dynamics of a qubit, described by a semigroup of single qubit quantum channels $\{T_t\}$ specified by a generator $\mathcal{L}$. This algorithm requires only single qubit and CNOT gates and approximates the channel $T_t = e^{t\mathcal{L}}$ up to chosen accuracy ϵ, with slightly superlinear cost $\mathcal{O}\big((||\mathcal{L}||_{(1\to 1)}t)^{1+1/2k}/\epsilon^{1/2k}\big)$ for any integer k. Inspired by developments in Hamiltonian simulation, a decomposition and recombination technique is utilised which allows for the exploitation of recently developed methods for the approximation of arbitrary single-qubit channels. In particular, as a result of these methods the algorithm requires only a single ancilla qubit, the minimal possible dilation for a non-unitary single-qubit quantum channel.

This chapter has been been previously published in [1].

2.1 Introduction

One of the primary motivations for the development of quantum computation is the possibility of efficiently simulating quantum systems [2–4], as suggested in Feynman's seminal paper on the topic [5]. The natural first step towards this vision is the simulation of closed quantum systems, undergoing Hamiltonian generated unitary evolution, and over the past two decades consistent progress has been made in this field. Initially, Lloyd demonstrated a technique for the efficient simulation of sufficiently local Hamiltonians [6], and over time new methods and techniques have been introduced which have generalised the class of Hamiltonians which can be efficiently simulated while simultaneously tightening the relevant cost and error bounds [7–14].

However, equally as important is the development of methods for the simulation of open quantum systems [15, 16], crucial for enhancing our understanding of non-equilibrium dynamics and thermalisation in a wide range of systems, from damped-driven spin-boson models to complex many fermion-boson models [3, 4]. In particular, one would like to begin by simulating quantum channels, representing the most general quantum dynamics possible, and dynamical semigroups of quantum channels, which describe Markovian dynamics - continuous time processes resulting from interactions with a Markovian environment in the Born approximation [17]. A straightforward methodology for the simulation of these systems is instantly suggested by the Stinespring dilation theorem [18], in which one introduces an initially pure state environment, with size the square of the system size in the general case, such that one may simulate the open system dynamics of the system via Hamiltonian dynamics of the larger system-environment combination. Initially Lloyd [6] conjectured that this approach may be improved by utilising environments initialised in a mixed state, but this conjecture was quickly falsfied by Terhal et al. [19], who prove that in the worst case an environment of dimension n^2 is necessary for the simulation of n dimensional quantum channels via the Stinespring dilation.

An important early contribution was also made by Bacon et al. [20], who provide a method for decomposing the generators of Markovian evolution into simpler "primitive" generators. In particular, they demonstrate that for the single qubit case universal simulation of Markovian dynamics requires only the ability to simulate a specific continuous one parameter family of generators, as well as the ability to implement the recombination methods of linear combination and unitary conjugation. The development of collision models [21] for understanding quantum decoherence processes also suggests a constructive approach for the simulation of open quantum systems, and combining these insights

with the results of Bacon et al. allowed for the development of collision model based methods for the simulation of single-qubit unital semigroups, generalised phase-damping processes and indivisible qubit channels [22, 23].

More recently the notion of dissipative quantum computation and state preparation [24] has been introduced, in which under the assumption of Markovian dynamics described by a Lindblad master equation, the interactions of a system with its environment are no longer considered destructive, but are instead utilised to drive a desired computational process. This formalism offers a natural setting for the simulation of open quantum systems and research in this direction has resulted in successful experimental demonstrations of the dissipative simulation of complex many-body spin models [25, 26]. In addition, dissipative quantum computation has allowed for alternative approaches to state preparation [27–36] and universal quantum computation [37, 38]. Importantly however, it has recently been shown that dissipative quantum computing is no more powerful than the traditional circuit model - the so called "Dissipative Church Turing Thesis" [39]. Specifically, it was shown that time evolution of an open quantum system can be efficiently simulated by a unitary quantum circuit of size scaling polynomially in the simulation time and size of the system.

Given these previous results we address in this paper the problem of constructing explicitly these efficient quantum circuits for the simulation of arbitrary Markovian processes within the traditional circuit model of quantum computation. In particular, we generalise into the super-operator regime recombination results, based on higher order Suzuki-Lie-Trotter formulae [40, 41], from recent Hamiltonian simulation approaches [9–11]. These results allow us to efficiently implement the recombination methods of Bacon et al. [20], such that in order to construct efficient quantum circuits for the simulation of arbitrary Markovian dynamics of a qubit it is only necessary to construct efficient circuits for the simulation of semigroups corresponding to the continuous one parameter family of generators defined by Bacon et al. [20]. Furthermore, recently Wang et al. [42] have shown how to utilise convex properties of the set of single-qubit quantum channels [43] to simulate any such channel via unitary circuits requiring only a single ancilla qubit, as opposed to the two-ancilla qubits required by straightforward implementations of the Stinespring dilation. We utilise these results for the construction of circuits for the simulation of the semigroups required by Bacon et al. [20], such that after recombination we obtain an explicit unitary circuit, with size scaling slightly superlinearly with respect to time, consisting only of CNOT gates and single qubit gates and requiring only a single ancilla qubit, for the simulation up to any desired accuracy of an arbitrary single-qubit quantum dynamical semigroup.

The structure of this chapter is as follows: We begin by introducing the setting and rigorously defining the problem we wish to address. Following this we proceed in Section 2.3 by presenting the method, introduced in [20], for the decomposition of an arbitrary generator of a single-qubit Markov semigroup. In Section 2.4 we generalise results from [10] into the setting applicable for the problem addressed here, effectively demonstrating a method for the efficient recombination of the generators decomposed in Section 2.3. Finally, in Section 2.5 we exploit the methods introduced in [42] in order to provide explicit efficient unitary circuits for the semigroups corresponding to the generators resulting from the decomposition in Section 2.3.

2.2 Problem and setting

Given a system with finite dimensional Hilbert space $\mathcal{H}_S = \mathbb{C}^d$, a quantum state of this system is described by a density matrix $\rho \in \mathcal{M}_d(\mathbb{C}) \cong \mathcal{B}(\mathcal{H}_S)$, where $\rho \geq 0$, $\mathrm{tr}[\rho] = 1$ and $\mathcal{B}(\mathcal{H}_S)$ is the algebra of bounded operators on $\mathcal{H}_S$. Quantum channels [17] provide the most general framework for describing the evolution of quantum states, and are given by completely positive, trace-preserving (CPT) maps,

$$T : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S). \tag{2.1}$$

Given any quantum channel T, there exists Kraus operators $\{K_j \in \mathcal{B}(\mathcal{H}_S)\}$, such that

$$T(\rho) = \sum_{j=1}^{r} K_j \rho K_j^\dagger. \tag{2.2}$$

In the above, $\sum_{j=1}^{r} K_j^\dagger K_j = \mathbb{1}$ and $r = \mathrm{rank}(\tau) \leq d^2$ is the minimal number of Kraus operators, with $\tau \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_S)$ the Jamiolkowski state,

$$\tau = (T \otimes \mathbb{1}_S)|\Omega\rangle\langle\Omega|, \tag{2.3}$$

where $\mathbb{1}_S$ is the identity on $\mathcal{H}_S$ and $|\Omega\rangle \in \mathcal{H}_S \otimes \mathcal{H}_S$ is any maximally entangled state [17]. Furthermore, it is always possible to dilate the total Hilbert space in order to include an environment, such that the action of the channel on the system can be viewed as arising from the Hamiltonian generated unitary evolution of the total system and environment. Technically, it is always possible to introduce a dilation space $\mathcal{H}_E$ with

$\dim(\mathcal{H}_E) = [\dim(\mathcal{H}_S)]^2$ such that there exists a unitary matrix $U \in \mathcal{M}_{d^3}(\mathbb{C})$ where

$$T(\rho) = \mathrm{tr}_E\big[U(|e_0\rangle\langle e_0| \otimes \rho)U^\dagger\big] \tag{2.4}$$

and $|e_0\rangle\langle e_0| \in \mathcal{H}_E$ is some initial state of the environment. However, in the case that d is a factor of $\mathrm{rank}(\tau)$ then it is possible to construct a dilation with $\dim(\mathcal{H}_E) = r$ and $U \in \mathcal{M}_{dr}(\mathbb{C})$ - such a dilation space is called a *minimal* dilation. Quantum channels as described above provide a complete picture of discrete time evolution. However, in this paper we are concerned with the simulation of Markovian continuous time evolutions, described by a continuous one parameter semigroup of quantum channels $\{T_t\}$ satisfying

$$T_t T_s = T_{t+s}, \qquad T_0 = \mathbb{1}, \tag{2.5}$$

for $t \in \mathbb{R}_+$, where $\rho(t) = T_t\big(\rho(0)\big)$. Every continuous one parameter semigroup of quantum channels $\{T_t\}$ has a unique generator

$$\mathcal{L} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S), \tag{2.6}$$

such that

$$T_t = e^{t\mathcal{L}} = \sum_{k=0}^{\infty} \frac{t^k \mathcal{L}^k}{k!} \tag{2.7}$$

and $\mathcal{L}$ satisfies the differential equation

$$\frac{d}{dt}\rho(t) = \mathcal{L}\big(\rho(t)\big), \tag{2.8}$$

known as a master equation. Furthermore, a linear super-operator $\mathcal{L} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$ is the generator of a continuous dynamical semigroup of quantum channels, if and only if it can be written in the form

$$\mathcal{L}(\rho) = i[\rho, H] + \sum_{k,l=1}^{d^2-1} A_{l,k}\big([F_k, \rho F_l^\dagger] + [F_k \rho, F_l^\dagger]\big), \tag{2.9}$$

where $H = H^\dagger \in \mathcal{M}_d(\mathbb{C})$ is Hermitian, $A \in \mathcal{M}_{d^2-1}(\mathbb{C})$ is positive semidefinite and $\{F_i\}$ is a basis for the space of traceless matrices in $\mathcal{M}_d(\mathbb{C})$. Eq. (2.9) is known as the Gorini, Kossakowsi, Sudarshan and Lindblad form of the quantum Markov master equation and we refer to A as the GKS matrix [17]. For the remainder of this paper we choose the basis $\{F_i\}$, without loss of generality, to be the normalized Pauli operators $\frac{1}{\sqrt{2}}\{\sigma_x, \sigma_y, \sigma_z\}$.

In order to quantify the error in approximations of quantum channels we will utilise the $(1 \to 1)$-norm for super-operators, where in general the $(p \to q)$-norm of a super-operator is defined as [44]

$$||T||_{p\to q} := \sup_{||A||_p=1} ||T(A)||_q. \tag{2.10}$$

The $(p \to q)$-norm defined above is induced from the Schatten p-norm of an operator, defined as $||A||_p := \big(\mathrm{tr}(|A|^p)\big)^{\frac{1}{p}}$. We use the $(1 \to 1)$-norm as this is induced by the Schatten 1-norm, which corresponds up to a factor of $1/2$ with the trace distance, $\mathrm{dist}(\rho, \sigma) := \sup_{0\leq A\leq 1} \mathrm{tr}\big(A(\rho - \sigma)\big)$, arising from a physical motivation of operational distinguishability of quantum states [37]. At this stage it is possible to succinctly state the problem which is addressed in this chapter.

Problem 2.1. *Given a continuous one parameter semigroup of single-qubit quantum channels $\{T_t\}$, generated by a generator $\mathcal{L}$, specified by a GKS matrix $A \geq 0 \in M_3(\mathbb{C})$ and a Hamiltonian $H = H^\dagger \in M_2(\mathbb{C})$, find a quantum circuit, acting on only the system qubit and a single ancilla qubit and using at most* $\mathrm{poly}\big(||\mathcal{L}||_{(1\to 1)}, t, 1/\epsilon\big)$ *single qubit and CNOT gates, that approximates the superoperator $T_t = e^{t\mathcal{L}}$ such that the maximum error in the final state, as quantified by the* 1*-norm, is at most ϵ.*

It is important to note that each member T_t of an arbitrary semigroup of single-qubit channels $\{T_t\}$ is itself a single-qubit channel, and therefore in principle, using the methods of Wang et al. [42], can be simulated within 1-norm distance ϵ using $\mathcal{O}(\log^{3.97}(1/\epsilon))$ gates from any specified single qubit set S and one CNOT, acting on only the system qubit and a single ancilla. However in order to utilise this method, which may even be improved [45, 46] to require only $\mathcal{O}(\log(1/\epsilon))$ such gates, it is necessary to first obtain a decomposition of the channel T_t into a convex sum of quasi-extreme channels, which in order to do explicitly requires specification of the generator. Therefore in order to exploit these methods for the simulation of a semigroup generated by an *arbitrary* generator, we utilise the decomposition/recombination strategy outlined in Section 4.1. This strategy is inspired by approaches in Hamiltonian simulation [9–11] and as such we simultaneously adopt the notion of efficiency developed within that context. Due to our restriction to the single qubit case our notion of efficiency has no dependence on the system size, which remains a constant. However, as in [42], we restrict ourselves to quantum circuits requiring only a single ancilla qubit, the smallest possible minimal dilation for a non-unitary single-qubit channel.

As we are restricting ourselves to single-qubit channels we begin by recalling some

geometric properties of single qubit states [43]. As $\{I, \sigma_x, \sigma_y, \sigma_z\}$ forms a basis for $\mathcal{M}_2(\mathbb{C})$, every density matrix ρ can be written in this basis as $\rho = 1/2(\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma})$ where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\mathbf{r} \in \mathbb{R}^3$ with $|\mathbf{r}| \leq 1$. Any single qubit quantum channel can then be represented in this basis by a unique 4×4 matrix M, with the following structure:

$$M = \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{m} & \tilde{M} \end{pmatrix}, \tag{2.11}$$

where $\tilde{M}$ is a 3×3 matrix, $\mathbf{0}$ and $\mathbf{m}$ are row and column vectors respectively, and if we define

$$T(\rho) = \rho' = 1/2(\mathbb{1} + \mathbf{r}' \cdot \boldsymbol{\sigma}), \tag{2.12}$$

then M defines an affine map via

$$\mathbf{r}' = \tilde{M} \cdot \mathbf{r} + \mathbf{m}. \tag{2.13}$$

At this stage we can proceed to develop the solution to the problem defined above, as per the strategy outlined in Section 2.1.

2.3 Decomposition of arbitrary generator

As outlined in the description of our strategy, the first step is to provide a decomposition of an arbitrary generator $\mathcal{L}$, specified as per (2.9) by a GKS matrix $A \geq 0 \in \mathcal{M}_3(\mathbb{C})$ and a Hamiltonian $H = H^\dagger \in \mathcal{M}_2(\mathbb{C})$, into the combination of generators of simpler semigroups. This problem was initially addressed by Bacon et al. [20] and we follow their strategy here. As $A \geq 0$ one can use the spectral decomposition to write,

$$A = \sum_{k=1}^{3} \lambda_k A_k, \tag{2.14}$$

and therefore via linearity of $\mathcal{L}$

$$\mathcal{L} = \mathcal{L}_H + \sum_{k=1}^{3} \lambda_k \mathcal{L}_k, \tag{2.15}$$

where

$$\mathcal{L}_H(\rho) = i[\rho, H] \tag{2.16}$$

and

$$\mathcal{L}_k(\rho) = \sum_{i,j=1}^{3} A_{k,(i,j)}\big([F_j, \rho F_i^\dagger] + [F_j \rho, F_i^\dagger]\big). \tag{2.17}$$

Relabelling $\mathcal{L}_0 := \mathcal{L}_H$ and defining $\lambda_0 = 1$ we can then write

$$\mathcal{L} = \sum_{k=0}^{3} \lambda_k \mathcal{L}_k, \tag{2.18}$$

giving us that,

$$T_t = e^{t\mathcal{L}} = \exp\Big(t \sum_{k=0}^{3} \lambda_k \mathcal{L}_k\Big). \tag{2.19}$$

Furthermore, defining $T_{t'}^{(k)} := e^{t'\mathcal{L}_k}$ we see via a straightforward implementation of the Lie-Trotter formula [40] that

$$T_t = \lim_{n\to\infty} \left[\prod_{k=0}^{3} e^{[t\lambda_k(\mathcal{L}_k/2)]/n} \prod_{k'=3}^{0} e^{[t\lambda_{k'}(\mathcal{L}_{k'}/2)]/n} \right]^n \tag{2.20}$$

$$= \lim_{n\to\infty} \left[\prod_{k=0}^{3} T^{(k)}_{\left(\frac{t\lambda_k}{2n}\right)} \prod_{k'=3}^{0} T^{(k')}_{\left(\frac{t\lambda_{k'}}{2n}\right)} \right]^n. \tag{2.21}$$

Using the language of [20] we say that T_t can be constructed via *linear combination* of the semigroups $\{T_{t'}^{(k)}\}$. In Section 2.4 we present a method for the efficient recombination of linear combinations - i.e. we provide a method for the approximation of T_t, up to arbitrary accuracy, using only a finite (polynomial in t) number of implementations of channels from the constituent semigroups $\{T_t^{(k)}\}$. Given such a method for the efficient simulation of linear combinations, it is then clear that one can obtain an efficient algorithm for the simulation of T_t, provided one can efficiently simulate the constituent channels $T_t^{(k)}$.

However, as per [20], we can utilise basis transformations to further decompose the constituent semigroups $\{T_t^{(k)}\}$, and hence simplify the task of implementing channels from these semigroups, which is tackled in Section 2.5. Firstly, note that for $k = 1$, $\mathcal{L}_k$ simply generates Hamiltonian evolution, which can be simulated using a single unitary operation on a single qubit. We therefore focus on the generators of dissipative evolution, for which $k \in [2, 4]$. We begin by defining *unitary conjugation* of a channel T_t as the procedure transforming T_t according to $\mathcal{U}^\dagger T_t \mathcal{U}$, where $\mathcal{U}(\rho) = U\rho U^\dagger$ for some unitary operator U. Unitary conjugation preserves all Markovian semigroup properties and is clear that the effect of unitary conjugation is to apply T_t in an alternative basis. In order

to use unitary conjugation to further decompose the semigroups $\{T_t^{(k)}\}$ we utilise the following theorem, due to [20], establishing the manner in which unitary conjugation of a semigroup $\{T_t\}$ effects the GKS matrix defining the corresponding generator.

Theorem 2.1. *For an N dimensional system, unitary conjugation of the semigroup* $\{T_t\}$ *by* $U \in \mathrm{SU(N)}$ *results in conjugation of the GKS matrix by a corresponding element in the adjoint representation of* SU(N).

One can then show [20] that given A_k, as per (2.14), there exists $G_k \in \mathrm{SO}(3)$, the adjoint representation of SU(2), such that

$$A_k = G_k A_{(\theta_k)} G_k^T, \tag{2.22}$$

where

$$A_{(\theta_k)} = \begin{pmatrix} \cos^2(\theta_k) & -i\cos(\theta_k)\sin(\theta_k) & 0 \\ i\cos(\theta_k)\sin(\theta_k) & \sin^2(\theta_k) & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.23}$$

for $\theta_k \in [0, \pi/4]$. Therefore, as a result of Theorem 2.1 there exist unitary matrices $U_k \in \mathrm{SU(2)}$ such that

$$T_t^{(k)}(\rho) = U_k^\dagger \big[T_t^{(\theta_k)}\big(U_k \rho U_k^\dagger\big)\big] U_k, \tag{2.24}$$

where $T_t^{(\theta_k)} := e^{t\mathcal{L}_{(\theta_k)}}$ and

$$\mathcal{L}_{(\theta_k)}(\rho) = \sum_{i,j=1}^{3} A_{(\theta_k),(i,j)}\big([F_j, \rho F_i^\dagger] + [F_j \rho, F_i^\dagger]\big). \tag{2.25}$$

In light of the above, we can then see that simulation of any channel from the semigroup $\{T_t^{(k)}\}$ requires only simulation of channels from the semigroup $\{T_t^{(\theta_k)}\}$, along with implementations of the single qubit unitary U_k.

2.4 Recombination

In this section we utilise methods developed within the context of Hamiltonian simulation [9–11] to show that higher order Suzuki integrators [40,41] can be used to simulate T_t up to arbitrary accuracy ϵ, using a finite sequence of implementations of $T_{t'}^{(j)} := e^{t'\mathcal{L}_j}$. In particular we wish to place an upper bound on the number of implementations of $T_{t'}^{(j)}$ required within this sequence.

Given the generator $\mathcal{L} = \sum_{j=1}^{m} \mathcal{L}_j$ of a dynamical semigroup of quantum channels,

as per (2.19) where $m = 4$, we begin by assuming that

$$||\mathcal{L}_1||_{1\to 1} \geq ||\mathcal{L}_2||_{1\to 1} \geq \cdots \geq ||\mathcal{L}_m||_{1\to 1} \tag{2.26}$$

and defining the normalised component generators $\hat{\mathcal{L}}_j = \mathcal{L}_j/L_1$, where we have defined $L_1 := ||\mathcal{L}_1||_{1\to 1}$. We then follow [10] and define the basic Lie-Trotter product formula [40, 41, 47] as,

$$S_2(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda) = \prod_{j=1}^{m} e^{(\frac{\lambda}{2})\hat{\mathcal{L}}_j} \prod_{j'=m}^{1} e^{(\frac{\lambda}{2})\hat{\mathcal{L}}_{j'}} \tag{2.27}$$

$$= \prod_{j=1}^{m} T_{t_\lambda}^{(j)} \prod_{j'=m}^{1} T_{t_\lambda}^{(j')}, \tag{2.28}$$

where $t_\lambda = \lambda/(2L_1)$. Suzuki's higher order integrators are then defined using the recursion relation

$$S_{2k}(\lambda) = [S_{2k-2}(p_k\lambda)]^2[S_{2k-2}((1-4p_k)\lambda)][S_{2k-2}(p_k\lambda)]^2, \tag{2.29}$$

where $p_k = (4-4^{1/(2k-1)})^{-1}$ for $k > 1$ and for notational convenience we have used $S_{2k}(\lambda)$ and $S_{2k-2}(\lambda)$ to denote $S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda)$ and $S_{2k-2}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda)$ respectively. Note that $S_{2k}(\lambda)$ consists of a product of

$$2(m-1)5^{k-1} + 1 \tag{2.30}$$

exponentials, so that we can define

$$N_{\text{exp}} = [2(m-1)5^{k-1} + 1]x \tag{2.31}$$

as the number of exponentials, and hence channels $T_{t'}^{(j)}$, appearing in the expression $[S_{2k}(t/r)]^x$. In order to obtain the desired result, we then prove the following theorem, a direct generalization of the work in [10] to the superoperator setting.

Theorem 2.2. *Let $1 \geq \epsilon > 0$ be such that $4met||\mathcal{L}_2||_{1\to 1} \geq \epsilon$, then for any $k \in \mathbb{N}$ there exists r such that*

$$\Big|\Big|\exp\Big(t\sum_{j=1}^{m}\mathcal{L}_j\Big) - \big[S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, t/r)\big]^{rL_1}\Big|\Big|_{1\to 1} \leq \epsilon \tag{2.32}$$

and the number of exponentials required is bounded by

$$\mathrm{N}_{\exp} \leq (2m-1)5^{k-1}\Big[L_1 t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/2k}\frac{4me}{3}\Big(\frac{5}{3}\Big)^{k-1}\Big] \tag{2.33}$$

where $L_2 := ||\mathcal{L}_2||_{1\to 1}$.

In order to prove Theorem 2.2 we first note that the following lemma can be proven using the exact same proof as described in [10], provided one replaces the 1-norm with the $(1 \to 1)$ norm and notes that $||T||_{1\to 1} = 1$ for any quantum channel T [39,44], as the proof relies only on properties of the Taylor expansion of exponentials and generic properties of the norm, which hold for both Schatten norms and the induced superoperator norms [44].

Lemma 2.1. *For* $k \in \mathbb{N}$, $d_k\lambda < k+1$, $d_k = m(4/3)k(5/3)^{k-1}$ *and*

$$||\hat{\mathcal{L}}_m||_{1\to 1} \leq \cdots \leq ||\hat{\mathcal{L}}_2||_{1\to 1} \leq ||\hat{\mathcal{L}}_1||_{1\to 1} = 1, \tag{2.34}$$

we have that

$$\Big|\Big|\exp\Big(\lambda\sum_{j=1}^{m}\hat{\mathcal{L}}_j\Big) - S_{2k}(\lambda)\Big|\Big|_{1\to 1} \leq \frac{4L_2}{(2k+1)!}(d_k\lambda)^{2k+1}, \tag{2.35}$$

where $S_{2k}(\lambda) = S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda)$.

In addition to Lemma 2.1, the following lemma is required:

Lemma 2.2. *Given quantum channels* T *and* V *we have that*

$$\big|\big|T^n - V^n\big|\big|_{1\to 1} \leq n\big|\big|T - V\big|\big|_{1\to 1}. \tag{2.36}$$

Lemma 2.2 is a direct generalisation to the superoperator setting of an important result describing the accumulation of errors due to gate approximations in unitary circuits. However, in the conventional operator setting the proof relies crucially on properties of Hermitian operators and as a result an alternative proof is required within this more general setting.

Proof (of Lemma 2.2). It is clear that in the case that $n = 1$ the lemma is true. Assume the lemma holds for $n = m$. We now show that it holds for $n = m + 1$ and as a result

prove the result by induction.

$$\begin{aligned}
\big|\big|T^{m+1} - V^{m+1}\big|\big|_{1\to 1} &= \big|\big|TT^m - TV^m + TV^m - V.V^m\big|\big|_{1\to 1} && (2.37)\\
&\leq \big|\big|T\big(T^m - V^m\big)\big|\big|_{1\to 1} + \big|\big|\big(T - V\big)V^m\big|\big|_{1\to 1} && (2.38)\\
&\leq \big|\big|T\big|\big|_{1\to 1}\big|\big|T^m - V^m\big|\big|_{1\to 1} + \big|\big|T - V\big|\big|_{1\to 1}\big|\big|V^m\big|\big|_{1\to 1} && (2.39)\\
&\leq \big|\big|T^m - V^m\big|\big|_{1\to 1} + \big|\big|T - V\big|\big|_{1\to 1} && (2.40)\\
&\leq (m+1)\big|\big|T - V\big|\big|_{1\to 1} && (2.41)
\end{aligned}$$

In the above (2.39) follows from (2.38) via submultiplicativity of the norm, and (2.40) follows from (2.39) due to the fact [39,44] that for any quantum channel T we have that $||T||_{1\to 1} = 1$. ■

Given these two lemmas it is now possible to follow [10] in order to prove Theorem 2.2.

Proof (of Theorem 2.2). First note that

$$\exp\Big(t\sum_{j=1}^{m}\mathcal{L}_j\Big) = \Big[\exp\Big(\frac{t}{r}\sum_{j=1}^{m}\hat{\mathcal{L}}_j\Big)\Big]^{rL_1}, \tag{2.42}$$

and as a result we can utilise Lemma 2.1 and Lemma 2.2 to obtain

$$\Big|\Big|\exp\Big(t\sum_{j=1}^{m}\mathcal{L}_j\Big) - \big[S_{2k}(\frac{t}{r})\big]^{rL_1}\Big|\Big|_{1\to 1} \leq 4tL_2\frac{d_k^{2k+1}}{(2k+1)!}\frac{t^{2k}}{r^{2k}}. \tag{2.43}$$

Therefore taking

$$r \geq t\Big(\frac{4tL_2d_k^{2k+1}}{\epsilon(2k+1)!}\Big)^{1/(2k)} \tag{2.44}$$

ensures that (2.32) is satisfied. Furthermore, via the argument in [10] it suffices to take

$$r \geq t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/(2k)}\frac{2ed_k}{2k+1}, \tag{2.45}$$

such that we can define r as the lower bound

$$r := t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/(2k)}\frac{2ed_k}{2k+1}, \tag{2.46}$$

which is easily seen to satisfy the assumptions of Lemma 2.1. From (2.31) one can then

see that the total number of exponentials required is

$$\mathrm{N}_{\mathrm{exp}} \leq (2m-1)5^{k-1} r L_1, \tag{2.47}$$

so that substituting in the values of r and d_k one obtains (2.33). ■

As calculated in [10], if $\epsilon \leq mtL_2$ then the minimum value of the right hand side in (2.33) is achieved for

$$k = \mathrm{round}\left(\sqrt{\frac{1}{2}\log_{25/3}\frac{4emtL_2}{\epsilon}}\right), \tag{2.48}$$

such that the number of exponentials required satisfies

$$N_{\mathrm{exp}} \leq \frac{8}{3}(2m-1)metL_1 e^{2\sqrt{\frac{1}{2}\ln(25/3)\ln(4emtL_2/\epsilon)}}. \tag{2.49}$$

Furthermore, by definition of the $(1 \to 1)$ norm we have that for any density matrix ρ and any superoperators P and Q,

$$||P(\rho) - Q(\rho)||_1 \leq ||P - Q||_{1\to 1} \tag{2.50}$$

and as such the results of Theorem 2.2 bound the error in the output state obtained when approximating T_t with $[S_{2k}(t/r)]^{rL_1}$. At this point we have then established that any channel T_t, a member of the semigroup $\{T_t\}$ generated by $\mathcal{L} = \sum_{j=1}^{m} \mathcal{L}_j$, can be simulated up to arbitrary accuracy using only a slightly super-linear, with respect to t, number of implementations of $T_{t'}^{(j)} = e^{t'\mathcal{L}_j}$.

2.5 Simulation of constituent semigroups

Given the results of Section 2.3 and Section 2.4, all that remains is to illustrate a method for the construction of unitary circuits, consisting only of single-qubit and CNOT gates and requiring only a single ancilla qubit, for the exact implementation of quantum channels from the semigroups $\{T_t^{(\theta_k)}\}$. We proceed by following the strategy, introduced in [42], of decomposing the channels $T_t^{(\theta_k)}$ into the convex sum of quasi-extreme channels. These quasi-extreme channels require only two Kraus operators for implementation, and hence can be simulated using a unitary circuit acting on only a single ancilla qubit. Furthermore, given a decomposition of $T_t^{(\theta_k)}$ into the convex sum of quasi-extreme channels, $T_t^{(\theta_k)}$ can be simulated using classical random sampling of these channels.

In order to obtain this convex decomposition we proceed via the following steps:

Firstly, we utilise the damping basis [48,49] in order to find the affine map representation of $T_t^{(\theta_k)}$. From this affine map representation it is then easy to construct the Jamiolkowski state, from which it is possible to obtain the desired convex decomposition [43].

Using damping basis methods [48,49] (details can be found in the Appendix, Section 2.7.1) we find, as per (2.11)-(2.13), that the affine map representation M of $T_t^{(\theta_k)}$ is given by

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \Lambda_1 & 0 & 0 \\ 0 & 0 & \Lambda_2 & 0 \\ m_3 & 0 & 0 & \Lambda_3 \end{pmatrix}, \tag{2.51}$$

where

$$\Lambda_1 = e^{(-2\sin^2(\theta_k)t)}, \tag{2.52}$$
$$\Lambda_2 = e^{(-2\cos^2(\theta_k)t)}, \tag{2.53}$$
$$\Lambda_3 = e^{(-2t)}, \tag{2.54}$$
$$m_3 = \sin(2\theta_k)(\Lambda_3 - 1). \tag{2.55}$$

Given this affine representation of $T_t^{(\theta_k)}$, the Jamiolkowski state

$$\tau_{(\theta_k)} = (T_t^{(\theta_k)} \otimes \mathbb{1}_S)|\psi_0\rangle\langle\psi_0|, \tag{2.56}$$

with $|\psi_0\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$, is then given by [43]

$$\tau_{(\theta_k)} = \frac{1}{4}\begin{pmatrix} a^2 & 0 & 0 & \Lambda_1 + \Lambda_2 \\ 0 & b^2 & \Lambda_1 - \Lambda_2 & 0 \\ 0 & \Lambda_1 - \Lambda_2 & c^2 & 0 \\ \Lambda_1 + \Lambda_2 & 0 & 0 & d^2 \end{pmatrix} \tag{2.57}$$

with

$$a = (1 + m_3 + \Lambda_3)^{1/2}, \tag{2.58}$$
$$b = (1 - m_3 - \Lambda_3)^{1/2}, \tag{2.59}$$
$$c = (1 + m_3 - \Lambda_3)^{1/2}, \tag{2.60}$$
$$d = (1 - m_3 + \Lambda_3)^{1/2}. \tag{2.61}$$

In order to utilise $\tau_{(\theta_k)}$ to obtain the desired convex decomposition of $T^{(\theta_k)}$, we

follow the procedure established in [43]. Firstly, for any quantum channel T we define $\beta(T) = 2\tau$ and note that $\beta(T)$ can always be written in the block form

$$\beta(T) = \begin{pmatrix} A & C \\ C^\dagger & B \end{pmatrix}. \tag{2.62}$$

Furthermore, if $\hat{T}$ is the adjoint [17] of T then

$$\beta(\hat{T}) = \overline{U_{23}^\dagger \beta(T) U_{23}} \tag{2.63}$$

$$= \begin{pmatrix} A & C \\ C^\dagger & I - A \end{pmatrix}, \tag{2.64}$$

where

$$U_{23} = U_{23}^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.65}$$

Given these facts we then utilise the following three results, all due to [43], in order to obtain the desired convex decomposition.

Theorem 2.3. *A quantum channel T is a generalised extreme point of the set of all quantum channels of the same dimension if and only if $\beta(\hat{T})$ is of the form*

$$\beta(\hat{T}) = \begin{pmatrix} A & \sqrt{A}U\sqrt{I-A} \\ \sqrt{I-A}U^\dagger\sqrt{A} & I - A \end{pmatrix}. \tag{2.66}$$

for some unitary matrix U.

Lemma 2.3. *A matrix*

$$\begin{pmatrix} A & C \\ C^\dagger & B \end{pmatrix} \tag{2.67}$$

is positive semidefinite if and only if $A \geq 0$, $B \geq 0$ and $C = \sqrt{A}R\sqrt{B}$ for some contraction R. Moreover, the set of positive semidefinite matrices with fixed A and B is a convex set whose extreme points satisfy $C = \sqrt{A}U\sqrt{B}$ for some unitary matrix U.

Lemma 2.4. *Any contraction in $M_2(\mathbb{C})$ can be written as the convex combination of two unitary matrices.*

In light of the above three results, our strategy for obtaining a convex decomposition of an arbitrary channel T is as follows: Given $\beta(T)$ we find $\beta(\hat{T})$ using (2.63). As T is

completely positive this ensures that $\beta(\hat{T}) \geq 0$ and as such we write $\beta(\hat{T})$ in the form described in Lemma 2.3. As R is a contraction we know, via Lemma 2.4, that R can be decomposed into the convex combination of two unitary matrices, and as a result we obtain that

$$\beta(\hat{T}) = \frac{1}{2}\beta(\hat{T}_1) + \frac{1}{2}\beta(\hat{T}_2), \tag{2.68}$$

where due to Theorem 2.3 we see that T_1 and T_2 are quasi-extreme channels (generalised extreme points of the set of quantum channels) providing the desired convex decomposition of T. Following these steps for $T_t^{(\theta_k)}$ we find that

$$\beta\big(\hat{T}_t^{(\theta_k)}\big) = \frac{1}{2}\beta\big(\hat{T}_{(t,1)}^{\theta_k}\big) + \frac{1}{2}\beta\big(\hat{T}_{(t,2)}^{\theta_k}\big), \tag{2.69}$$

where

$$\beta\big(\hat{T}_{(t,i)}^{\theta_k}\big) = \begin{pmatrix} A & \sqrt{A}U_i\sqrt{I-A} \\ \sqrt{I-A}U_i^\dagger\sqrt{A} & I-A \end{pmatrix}, \tag{2.70}$$

with

$$U_1 = \begin{pmatrix} 0 & e^{i\phi_1} \\ e^{i\phi_2} & 0 \end{pmatrix}, \qquad U_2 = \begin{pmatrix} 0 & e^{-i\phi_1} \\ e^{-i\phi_2} & 0 \end{pmatrix}, \tag{2.71}$$

$$\phi_1 = \arccos\Big(\frac{\Lambda_1 + \Lambda_2}{ad}\Big), \tag{2.72}$$

$$\phi_2 = \arccos\Big(\frac{\Lambda_1 - \Lambda_2}{bc}\Big), \tag{2.73}$$

and

$$A = \frac{1}{2}\begin{pmatrix} a^2 & 0 \\ 0 & c^2 \end{pmatrix}. \tag{2.74}$$

As in [42], in order to construct the unitary circuits implementing $T_{(t,i)}^{\theta_k}$ it is necessary to first find the Kraus operators K_1^i and K_2^i, where

$$T_{(t,i)}^{\theta_k}(\rho) = \sum_{j=1}^{2} \big(K_j^i\big)\rho\big(K_j^i\big)^\dagger. \tag{2.75}$$

To find these Kraus operators one then uses (2.63) to find the relevant Jamiolkowski state, before exploiting the standard Choi-Jamiolkowski correspondence [17]. Following

these steps one obtains

$$K_1^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & c \\ be^{i\phi_2} & 0 \end{pmatrix} \qquad K_2^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} ae^{-i\phi_1} & 0 \\ 0 & d \end{pmatrix} \tag{2.76}$$

and

$$K_1^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & c \\ be^{-i\phi_2} & 0 \end{pmatrix} \qquad K_2^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} ae^{i\phi_1} & 0 \\ 0 & d \end{pmatrix}. \tag{2.77}$$

Given these Kraus operators it is then possible to find a constant size unitary circuit implementing $T^{\theta_k}_{(t,i)}$, consisting only of CNOT's and single qubit gates, in a variety of ways. A first method is to apply directly the results of [42] (requiring an additional two basis transformations), or alternatively one can construct from the Kraus operators unitary matrices $U_i^{(\theta_k)}$, such that

$$T^{\theta_k}_{(t,i)}(\rho) = \mathrm{tr}_E\big[\big(U_i^{(\theta_k)}\big)(|0\rangle\langle 0| \otimes \rho)\big(U_i^{(\theta_k)}\big)^\dagger\big], \tag{2.78}$$

and proceed by obtaining a circuit decomposition of these unitary matrices. We provide an explicit demonstration of the latter strategy here. It is important to note that these unitary matrices are *not* unique [17], however for the purposes of this paper we choose to work with the following form for the unitary $U_1^{(\theta_k)}$,

$$U_1^{(\theta_k)} = \begin{pmatrix} e^{-i\phi_1}\cos(\beta) & 0 & 0 & -e^{-i\phi_2}\sin(\beta) \\ 0 & \cos(\alpha) & -\sin(\alpha) & 0 \\ 0 & \sin(\alpha) & \cos(\alpha) & 0 \\ e^{i\phi_2}\sin(\beta) & 0 & 0 & e^{i\phi_1}\cos(\beta) \end{pmatrix}, \tag{2.79}$$

where we have written

$$\cos(\beta) = \frac{1}{\sqrt{2}}a, \qquad \sin(\beta) = \frac{1}{\sqrt{2}}b, \tag{2.80}$$

$$\cos(\alpha) = \frac{1}{\sqrt{2}}d, \qquad \sin(\alpha) = \frac{1}{\sqrt{2}}c, \tag{2.81}$$

as a result of the observation that $a^2 + b^2 = 2$ and $c^2 + d^2 = 2$. Furthermore, note that $U_2^{(\theta_k)}$ can be simply obtained by swapping the signs occurring within each exponential function in $U_1^{(\theta_k)}$, and as such is not presented explicitly. In order to obtain an explicit circuit decomposition for $U_1^{(\theta_k)}$ we note that we can write $U_1^{(\theta_k)} = U_{1,A}^{(\theta_k)} U_{1,B}^{(\theta_k)}$, where

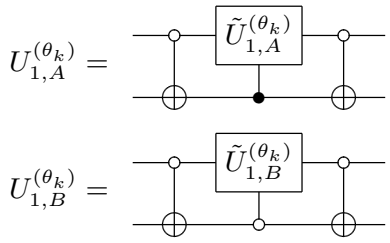

Figure 2.1: Circuit decompositions for the unitary operators $U_{1,A}^{(\theta_k)}$ and $U_{1,B}^{(\theta_k)}$, where the unitary operator $U_1^{(\theta_k)}$, implementing the quasi-extreme channel $T_{(t,i)}^{\theta_k}$ via (2.78), is given by $U_1^{(\theta_k)} = U_{1,A}^{(\theta_k)} U_{1,B}^{(\theta_k)}$. The single qubit unitary operations $\tilde{U}_{1,A}^{(\theta_k)}$ and $\tilde{U}_{1,B}^{(\theta_k)}$ are defined in Eqs. (2.84) and (2.85) respectively.

$U_{1,A}^{(\theta_k)}$ and $U_{1,B}^{(\theta_k)}$ are the two-level unitary matrices

$$U_{1,A}^{(\theta_k)} = \begin{pmatrix} e^{-i\phi_1}\cos(\beta) & 0 & 0 & -e^{-i\phi_2}\sin(\beta) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ e^{i\phi_2}\sin(\beta) & 0 & 0 & e^{i\phi_1}\cos(\beta) \end{pmatrix} \tag{2.82}$$

and

$$U_{1,B}^{(\theta_k)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\alpha) & -\sin(\alpha) & 0 \\ 0 & \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.83}$$

Furthermore, if we define the unitary matrices,

$$\tilde{U}_{1,A}^{(\theta_k)} = \begin{pmatrix} e^{-i\phi_1}\cos(\beta) & -e^{-i\phi_2}\sin(\beta) \\ e^{i\phi_2}\sin(\beta) & e^{i\phi_1}\cos(\beta) \end{pmatrix} \tag{2.84}$$

and

$$\tilde{U}_{1,B}^{(\theta_k)} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}, \tag{2.85}$$

then we can implement $U_{1,A}^{(\theta_k)}$ and $U_{1,B}^{(\theta_k)}$ using the circuits given in Figure 2.1.

At this stage all that remains is to obtain circuit decompositions of the controlled-$\tilde{U}_{1,i}^{(\theta_k)}$ gates. In order to implement the controlled-$\tilde{U}_{1,B}^{(\theta_k)}$ gate we note the equivalence depicted in Figure 2.2, where $A_B = R_y(\alpha)$ and $B_B = R_y(-\alpha)$, with R_y the standard

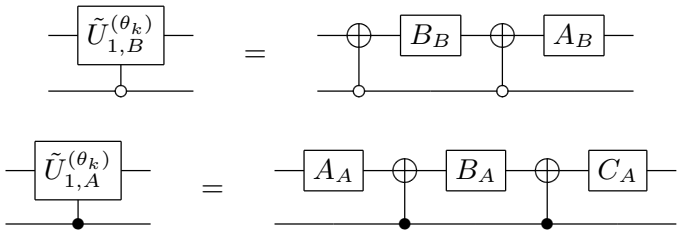

Figure 2.2: Circuit decomposition for the controlled-$\tilde{U}_{1,i}^{(\theta_k)}$ operations, required for implementation of the unitary operators $U_{1,i}^{(\theta_k)}$, into only single qubit and controlled-NOT gates. The single qubit unitary gates are defined as $A_B = R_y(\alpha)$, $B_B = R_y(-\alpha)$, $A_A = R_z(\phi_1 + \phi_2)R_y(\beta)$, $B_A = R_y(-\beta)R_z(-\phi_1)$ and $C_A = R_z(-\phi_2)$, where $R_y(\theta)$ and $R_z(\theta)$ are defined in Eqs. (2.86) and (2.87) respectively.

exponentiation of the Pauli y matrix, given by

$$R_y(\theta) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}. \tag{2.86}$$

Similarly, in order to implement the controlled-$\tilde{U}_{1,A}^{(\theta_k)}$ gate we note the equivalence depicted in Figure 2.2, where $A_A = R_z(\phi_1 + \phi_2)R_y(\beta)$, $B_A = R_y(-\beta)R_z(-\phi_1)$ and $C_A = R_z(-\phi_2)$ with R_z the standard exponentiation of the Pauli z matrix, given by

$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}. \tag{2.87}$$

2.6 Conclusions and outlook

Combining the results of the previous three sections we obtain the following algorithm, requiring only $\mathcal{O}\big((||\mathcal{L}||_{1\to 1}t)^{1+1/2j}/\epsilon^{1/2j}\big)$ single qubit and CNOT gates, as a solution to the problem defined in Section 4.2:

1. Given $\mathcal{L}$, obtain as per Section 2.3 the spectral decomposition

$$\mathcal{L} = \sum_{k=0}^{4} \lambda_k \mathcal{L}_k, \tag{2.88}$$

as well as G_k and θ_k specifying the decomposition

$$A_k = G_k A_{(\theta_k)} G_k^T, \tag{2.89}$$

for all $k \in [1, 3]$.

2. Choose the desired approximation accuracy ϵ as well as the simulation time t. Using Eqs. (2.28) and (2.29) construct $S_{2j}(t/r)$ with

$$j = \text{round}\left(\sqrt{\log_{25/3}\frac{8etL_2}{\epsilon}}\right) \tag{2.90}$$

and

$$r = t\Big(\frac{16etL_2}{\epsilon}\Big)^{1/(2j)}\frac{2ed_j}{2j+1}. \tag{2.91}$$

3. Implement $S_{2j}(t/r)$ $L_1 r$ times using

$$T_{t'}^{(k)}(\rho) = U_k^\dagger\big[T_{t'}^{(\theta_k)}\big(U_k\rho U_k^\dagger\big)\big]U_k, \tag{2.92}$$

where λ_k, L_1 and r have been incorporated into t', U_k is obtained from G_k as per Section 2.3 and $T_{t'}^{(\theta_k)}$ is implemented via classical random sampling of the circuits derived in Section 2.5.

In light of this result two natural avenues arise for extension of this work. The first is investigation of improvements to the method presented here for the simulation of arbitrary single-qubit Markovian open quantum systems. However, in light of a very recently proven "no fast-forwarding" theorem for Markovian open quantum systems [50], which shows that simulation of Markovian systems with sublinear time complexity is not possible, it is now clear that the time complexity of this method is very close to optimal. It would however be of interest to investigate methods for improving the dependency of the complexity on the error tolerance. The second natural extension of this work is development of methods allowing for the construction of explicit algorithms for the simulation of multi-qubit and multi-qudit Markovian open systems. However, the work presented in this paper relies heavily on geometric properties of single-qubit channels and as such generalisation of this work would require investigation into the geometric and convex structure of multi-particle quantum channels. These questions are explicitly addressed in the following Chapter.

2.7 Appendix

2.7.1 Damping basis derivation of affine map representation

Given the generator $\mathcal{L}$ of a semigroup of quantum channels (with $H = 0$) one can find the left and right eigenoperators L_i and R_i satisfying [49],

$$L_i\mathcal{L} = \lambda_{(L,i)}L_i \tag{2.93}$$

$$\mathcal{L}R_i = \lambda_{(R,i)}R_i, \tag{2.94}$$

where the left action of a superoperator is defined so that

$$\mathrm{tr}\big[(X\mathcal{L})\rho\big] = \mathrm{tr}\big[(\mathcal{L}(\rho))X\big] \tag{2.95}$$

for any Hermitian operator X and for all density matrices ρ. Using this left action one finds that $\mathrm{tr}[L_iR_j] = \delta_{ij}$ and $\lambda_{(L,i)} = \lambda_{(R,i)}$. Furthermore, any density matrix $\rho(0)$ can be expressed in this basis (known as the damping basis), such that [48]

$$\rho(0) = \sum_i \mathrm{tr}\big[L_i\rho(0)\big]R_i \tag{2.96}$$

and

$$\rho(t) = e^{\mathcal{L}t}[\rho(0)] \tag{2.97}$$

$$= \sum_i \mathrm{tr}\big[L_i\rho(0)\big]\Lambda_iR_i \tag{2.98}$$

with $\Lambda_i = e^{\lambda_i t}$. Furthermore, the sub-matrix $\tilde{M}$ in the affine map representation of $T_t = e^{t\mathcal{L}}$ is then given by

$$\tilde{M} = \begin{pmatrix} \Lambda_2 & 0 & 0 \\ 0 & \Lambda_3 & 0 \\ 0 & 0 & \Lambda_4 \end{pmatrix}. \tag{2.99}$$

Utilising these methods for the semigroup $T_t^{(\theta_k)}$ generated by $\mathcal{L}_{(\theta_k)}$, as per (2.25), we find that

$$\lambda_2 = -2\sin^2(\theta_k) \tag{2.100}$$

$$\lambda_3 = -2\cos^2(\theta_k) \tag{2.101}$$

$$\lambda_4 = -2. \tag{2.102}$$

The full affine representation, (2.51)-(2.55), is then found using (2.99) and constructing $\mathbf{m}$ in (2.11) such that (2.12) and (2.13) hold.

Bibliography

[1] R. Sweke, I. Sinayskiy, and F. Petruccione. Simulation of single-qubit open quantum systems. *Phys. Rev. A*, 90:022331, 2016.

[2] B. C. Sanders. Efficient Algorithms for Universal Quantum Simulation. In G. W. Dueck and D. M. Miller, editors, *Reversible Computation: 5th International Conference, RC 2013, Victoria, BC, Canada, July 4-5, 2013. Proceedings*, pages 1–10. Springer, 2013.

[3] K. L. Brown, W. J. Munro, and V. M. Kendon. Using quantum computers for quantum simulation. *Entropy*, 12:2268, 2010.

[4] I. M. Georgescu, S. Ashhab, and F. Nori. Quantum simulation. *Rev. Mod. Phys.*, 86:153, 2014.

[5] R. P. Feynman. Simulating physics with computers. *Int. J. Theoret. Phys.*, 21:467, 1982.

[6] S. Lloyd. Universal Quantum Simulators. *Science*, 273:1073, 1996.

[7] D. Aharonov and A. Ta-Shma. Adiabatic quantum state generation and statistical zero knowledge. In L. L. Larmore and M. X. Goemans, editors, *Proc. 35th Annual ACM Symp. on Theory of Computing*, pages 20–29. ACM: New York, 2003.

[8] A. M. Childs. *Quantum information processing in continuous time.* PhD thesis, Massachusetts Institute of Technology, 2004.

[9] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders. Efficient Quantum Algorithms for Simulating Sparse Hamiltonians. *Comm. Math. Phys.*, 270(2):359, 2007.

[10] A. Papageorgiou and C. Zhang. On the efficiency of quantum algorithms for Hamiltonian simulation. *Quant. Inf. Proc.*, 11:541, 2012.

[11] N. Wiebe, D. Berry, P. Høyer, and B. C. Sanders. Higher order decompositions of ordered operator exponentials. *J. Phys. A: Math. Theor.*, 43:065203, 2010.

[12] A. M. Childs and R. Kothari. Simulating sparse Hamiltonians with star decompositions. In *Theory of Quantum Computation, Communication and Cryptography (TQC 2010)*, volume 6519 of *Lecture Notes in Computer Science*, page 94. Springer, 2011.

[13] D. W. Berry and A. M. Childs. Black-box Hamiltonian simulation and unitary implementation. *Quantum Information and Computation*, 12:29, 2012.

[14] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma. Exponential improvement in precision for simulating sparse Hamiltonians. In D. Shmoys, editor, *Proc. of the 46th Annual ACM Symposium on Theory of Computing*, pages 283–292. ACM: New York, 2014.

[15] H. P. Breuer and F. Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press, 2002.

[16] H. Wang, S. Ashhab, and F. Nori. Quantum algorithm for simulating the dynamics of an open quantum system. *Phys. Rev. A*, 83:062317, 2011.

[17] M. M. Wolf. Quantum channels and operations guided tour. http://www-m5.ma.tum.de/foswiki/pub/M5/Allgemeines/MichaelWolf/2012, 2012.

[18] W. F. Stinespring. Positive functions on C^*-algebras. *Proc. Am. Math. Soc.*, 6:211, 1955.

[19] B. M. Terhal, I. L. Chuang, D.P. DiVincenzo, M. Grassl, and J. A. Smolin. Simulating quantum operations with mixed environments. *Phys. Rev. A*, 60:881, 1999.

[20] D. Bacon, A. M. Childs, I. L. Chuang, J. Kempe, D. W. Leung, and X. Zhou. Universal simulation of Markovian quantum dynamics. *Phys. Rev. A*, 64:062302, 2001.

[21] M. Ziman, P. Štelmachovič, and V. Bužek. Description of Quantum Dynamics of Open Systems Based on Collision-Like Models. *Open systems and information dynamics*, 12:81, 2005.

[22] M. Koniorczyk, V. Bužek, P. Adam, and A. Lázló. Simulation of Markovian quantum dynamics on quantum logic networks. arXiv:quant-ph/0205008, 2005.

[23] T. Rybár, S. N. Filippov, M. Ziman, and V. Bužek. Simulation of indivisible qubit channels in collision models. *J. Phys. B: At. Mol. Opt. Phys.*, 45:154006, 2012.

[24] F. Verstraete, M. M. Wolf, and J. I. Cirac. Quantum computation and quantum-state engineering driven by dissipation. *Nature Physics*, 5:633, 2009.

[25] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C.F. Roos, P. Zoller, and R. Blatt. An open-system quantum simulator with trapped ions. *Nature*, 470:486, 2011.

[26] P. Schindler, M. Müller, D. Nigg, J. T. Barreiro, E. A. Martinez, M. Hennrich, T. Monz, S. Diehl, P. Zoller, and R. Blatt. Quantum simulation of dynamical maps with trapped ions. *Nature Physics*, 9:361, 2013.

[27] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller. Preparation of entangled states by quantum Markov processes. *Phys. Rev. A*, 78:042307, 2008.

[28] M. J. Kastoryano, F. Reiter, and A. S. Sørensen. Dissipative Preparation of Entanglement in Optical Cavities. *Phys. Rev. Lett.*, 106:090502, 2011.

[29] F. Reiter, M. J. Kastoryano, and A. S. Sorensen. Entangled steady-states of two atoms in an optical cavity by engineered decay. arXiv:1110.1024v1 [quant-ph], 2011.

[30] L. Shen, X. Chen, Z. Yang, H. Wu, and S. Zheng. Steady-state entanglement for distant atoms by dissipation in coupled cavities. *Phys. Rev. A*, 84:064302, 2011.

[31] S. G. Schirmer and X. Wang. Stabilizing open quantum systems by Markovian reservoir engineering. *Phys. Rev. A*, 81:062306, 2010.

[32] X. Chen, L. Shen, Z. Yang, H. Wu, and M. Chen. Engineering W-type steady states for three atoms via dissipation in an optical cavity. *J. Opt. Soc. Am. B*, 29:1535, 2012.

[33] R. Sweke, I. Sinayskiy, and F. Petruccione. Dissipative preparation of generalised Bell states. *J. Phys. B: At. Mol. Opt. Phys.*, 46:104004, 2013.

[34] G. Vacanti and A. Beige. Cooling atoms into entangled states. *New J. Phys.*, 11(8):083008, 2009.

[35] J. Busch, S. De, S. S. Ivanov, B. T. Torosov, T. P. Spiller, and A. Beige. Cooling atom-cavity systems into entangled states. *Phys. Rev. A*, 84:022316, 2011.

[36] R. Sweke, I. Sinayskiy, and F. Petruccione. Dissipative preparation of large W states in optical cavities. *Phys. Rev. A*, 87:042323, 2013.

[37] M. J. Kastoryano. *Quantum Markov Chain Mixing and Dissipative Engineering.* PhD thesis, University of Copenhagen, 2012.

[38] I. Sinayskiy and F. Petruccione. Efficiency of open quantum walk implementation of dissipative quantum computing algorithms. *Quant. Inf. Proc.*, 11:1301, 2012.

[39] M. Kliesch, T. Barthel, C. Gogolin, M. J. Kastoryano, and J. Eisert. Dissipative Quantum Church-Turing Theorem. *Phys. Rev. Lett.*, 107:120501, 2011.

[40] M. Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and Monte-Carlo simulations. *Phys. Lett. A*, 146:319, 1990.

[41] M. Suzuki. General theory of fractal path integrals with applications to many-body theories and statistical physics. *J. Math. Phys.*, 32:400, 1991.

[42] D. S. Wang, D. W. Berry, M. C. de Oliveira, and B. C. Sanders. Solovay-Kitaev Decomposition Strategy for Single-Qubit Channels. *Phys. Rev. Lett.*, 111:130504, 2013.

[43] M. B. Ruskai, S. Szarek, and E. Werner. An analysis of completely-positive trace-preserving maps on 2×2 matrices. *Lin. Alg. Appl.*, 347:159, 2002.

[44] J. Watrous. Notes on super-operator norms induced by schatten norms. *Quantum Information and Computation*, 5:58, 2005.

[45] V. Kliuchnikov, D. Maslov, and M. Mosca. Asymptotically optimal approximation of single qubit unitaries by Clifford and T circuits using a constant number of ancillary qubits. *Phys. Rev. Lett.*, 110:190502, 2013.

[46] P. Selinger. Efficient Clifford $+T$ approximation of single-qubit operators. arXiv:1212.6253 [quant-ph], 2012.

[47] H. F. Trotter. On the product of semi-groups of operators. *Proc. Amer. Math. Soc.*, 10:545, 1959.

[48] S. Daffer, K. Wódkiewicz, and J. K. McIver. Quantum markov channels for qubits. *Phys. Rev. A*, 67:062312, 2003.

[49] H. Briegel and B. Englert. Quantum optical master equations: The use of damping bases. *Phys. Rev. A*, 47:3311, 1993.

[50] A. M. Childs and T. Li. Efficient simulation of sparse Markovian quantum dynamics. arXiv:1611.05543 [quant-ph], 2016.

Chapter 3

Universal simulation of Markovian open quantum systems

We consider the problem of constructing a "universal set" of Markovian processes, such that any Markovian open quantum system, described by a one-parameter semigroup of quantum channels, can be simulated through sequential simulations of processes from the universal set. In particular, for quantum systems of dimension d, we explicitly construct a universal set of semigroup generators, parametrized by $d^2 - 3$ continuous parameters, and prove that a necessary and sufficient condition for the dynamical simulation of a d dimensional Markovian quantum system is the ability to implement a) quantum channels from the semigroups generated by elements of the universal set of generators, and b) unitary operations on the system. Furthermore, we provide an explicit algorithm for simulating the dynamics of a Markovian open quantum system using this universal set of generators, and show that it is efficient, with respect to this universal set, when the number of distinct Lindblad operators (representing physical dissipation processes) scales polynomially with respect to the number of subsystems.

This chapter has been been previously published in [1].

3.1 Introduction

All quantum systems are invariably in contact with some environment to some extent. As a result, the development of tools for the study of such open quantum systems, undergoing non-unitary dynamics as a result of system-environment interactions, is of importance for understanding a rich variety of phenomena [2,3]. In particular, the study of open quantum systems allows us to better understand the nature of dissipation and decoherence [2, 3], thermalisation and equilibration [4, 5], non-equilibrium phase transitions [6, 7] and transport phenomena in both strongly-correlated [8–10] and biological systems [11–13]. Furthermore, it has been shown that dissipation and decoherence, traditional enemies of quantum information processing, can be exploited as a resource for quantum computation [14, 15], the preparation of topological phases [16–18] and the preparation of entangled states [19, 20].

Simulations on controllable quantum devices promise to be one of the most effective tools for the study of open quantum systems, and while the majority of effort over the past twenty years has focused on the development of methods for the simulation of closed quantum systems [21–24], which undergo Hamiltonian generated unitary evolution, a plethora of methods have also been developed for the quantum simulation of open quantum systems, on a wide variety of quantum devices. These methods include collision model based approaches [25–27], simulation algorithms designed for conventional unitary gate based universal quantum computers [28–43] and simulation algorithms designed for more general quantum simulators incorporating feedback and dissipative elements in addition to unitary gates [44–51].

However, despite the wide variety of methods for the simulation of open quantum systems, there exists no "universal set" of non-unitary processes through which all such processes can be simulated via sequential simulations from the universal set. This is in clear contrast with the situation for Hamiltonian generated unitary evolution, for which it is well known that any unitary operation can be implemented, up to arbitrary precision, using some (not necessarily efficient) sequence of unitary gates from a finite universal set [52]. Such universal sets are interesting not only from a fundamental perspective, but also from a pragmatic perspective, as they allow for experimental development to be focused on developing the capability of implementing a reduced set of significantly simpler processes.

One natural response to this problem is via the Stinespring dilation [53]. Given any non-unitary dynamics of some particular system, it is always possible to introduce some environment, with size the square of the system size in the general case, such that

the non-unitary dynamics of the system may be simulated through unitary evolution of the total system and environment [28, 29, 36, 40, 41, 43]. However, it is important to note that for an arbitrary non-unitary process, there is no guarantee that the dilated unitary admits an *efficient* decomposition into some sequence of unitary gates from a universal set [52], and as such this strategy offers an advantage for the construction of efficient simulation algorithms only when the original non-unitary process exhibits some useful structure, such as local interactions [36]. Furthermore, in line with the spirit of dissipative state preparation [19, 20], we would like to investigate the possibility of developing a universal set which might allow us to exploit the natural dissipation and decoherence present in any controlled quantum device.

Therefore, as an alternative approach, one can consider the problem of identifying the smallest set of non-unitary dynamics, applied to the system only, such that if one has the resources to simulate dynamics from this set, and implement unitary operations on the system, then one will be able to simulate any non-unitary dynamics up to arbitrary precision. This problem has been considered before. In particular, Wang et al. have constructed a method for the simulation of arbitrary quantum channels through the simulation of extreme channels [40, 41], and in effect identified such a universal set for discrete time evolution of open quantum systems. However, for systems evolving continuously in time, even in the simplest case of Markovian semigroup dynamics it is necessary to first exponentiate the generator of the semigroup in order to obtain the quantum channels describing time evolution. This is infeasible for an arbitrary semigroup generator and in order to address this problem Bacon et al. [31] have constructed a composition framework for the combination and transformation of semigroup generators. Using this framework they were able to identify a continuous one-parameter set of semigroup generators and demonstrate that one can efficiently simulate arbitrary Markovian dynamics of a single qubit through simulations of quantum channels from the semigroups generated by this one parameter set of generators [31, 43].

Despite this initial progress, extending these results to arbitrary Markovian open quantum systems has remained a challenging open problem. In this work we address this problem by using the composition framework of [31] to construct a continuous d^2-3 parameter set of generators, which is universal in the sense that given the ability to implement quantum channels from the semigroups generated by elements of this set of generators, along with unitary operations on the system, one can simulate the dynamics of an arbitrary d dimensional Markovian quantum system up to arbitrary precision. This set of generators is minimal within this particular composition framework, and by construction of this set we complete the program initiated in [31], proving that the

dimension of this universal set is indeed as originally conjectured.

Furthermore, assuming the ability to implement unitary operations on the system along with quantum channels from the semigroups generated by elements of the universal set, we utilise recent error bounds for superoperator Suzuki-Lie-Trotter expansions [43] to construct an explicit algorithm for the simulation of arbitrary Markovian open quantum systems, and analyse the conditions under which a Markovian open quantum system may be efficiently simulated, with respect to the constructed universal set, using this algorithm.

This chapter is structured as follows: We begin in Section 3.2 by introducing the formalism of Markovian semigroup dynamics and formulating the problem of simulating such dynamics. We then proceed, in Section 3.3, to introduce the composition framework of *linear combination* and *unitary conjugation*, introduced in [31], for the combination of Markovian semigroup generators. Given this framework, we then present our main result in Section 3.4, the construction of a universal set of generators for arbitrary Markovian dynamics. A detailed proof of the main result is then given in Section 3.5, before discussing in Section 3.6 the consequences for simulation of Markovian open quantum systems.

3.2 Setting

Given a quantum system with Hilbert space $\mathcal{H}_S \cong \mathbb{C}^d$, we are concerned with Markovian semigroup dynamics, in which the state of the system $\rho(t) \in \mathcal{B}(\mathcal{H}_S)$ evolves according to a quantum Markov master equation

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t), \tag{3.1}$$

where $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$ is the generator of a uniformly continuous one parameter semigroup of quantum channels $\{T(t)\}$, which we refer to as a Markovian semigroup [2]. The state of the system at time $t > t_0$ is then given by $\rho(t) = T(t - t_0)\rho(t_0) = e^{(t-t_0)\mathcal{L}}\rho(t_0)$. Furthermore, (3.1) may always be written in the form

$$\mathcal{L}(\rho) = i[\rho, H] + \sum_{l,k=1}^{d^2-1} A_{l,k}\left(F_l \rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}_+\right), \tag{3.2}$$

for some Hermitian operator $H = H^\dagger \in \mathcal{M}_d(\mathbb{C})$ and some positive semidefinite $A \in \mathcal{M}_{d^2-1}(\mathbb{C})$, where $\{F_i\}$ is some basis for the space of traceless matrices in $\mathcal{M}_d(\mathbb{C})$, and

without loss of generality from this point we will always utilise the Hermitian traceless basis which generalises the Gell-Mann basis for su(3). Eq. (3.2) is known as the Gorini, Kossakowski, Sudarshan and Lindblad (GKSL) form of the quantum Markov master equation and we refer to A as the GKS matrix. Additionally, note that via diagonalisation of the GKS matrix A, Eq. (3.2) can always be brought into, and is often specified in, the so called diagonal form,

$$\mathcal{L}(\rho) = i[\rho, H] + \sum_{k=1}^{m} \gamma_k \bigg(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \bigg), \tag{3.3}$$

where m is the number of non-zero eigenvalues of A, and typically each Lindblad operator L_k represents some physical dissipation process [2].

In order to discuss simulations of Markovian semigroups it is necessary to have some means for quantifying the error in approximations of generators and quantum channels. To achieve this we will utilise the $(1 \to 1)$-norm for super-operators, where in general the $(p \to q)$-norm of a super-operator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is defined as [54]

$$||T||_{p\to q} := \sup_{||A||_p = 1} ||T(A)||_q. \tag{3.4}$$

The $(p \to q)$-norm defined above is induced from the Schatten p-norm of an operator, defined as $||A||_p := \big(\mathrm{tr}(|A|^p)\big)^{\frac{1}{p}}$ for all $A \in \mathcal{B}(\mathcal{H})$. We use the $(1 \to 1)$-norm as this is induced by the Schatten 1-norm, which corresponds up to a factor of $1/2$ with the trace distance, $\mathrm{dist}(\rho, \sigma) := \sup_{0 \leq A \leq 1} \mathrm{tr}\big(A(\rho - \sigma)\big)$, arising from a physical motivation of operational distinguishability of quantum states [52], which is relevant when working in the Schrödinger picture.

At this stage, given a Markovian semigroup $\{T(t)\}$, generated by $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$ with $\dim(\mathcal{H}_s) = d$, we say that the semigroup can be *efficiently simulated* if given any initial state $\rho(0) \in \mathcal{B}(\mathcal{H}_\mathcal{S})$, any $\epsilon > 0$ and any $t > 0$, there exists a well defined procedure, requiring at most $\mathrm{poly}\big(||\mathcal{L}||_{(1\to1)}, t, 1/\epsilon, \ln(d)\big)$ applications of standard resources, such that the output of the procedure is a state $\tilde{\rho}$ satisfying $||\tilde{\rho} - \rho(t)||_1 < \epsilon$. Note that poly denotes any polynomial function and that for many-body systems $\ln(d)$ is proportional to the number of subsystems. Furthermore, note that the standard resources depend on the simulator on which the well defined procedure, or algorithm, is executed. If we are considering simulations on a universal quantum computer, then the procedure would be a quantum circuit, and the resources would be unitary gates from some finite universal set. However, motivated by the spirit of dissipative state preparation, in this chapter

we are considering more general simulators whose standard resources might include additional non-unitary elements capable of exploiting natural or engineered dissipation. In particular, under the understanding that we are considering this more general context, we will consider as standard resources all quantum channels from semigroups generated by elements of the universal set constructed in Section 3.4, in addition to arbitrary unitary operations.

3.3 Composition framework

In this section, following [31], we present a composition and transformation framework through which one can combine and transform the generators of Markovian semigroups to form the generator of a new Markovian semigroup. As described in Section 3.1, this composition framework will allow us to identify in Section 3.4 a parametrized universal set of semigroup generators, through which all Markovian semigroups of a given dimension can be simulated, up to arbitrary precision.

This composition framework consists of two procedures, *linear combination* and *unitary conjugation*. Firstly, let $\mathcal{L}_a$ and $\mathcal{L}_b$ be the generators of Markovian semigroups $\{T^{(a)}(t)\}$ and $\{T^{(b)}(t)\}$ respectively. The *linear combination* of $\mathcal{L}_a$ and $\mathcal{L}_b$ is then quite simply defined as the super-operator $\mathcal{L}_{a+b} = \mathcal{L}_a + \mathcal{L}_b$, the generator of a Markovian semigroup $\{T^{(a+b)}(t)\}$ [31]. From a generalisation of the Lie-Trotter theorem [55] into the superoperator regime [36, 43], we see that

$$T^{(a+b)}(t) = e^{t\mathcal{L}_{a+b}} = \lim_{n\to\infty} \left[T^{(a)}(t/n)T^{(b)}(t/n)\right]^n. \tag{3.5}$$

The generalisation of this procedure to the linear combination of multiple generators is then straightforward. Furthermore, as discussed in detail in Appendix 3.9.1, using Suzuki-Lie-Trotter techniques [56, 57], generalised from the context of Hamiltonian simulation [58, 59], one can show that the infinite sum in Eq. (3.5) can be effectively truncated, such that any channel from the semigroup generated by the linear combination $\mathcal{L}_{a+b}$ can be implemented, up to arbitrary precision, through a finite number of implementations of channels from the semigroups generated by the constituent generators $\mathcal{L}_a$ and $\mathcal{L}_b$ [36, 43]. A discussion of when the Markovian semigroup generated by the linear combination of multiple generators can be *efficiently* simulated is postponed until Section 3.6.

Note that given any generator $\mathcal{L}$ we can always rewrite (3.2) as

$$\mathcal{L}(\rho) = \mathcal{L}_H(\rho) + \mathcal{L}_A(\rho), \tag{3.6}$$

where

$$\mathcal{L}_H(\rho) = i[\rho, H] \tag{3.7}$$

and

$$\mathcal{L}_A(\rho) = \sum_{l,k=1}^{d^2-1} A_{l,k}\bigg(F_l\rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}_+\bigg). \tag{3.8}$$

Therefore, if we assume the ability to implement arbitrary unitary operations on the system, then without loss of generality we can set $H = 0$, as we can always reintroduce the unitary contribution and implement the total generator $\mathcal{L}$ through linear combination of $\mathcal{L}_H$ and $\mathcal{L}_A$.

The second transformation procedure, *unitary conjugation*, is defined as follows: Given a Hilbert space $\mathcal{H}_S \cong \mathbb{C}^d$ and a Markovian semigroup $\{T(t)\}$ with generator $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$, for any unitary operator $U \in \mathrm{SU}(d)$ the unitary conjugation via U of the semigroup $\{T(t)\}$ is the new Markovian semigroup

$$\{T_U(t)\} \equiv \{\mathcal{U}^\dagger T(t)\mathcal{U}\}, \tag{3.9}$$

where $\mathcal{U}(\rho) = U\rho U^\dagger$. The following theorem, due to [31], is particularly important, as it describes the manner in which the GKS matrix specifying $\mathcal{L}$ is transformed as a result of unitary conjugation of the semigroup $\{T(t)\}$. The statement of this theorem relies on notions related to the adjoint representation of a Lie group, presented in detail in Appendix 3.9.2. Note in particular that $\mathrm{Int}\big(\mathrm{su}(d)\big)$ denotes the image of the adjoint representation of $\mathrm{SU}(d)$, a Lie group itself, while $\mathfrak{Int}\big(\mathrm{su}(d)\big)$ is the Lie algebra of $\mathrm{Int}\big(\mathrm{su}(d)\big)$.

Theorem 3.1. *Assume $\mathcal{H}_S \simeq \mathbb{C}^d$ and that $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$ is the generator of a Markovian semigroup with $H = 0$, such that*

$$\mathcal{L}(\rho) = \mathcal{L}_A(\rho) \tag{3.10}$$

$$= \sum_{l,k=1}^{d^2-1} A_{l,k}\bigg(F_l\rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}_+\bigg). \tag{3.11}$$

Furthermore, assume that $\{F_\gamma\}|_{\gamma=1}^{d^2-1}$ is a Hermitian basis for the space of traceless matrices in $\mathcal{M}_d(\mathbb{C})$, such that $\{iF_\gamma\}|_{\gamma=1}^{d^2-1}$ is a basis for $\mathrm{su}(d)$ and $U = \exp\big(\sum_{\gamma=1}^{d^2-1} ir_\gamma F_\gamma\big) \in$

$\mathrm{SU}(d)$ *for any* $\vec{r} \in \mathbb{R}^{d^2-1}$. *Then,*

$$\mathcal{U}^\dagger T_t \mathcal{U} = \mathcal{U}^\dagger e^{t\mathcal{L}_A}\mathcal{U} \tag{3.12}$$

$$= e^{t\mathcal{L}_{\tilde{A}}} \tag{3.13}$$

$$= T_U(t), \tag{3.14}$$

where,

$$\mathcal{L}_{\tilde{A}}(\rho) = \sum_{l,k=1}^{d^2-1} \tilde{A}_{l,k}\Big(F_l \rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}_+\Big), \tag{3.15}$$

with $\tilde{A} = G_{(U)} A G_{(U)}^T$, *where* $G_{(U)} \in \mathrm{Int}\big(\mathrm{SU}(d)\big)$ *is given by*

$$G_{(U)} = \hat{\mathrm{Ad}}\big(U\big) = \exp\big(\sum_{\gamma=1}^{d^2-1} i r_\gamma G_\gamma\big), \tag{3.16}$$

and $\{iG_\gamma\}$ *is a basis for* $\mathfrak{Int}\big(\mathrm{su}(d)\big)$, *with matrix elements* $[G_\gamma]_{\alpha\beta} = i f_{\gamma\alpha\beta}$, *where* $f_{\gamma\alpha\beta}$ *are the real structure constants of* $\mathrm{su}(d)$, *defined via*

$$[F_\gamma, F_\alpha] = i \sum_{\beta=1}^{d^2-1} f_{\gamma\alpha\beta} F_\beta. \tag{3.17}$$

Colloquially, Theorem 3.1 states that unitary conjugation of the semigroup results in conjugation of the GKS matrix by an element of the adjoint representation of $\mathrm{SU}(d)$. As such, we see that by adding together the generators of Markovian semigroups (linear combination), or conjugating the generators via elements of $\mathrm{Int}(\mathrm{SU}(d))$ (unitary conjugation), we obtain the generators of new Markovian semigroups which can be simulated (though perhaps not necessarily efficiently), provided the semigroups corresponding to the original constituent generators can be simulated and arbitrary unitary operations can be implemented on the system.

3.4 Main result

Given the composition framework of Section 3.3, we can now present our main result, the construction of a universal set of Markovian semigroup generators, parameterised by $d^2 - 3$ continuous parameters, for Markovian open quantum systems of any dimension d. For $d = 2$ this set was first constructed in [31], and our construction, presented as Theorem 3.2, generalises this original method to arbitrary dimension. As per the

statement of the theorem, the constructed set is universal with respect to the composition framework of linear combination and unitary conjugation, i.e. universal in the sense that in order to simulate any Markovian semigroup it is necessary and sufficient to be able to implement arbitrary unitary operations on the system, along with all quantum channels from the semigroups generated by the d^2-3 parameter family of generators. It is important to note however that, as in the unitary case, if we consider operations from the universal set as our "standard resources", we do not necessarily expect to be able to *efficiently* simulate all Markovian semigroups in terms of these resources. In Section 3.6 we utilise the construction of the proof of Theorem 3.2, presented in Section 3.5, to construct an explicit algorithm for the (not necessarily efficient) simulation of an arbitrary Markovian semigroup via simulations of semigroups from the universal set, and then analyse the conditions under which a class of Markovian open quantum systems may be efficiently simulated using this particular algorithm.

Theorem 3.2. *In order to simulate, using linear combination and conjugation by unitaries, an arbitrary Markovian semigroup generated by $\mathcal{L} \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$ with $\mathcal{H}_S \simeq \mathbb{C}^d$, it is necessary and sufficient to be able to simulate all Markovian semigroups whose generator is specified by a GKS matrix from the d^2-3 parameter family*

$$A(\theta, \vec{\alpha}^R, \vec{\alpha}^I) = \vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)^\dagger, \tag{3.18}$$

where

$$\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I) = \cos(\theta)\tilde{a}^R(\vec{\alpha}^R) + i\sin(\theta)\tilde{a}^I(\vec{\alpha}^I) \tag{3.19}$$

for $\theta \in [0, \pi/4]$, with $\tilde{a}^R(\vec{\alpha}^R), \tilde{a}^I(\vec{\alpha}^I) \in \mathbb{R}^{d^2-1}$ given by

$$\tilde{a}^R(\vec{\alpha}^R) = \begin{pmatrix} a_1^R \\ \vdots \\ a_{d-1}^R \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix} \qquad \tilde{a}^I(\vec{\alpha}^I) = \begin{pmatrix} a_1^I \\ \vdots \\ \vdots \\ a_{d^2-d}^I \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{3.20}$$

with

$$|\tilde{a}^R(\vec{\alpha}^R)| = |\tilde{a}^I(\vec{\alpha}^I)| = 1 \tag{3.21}$$
$$\tilde{a}^R(\vec{\alpha}^R) \cdot \tilde{a}^I(\vec{\alpha}^I) = 0, \tag{3.22}$$

such that for $d \geq 3$,

$$a_1^R = \cos(\alpha_1^R) \tag{3.23}$$
$$a_2^R = \sin(\alpha_1^R)\cos(\alpha_2^R) \tag{3.24}$$
$$\vdots$$
$$a_{d-2}^R = \sin(\alpha_1^R)\ldots\sin(\alpha_{d-3}^R)\cos(\alpha_{d-2}^R) \tag{3.25}$$
$$a_{d-1}^R = \sin(\alpha_1^R)\ldots\sin(\alpha_{d-3}^R)\sin(\alpha_{d-2}^R) \tag{3.26}$$

and

$$a_1^I = \cos(\alpha_1^I) \tag{3.27}$$
$$a_2^I = \sin(\alpha_1^I)\cos(\alpha_2^I) \tag{3.28}$$
$$\vdots$$
$$a_{d^2-d-1}^I = \sin(\alpha_1^I)\ldots\sin(\alpha_{d^2-d-2}^I)\cos(\alpha_{d^2-d-1}^I) \tag{3.29}$$
$$a_{d^2-d}^I = \sin(\alpha_1^I)\ldots\sin(\alpha_{d^2-d-2}^I)\sin(\alpha_{d^2-d-1}^I) \tag{3.30}$$

where,

$$\alpha_j^R \in [0,\pi] \quad \text{for} \quad j \in [1, d-3], \tag{3.31}$$
$$\alpha_k^I \in [0,\pi] \quad \text{for} \quad k \in [1, d^2-d-2], \tag{3.32}$$
$$\alpha_{d-2}^R \in [0, 2\pi], \tag{3.33}$$
$$\alpha_{d^2-d-1}^I \in [0, 2\pi], \tag{3.34}$$

and

$$\cos(\alpha_1^I) = \frac{1}{a_1^R}\left(\sum_{j=2}^{d-1} a_j^R a_j^I\right) \tag{3.35}$$

is constrained by orthogonality, and for $d = 2$*,*

$$\tilde{a}^R(\vec{\alpha}^R) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \tilde{a}^I(\vec{\alpha}^I) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{3.36}$$

3.5 Proof of Theorem 3.2

3.5.1 Proof of sufficiency

Firstly, without any loss of generality we assume $H = 0$. Let $A \geq 0 \in \mathcal{M}_{d^2-1}(\mathbb{C})$ then be the GKS matrix specifying the generator of the Markovian semigroup we wish to simulate. A is positive semidefinite and therefore via the spectral decomposition one can express A as

$$A = \sum_k^m \lambda_k \vec{a}_k \vec{a}_k^\dagger, \tag{3.37}$$

where $\lambda_k \geq 0$, m is the number of non-zero eigenvalues of A and $|\vec{a}_k| = 1$ for all k. By linear combination it is therefore sufficient to be able to simulate all GKS matrices $\vec{a}\vec{a}^\dagger$ with $|\vec{a}| = 1$. Any such vector $\vec{a}$ can be split into real and imaginary part,

$$\vec{a} = \vec{a}^R + i\vec{a}^I, \tag{3.38}$$

where $\vec{a}^R, \vec{a}^I \in \mathbb{R}^{d^2-1}$. Furthermore, $\vec{a}$ appears only in outer products and as such the phase of $\vec{a}$ is irrelevant, i.e. if we define $\vec{a}' = e^{i\psi}\vec{a}$, then we see that $\vec{a}\vec{a}^\dagger = \vec{a}'\vec{a}'^\dagger$, and therefore to simulate $\vec{a}\vec{a}^\dagger$ we could simulate $\vec{a}'\vec{a}'^\dagger$ for any value of ψ. If we now define the two parameters

$$k_1 \equiv |\vec{a}^R|^2 - |\vec{a}^I|^2 \tag{3.39}$$

$$k_2 \equiv 2\vec{a}^R \cdot \vec{a}^I, \tag{3.40}$$

then we can see that a phase transformation

$$\vec{a}' = e^{i\psi}\vec{a} \tag{3.41}$$

$$= (\vec{a}^R \cos\psi - \vec{a}^I \sin\psi) + i(\vec{a}^R \sin\psi + \vec{a}^I \cos\psi) \tag{3.42}$$

maps k_1 and k_2 according to

$$\begin{pmatrix} k_1' \\ k_2' \end{pmatrix} = \begin{pmatrix} \cos 2\psi & -\sin 2\psi \\ \sin 2\psi & \cos 2\psi \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}. \tag{3.43}$$

As we can choose ψ arbitrarily, we can always choose

$$\tan 2\psi = -k_2/k_1, \tag{3.44}$$

such that $k_2' = 0$, in which case $\vec{a}'^R$ and $\vec{a}'^I$ are orthogonal. In addition, we can always choose $k_1' = k_1/\cos 2\psi \geq 0$ such that $|\vec{a}'^R| \geq |\vec{a}'^I|$. Therefore, via the phase freedom in $\vec{a}$, we can assume, without loss of generality, that $\vec{a}^R \cdot \vec{a}^I = 0$ and that $|\vec{a}^R| \geq |\vec{a}^I|$. Taking into account the fact that $|\vec{a}| = 1$, we see that in order to simulate any GKS matrix $\vec{a}\vec{a}^\dagger$, it is sufficient to consider only

$$\vec{a} = \vec{a}^R + i\vec{a}^I \tag{3.45}$$

$$= \cos(\theta)\hat{a}^R + i\sin(\theta)\hat{a}^I \tag{3.46}$$

with $|\hat{a}^R| = |\hat{a}^I| = 1$, $\theta \in [0, \pi/4]$ and $\hat{a}^R \cdot \hat{a}^I = 0$.

Now, as per Theorem 3.1, we see that conjugation via $U \in \mathrm{SU}(d)$, of the semigroup whose generator is specified by GKS matrix $\vec{a}\vec{a}^\dagger$, results in the transformation

$$\vec{a}\vec{a}^\dagger \to G_{(U)}\vec{a}\vec{a}^\dagger G_{(U)}^T = (G_{(U)}\vec{a})(G_{(U)}\vec{a})^\dagger, \tag{3.47}$$

where $G_{(U)} = \hat{\mathrm{Ad}}(U) \in \mathrm{Int}\big(\mathrm{SU}(d)\big)$ is a real matrix. Furthermore, using the natural basis isomorphism $f : \mathrm{su}(d) \to \mathbb{R}^{d^2-1}$, we see that

$$\begin{aligned} G_{(U)}\vec{a} &= \cos(\theta) f\big[\mathrm{Ad}(U)(\hat{A}^R)\big] + i\sin(\theta) f\big[\mathrm{Ad}(U)(\hat{A}^I)\big] \\ &= \cos(\theta) f\big[U\hat{A}^R U^\dagger\big] + i\sin(\theta) f\big[U\hat{A}^I U^\dagger\big], \end{aligned} \tag{3.48}$$

where we have defined $\hat{A}^R \equiv f^{-1}(\hat{a}^R)$ and $\hat{A}^I \equiv f^{-1}(\hat{a}^I)$.

At this stage it is useful to define an explicit basis for $\mathrm{su}(d)$. To this end, let $\{|j\rangle\}|_{j=1}^d$

be a basis for $\mathbb{R}^d$ and define the Hermitian traceless matrices

$$d^{(l)} = \frac{1}{\sqrt{l(l+1)}}\Big[\sum_{j=1}^{l} |j\rangle\langle j| - l|l+1\rangle\langle l+1|\Big], \tag{3.49}$$

$$\sigma_x^{(j,k)} = \frac{1}{\sqrt{2}}\Big(|j\rangle\langle k| + |k\rangle\langle j|\Big), \tag{3.50}$$

$$\sigma_y^{(j,k)} = \frac{1}{\sqrt{2}}\Big(-i|j\rangle\langle k| + i|k\rangle\langle j|\Big), \tag{3.51}$$

such that

$$\Big\{\{id^{(l)}\}\big|_{l=1}^{d-1}, \{i\sigma_x^{(j,k)}, i\sigma_y^{(j,k)}\}\big|_{j=1}^{d-1}\big|_{j<k\leq d}\Big\} \tag{3.52}$$

is a basis for $\mathrm{su}(d)$ and $\{id^{(l)}\}\big|_{l=1}^{d-1}$ is a basis for the diagonal Cartan subalgebra of $\mathrm{su}(d)$.

As $\hat{A}^R \in \mathrm{su}(d)$, we can always find $U_1 \in \mathrm{SU}(d)$ which diagonalises $\hat{A}^R$, such that

$$U_1\hat{A}^R U_1^\dagger \equiv \tilde{A}_d^R = \sum_{l=1}^{d-1} d_l^R(id^{(l)}), \tag{3.53}$$

with real components $\{d_l^R\}$. Defining $\tilde{A}^I \equiv U_1\hat{A}^I U_1^\dagger$, we can also write

$$\tilde{A}^I \equiv \tilde{A}_d^I + \tilde{A}_\sigma^I \tag{3.54}$$

$$= \sum_{l=1}^{d-1} d_l^I(id^{(l)}) + \sum_{j=1}^{d-1}\sum_{k=j+1}^{d}\Big(a_{(j,k)}^x(i\sigma_x^{(j,k)}) + a_{(j,k)}^y(i\sigma_y^{(j,k)})\Big), \tag{3.55}$$

with real components $\{d_l^I\}$, $\{a_{(j,k)}^x\}$ and $\{a_{(j,k)}^y\}$.

Now, let $U_2 = \exp(i\sum_{l=1}^{d-1} h_l d^{(l)})$ for some $\vec{h} \in \mathbb{R}^{d-1}$ with components h_l. One can then see that for any $\vec{h} \in \mathbb{R}^{d-1}$,

$$U_2\tilde{A}_d^R U_2^\dagger = \tilde{A}_d^R, \tag{3.56}$$

$$U_2\tilde{A}_d^I U_2^\dagger = \tilde{A}_d^I, \tag{3.57}$$

so that if we define $\tilde{B}_\sigma^I \equiv U_2\tilde{A}_\sigma^I U_2^\dagger$ and take $G_{(U_2U_1)} \equiv \hat{\mathrm{Ad}}(U_2U_1)$, then we obtain,

$$G_{(U_2U_1)}\vec{a} = \cos(\theta)f\big(\tilde{A}_d^R\big) + i\sin(\theta)f\big(\tilde{A}_d^I + \tilde{B}_\sigma^I\big). \tag{3.58}$$

In order to obtain an explicit expression for $\tilde{B}_\sigma^I$ let us define the matrices $\sigma^{(j,k)} \equiv$

$(1/\sqrt{2})|j\rangle\langle k|$, and rewrite $\tilde{A}^I_\sigma$ as

$$\tilde{A}^I_\sigma = \sum_{j=1}^{d-1}\sum_{k=j+1}^{d}\Big(a_{(j,k)}(i\sigma^{(j,k)}) + \overline{a}_{(j,k)}(i\sigma^{(k,j)})\Big), \tag{3.59}$$

where

$$a_{(j,k)} = a^x_{(j,k)} - ia^y_{(j,k)} \equiv m_{(j,k)}e^{i\phi_{(j,k)}}, \tag{3.60}$$

and $\overline{a}_{(j,k)}$ denotes the complex conjugate of $a_{(j,k)}$. The matrices $\sigma^{(j,k)}$ are eigenvectors of the map which conjugates by U_2, so that some algebra yields,

$$\tilde{B}^I_\sigma = \sum_{j=1}^{d-1}\sum_{k=j+1}^{d} i\Big[m_{(j,k)}e^{if_{(j,k)}}(\sigma^{(j,k)}) + \text{H.C}\Big], \tag{3.61}$$

where H.C denotes the Hermitian conjugate, and

$$f_{(j,k)} = \phi_{(j,k)} - (j-1)\varphi(j-1)h_{j-1} + \sum_{l=j}^{k-2}\big(\varphi(l)h_l\big) + k\varphi(k-1)h_{k-1}, \tag{3.62}$$

with $\varphi(j) \equiv 1/(\sqrt{j(j+1)})$ and $h_0 \equiv 0$. If we choose

$$h_1 = -\frac{1}{2\varphi(1)}\phi_{(1,2)}, \tag{3.63}$$

and then inductively set

$$h_l = -\frac{1}{(l+1)\varphi(l)}\big[\phi_{1,l+1} + \sum_{x=1}^{l-1}\varphi(x)h_x\big], \tag{3.64}$$

we see that $f_{(1,k)} = 0$ for all $k \in [2,d]$. As a result, we obtain that

$$\tilde{B}^I_\sigma = \sum_{k=2}^{d} m_{(1,k)}i(\sigma^{(1,k)} + \sigma^{(k,1)}) + \sum_{j=2}^{d-1}\sum_{k=j+1}^{d} i\Big[m_{(j,k)}e^{if_{(j,k)}}(\sigma^{(j,k)}) + \text{H.C}\Big] \tag{3.65}$$

$$= \sum_{k=2}^{d} m_{(1,k)}(i\sigma_x^{(1,k)}) + \sum_{j=2}^{d-1}\sum_{k=j+1}^{d}\Big(b^x_{(j,k)}(i\sigma_x^{(j,k)}) + b^y_{(j,k)}(i\sigma_y^{(j,k)})\Big). \tag{3.66}$$

If we now define $\tilde{a}^R = f(\tilde{A}^R_d)$ and $\tilde{a}^I = f(\tilde{A}^I_d + \tilde{B}^I_\sigma)$, then by fixing an appropriate order for the basis vectors in (3.52), and relabelling the components in (3.53), (3.55), (3.66),

we can write

$$\tilde{a}^R = \begin{pmatrix} a_1^R \\ \vdots \\ a_{d-1}^R \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix} \qquad \tilde{a}^I = \begin{pmatrix} a_1^I \\ \vdots \\ \vdots \\ a_{d^2-d}^R \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{3.67}$$

Furthermore, via complete antisymmetry of the structure constants of $\mathrm{su}(d)$ one can prove that $\mathrm{Int}(\mathrm{SU}(d)) \subseteq \mathrm{SO}(d^2-1)$, and therefore that the adjoint action preserves orthogonality and normalisation. As a result, we have now successfully shown that for any GKS matrix $\vec{a}\vec{a}^\dagger$, with $\vec{a} \in \mathbb{C}^{d^2-1}$ and $|\vec{a}| = 1$, there always exists $U = U_2 U_1 \in \mathrm{SU}(d)$ such that

$$G_{(U)}\vec{a} = \cos(\theta)\tilde{a}^R + i\sin(\theta)\tilde{a}^I, \tag{3.68}$$

where $G_{(U)} = \hat{\mathrm{Ad}}(U)$ and $\tilde{a}^R, \tilde{a}^I \in \mathbb{R}^{d^2-1}$ are given by (3.67), with $|\tilde{a}^R| = |\tilde{a}^I| = 1$ and $\tilde{a}^R.\tilde{a}^I = 0$. Exploiting orthogonality and normalisation we can always find angles $\{\alpha_j^R\}|_{j=1}^{d-2}$ and $\{\alpha_k^I\}|_{k=1}^{d^2-(d+1)}$ such that the parametrisation given in the statement of the theorem exists. Finally, using the definition of $G_{(U)}$, along with complete antisymmetry of the structure constants, one can show that $G_{(U)}^T = G_{(U^\dagger)} = \hat{\mathrm{Ad}}(U^\dagger)$, and therefore as $G_{(U)} \in \mathrm{SO}(d^2-1)$ we have that

$$\vec{a}\vec{a}^\dagger = G_{(U^\dagger)}\big[G_{(U)}\vec{a}\vec{a}^\dagger G_{(U)}^T\big]G_{(U)^\dagger}^T, \tag{3.69}$$

and as a result the semigroup generated by $\vec{a}\vec{a}^\dagger$ can be simulated through the semigroup generated by $G_{(U)}\vec{a}\vec{a}^\dagger G_{(U)}^T$, a member of the universal set, using unitary conjugation via $U^\dagger$.

3.5.2 Proof of necessity

We show here that using linear combination and unitary conjugation it is not possible to simulate the Markovian semigroup specified by some GKS matrix $A(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$, satisfying the restrictions of the theorem statement, through simulation of some other combination/transformation of Markovian semigroups specified by GKS matrices satisfying the same conditions for some different set of parameters.

Firstly, all $A(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$, as projections onto the eigenspace of a single eigenvector of

A, a basis vector of $\mathbb{C}^{d^2-1}$, are rank one matrices. As rank one matrices are extreme in the convex cone of positive matrices, no such $A(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$ can be simulated through the linear combination of Markovian semigroups specified by other such GKS matrices. Note also that a phase transformation of $\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$ commutes with a rotation via $G \in \mathrm{Int}(\mathrm{SU}(d))$, and as such we only need to prove that if $\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$ and $\vec{a}(\theta', \vec{\alpha}'^R, \vec{\alpha}'^I)$ satisfy the restrictions (3.23)-(3.35), but for different sets of parameters, and

$$e^{i\psi} G\big[\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)\big] = \vec{a}(\theta', \vec{\alpha}'^R, \vec{\alpha}'^I), \tag{3.70}$$

for some $\psi \in [0, 2\pi]$ and some $G \in \mathrm{Int}(\mathrm{SU}(d))$, then $(\theta, \vec{\alpha}^R, \vec{\alpha}^I) = (\theta', \vec{\alpha}'^R, \vec{\alpha}'^I)$. In order to simplify the presentation of the proof, in what follows we drop from our notation the explicit dependency of vectors on their parameters by defining

$$\begin{aligned}
\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I) &= \cos(\theta)\tilde{a}^R(\vec{\alpha}^R) + i\sin(\theta)\tilde{a}^I(\vec{\alpha}^I) && (3.71)\\
&\equiv \cos(\theta)\tilde{a}^R + i\sin(\theta)\tilde{a}^I && (3.72)\\
&\equiv \vec{a}^R + \vec{a}^I && (3.73)\\
&\equiv \vec{a}, && (3.74)
\end{aligned}$$

and

$$\begin{aligned}
\vec{a}(\theta', \vec{\alpha}'^R, \vec{\alpha}'^I) &= \cos(\theta')\tilde{a}^R(\vec{\alpha}'^R) + i\sin(\theta')\tilde{a}'^I(\vec{\alpha}'^I) && (3.75)\\
&\equiv \cos(\theta')\tilde{a}'^R + i\sin(\theta')\tilde{a}'^I && (3.76)\\
&\equiv \vec{a}'^R + \vec{a}'^I && (3.77)\\
&\equiv \vec{a}', && (3.78)
\end{aligned}$$

with the goal of proving that if $e^{i\psi}G\vec{a} = \vec{a}'$ then $\vec{a} = \vec{a}'$. In this simplified notation we can write,

$$e^{i\psi} G\big[\vec{a}\big] = e^{i\psi}\big[\cos(\theta)\big(G\tilde{a}^R\big) + i\sin(\theta)\big(G\tilde{a}^I\big)\big], \tag{3.79}$$

where, as $G \in \mathrm{Int}(\mathrm{SU}(d)) \subseteq \mathrm{SO}(d^2-1)$, we see that rotation of $\vec{a}(\theta, \vec{\alpha}^R, \vec{\alpha}^I)$ via G leaves θ unchanged. Furthermore, if we define

$$\begin{aligned}
\tilde{k}_1 &\equiv |\cos(\theta)\big(G\hat{a}^R\big)|^2 - |\sin(\theta)\big(G\hat{a}^I\big)|^2 && (3.80)\\
\tilde{k}_2 &\equiv 2\big[\cos(\theta)\big(G\hat{a}^R\big)\big] \cdot \big[\sin(\theta)\big(G\hat{a}^I\big)\big] && (3.81)
\end{aligned}$$

then via the fact that $G \in \mathrm{SO}(d^2-1)$ we obtain that $\tilde{k}_1 = k_1 \geq 0$ and $\tilde{k}_2 = k_2 = 0$,

where k_1 and k_2 are defined in (3.39) and (3.40). Let us now define

$$k_1' \equiv |\vec{a}'^R|^2 - |\vec{a}'^I|^2 \tag{3.82}$$
$$k_2' \equiv 2\vec{a}'^R \cdot \vec{a}'^I. \tag{3.83}$$

(k_1', k_2') is related to $(\tilde{k}_1, \tilde{k}_2)$ via an expression such as (3.43), but as $k_1' \geq 0$ and $k_2' = 0$ by assumption, we see that we must have $\psi = 0$, i.e. the phase transformation must be trivial. As neither the phase transformation nor rotation via G effects θ, we have that $\theta = \theta'$ and we can then write

$$\vec{a}' = \cos(\theta)\big(G\tilde{a}^R\big) + i\sin(\theta)\big(G\tilde{a}^I\big) \tag{3.84}$$
$$= \cos(\theta)\tilde{a}'^R + i\sin\theta\tilde{a}'^I. \tag{3.85}$$

Furthermore, again because $G \in \mathrm{Int}(\mathrm{SU}(d)) \subseteq \mathrm{SO}(d^2-1)$ is real, $e^{i\psi}G\vec{a} = \vec{a}'$ implies that $G\tilde{a}^R = \tilde{a}'^R$ and $G\tilde{a}^I = \tilde{a}'^I$, and therefore all that remains is to prove that $G\tilde{a}^R = \tilde{a}^R$ and $G\tilde{a}^I = \tilde{a}^I$.

To this end, let us define

$$\tilde{A}^R = f^{-1}(\tilde{a}^R), \tag{3.86}$$
$$\tilde{A}'^R = f^{-1}(\tilde{a}'^R). \tag{3.87}$$

If $G = \hat{\mathrm{Ad}}(U)$, for some $U \in \mathrm{SU}(d)$, then from $G\tilde{a}^R = \tilde{a}'^R$ we have that

$$\tilde{A}'^R = U\tilde{A}^R U^\dagger. \tag{3.88}$$

However, also by assumption, both $\tilde{A}'^R$ and $\tilde{A}^R$ are diagonal, and therefore U must also be diagonal, i.e. we must have that $U = \exp(i\sum_{l=1}^{d-1} p_l d^{(l)})$, for some $\vec{p} \in \mathbb{R}^{d-1}$ with components p_l. However, in this case one can show that

$$U\tilde{A}^R U^\dagger = \tilde{A}^R, \tag{3.89}$$

and therefore $G\tilde{a}^R = \tilde{a}^R$. To prove that $G\tilde{a}^I = \tilde{a}^I$ we define

$$f^{-1}(\tilde{a}^I) \equiv \tilde{A}_d^I + \tilde{B}_\sigma^I, \tag{3.90}$$

where

$$\tilde{A}_d^I = \sum_{l=1}^{d-1} d_l^I(id^{(l)}), \tag{3.91}$$

is diagonal and

$$\tilde{B}_\sigma^I = \sum_{k=2}^{d} m_{(1,k)} i(\sigma^{(1,k)} + \sigma^{(k,1)}) + \sum_{j=2}^{d-1}\sum_{k=j+1}^{d} i\Big[m_{(j,k)} e^{if_{(j,k)}}(\sigma^{(j,k)}) + \text{H.C}\Big]. \tag{3.92}$$

We then have that

$$G\tilde{a}^I = f(U\tilde{A}_d^I U^\dagger + U\tilde{B}_\sigma^I U^\dagger), \tag{3.93}$$

but given diagonal U we again see that

$$U\tilde{A}_d^I U^\dagger = \tilde{A}_d^I, \tag{3.94}$$

and as such all that remains is to prove that $U\tilde{B}_\sigma^I U^\dagger = \tilde{B}_\sigma^I$. To show this, note that via our assumptions we can write

$$f^{-1}(\tilde{a}'^I) \equiv \tilde{A}_d'^I + \tilde{B}_\sigma'^I, \tag{3.95}$$

with $\tilde{A}_d'^I$ diagonal and

$$\tilde{B}_\sigma'^I = \sum_{k=2}^{d} m'_{(1,k)} i(\sigma^{(1,k)} + \sigma^{(k,1)}) + \sum_{j=2}^{d-1}\sum_{k=j+1}^{d} i\Big[m'_{(j,k)} e^{if'_{(j,k)}}(\sigma^{(j,k)}) + \text{H.C}\Big]. \tag{3.96}$$

However, from (3.93)-(3.95) and the fact that $G\tilde{a}^I = \tilde{a}'^I$, we can also see that

$$\tilde{B}_\sigma'^I = U\tilde{B}_\sigma^I U^\dagger, \tag{3.97}$$

and therefore that

$$\tilde{B}_\sigma'^I = \sum_{j=1}^{d-1}\sum_{k=j+1}^{d} i\Big[m_{(j,k)} e^{i\gamma_{(j,k)}}(\sigma^{(j,k)}) + \text{H.C}\Big], \tag{3.98}$$

where

$$\gamma_{(j,k)} = f_{(j,k)} - (j-1)\varphi(j-1)p_{j-1} + \sum_{l=j}^{k-2}\big(\varphi(l)p_l\big) + k\varphi(k-1)p_{k-1}, \tag{3.99}$$

and from (3.92) we have that $f_{(1,k)} = 0$ for $k \in [2, d]$. By comparison of (3.96) and (3.98) we see that we must have $\gamma_{(1,k)} = 0$ for $k \in [2, d]$, and therefore from (3.99) and (3.92) we can show that we must have $p_l = 0$ for $l \in [1, d-1]$. This implies that $U = \mathbb{1}$, and therefore $G = \mathbb{1}$ and $G\vec{a} = \vec{a}$. ■

3.6 Simulation algorithm

If we assume the ability to implement the necessary and sufficient set of resources implied by Theorem 3.2, or in other words, if we consider arbitrary unitary operations on our system along with quantum channels from the semigroups generated by elements of the universal set as "standard resources", then the construction of Theorem 3.2, along with previous work on simulation of linear combinations [43] (described in Appendix 3.9.1), implies a natural algorithm for the simulation of arbitrary Markovian open quantum systems. This algorithm is not necessarily efficient for an arbitrary system, however after presentation of the algorithm we discuss the conditions under which a Markovian open quantum system can be efficiently simulated, with respect to the constructed universal set, using this algorithm. This discussion of efficiency relies on the details concerning simulation of linear combinations [43], as presented in detail in Appendix 3.9.1.

The algorithm, illustrated in Fig. 3.1 is as follows:

1. Given $\mathcal{H}_S \cong \mathbb{C}^d$ and $\mathcal{L} = \mathcal{L}_H + \mathcal{L}_A \in \mathcal{B}(\mathcal{B}(\mathcal{H}_S))$, the generator of a Markovian semigroup, obtain the spectral decomposition of A such that

$$\mathcal{L} = \mathcal{L}_H + \sum_{k=1}^{m} \lambda_k \mathcal{L}_{\vec{a}_k \vec{a}_k^\dagger} \equiv \sum_{k=0}^{m} \lambda_k \mathcal{L}_k, \tag{3.100}$$

   where $\lambda_0 = 1$ and $\mathcal{L}_0 \equiv \mathcal{L}_H$.

2. For each $k \in [1, m]$ use phase freedom to find θ_k, and construct $U_1^{(k)}$ and $U_2^{(k)}$ as per the proof of Theorem 3.2, such that by defining $U^{(k)} = U_1^{(k)\dagger} U_2^{(k)\dagger}$,

$$\vec{a}_k \vec{a}_k^\dagger = G_{(U^{(k)})} \big[A^{(k)}(\theta_k, \vec{\alpha}_k^R, \vec{\alpha}_k^I) \big] G^T_{(U^{(k)})}, \tag{3.101}$$

   where $A^{(k)}(\theta_k, \vec{\alpha}_k^R, \vec{\alpha}_k^I)$ is an element of the universal set of semigroup generators.

3. Given $\epsilon > 0$ and $t > 0$, construct, as described in Appendix 3.9.1, the Suzuki

higher order integrator $S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, t/r)$ [43, 58], with

$$k = \text{round}\left(\sqrt{\frac{1}{2}\log_{25/3}\frac{4emtL_2}{\epsilon}}\right), \tag{3.102}$$

and

$$r = t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/(2k)}\frac{2ed_k}{2k+1}, \tag{3.103}$$

where $L_2 := ||\mathcal{L}_2||_{1\to 1}$ and $d_k = m(4/3)k(5/3)^{k-1}$.

4. Given $\rho(0)$, implement $S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, t/r)$ consecutively rL_1 times, in order to recombine the linear combination (3.100) through sequential implementations of $T_k(\tilde{t}) = e^{\tilde{t}\mathcal{L}_k}$. Each implementation of $T_k(\tilde{t})$ is achieved via

$$T_k(\tilde{t}) = \mathcal{U}_k^\dagger\big(T_{A^{(k)}}(\tilde{t})\big)\mathcal{U}_k, \tag{3.104}$$

where $\mathcal{U}_k(\rho) = U^{(k)}(\rho)U^{(k)\dagger}$ and $T_{A^{(k)}}(t) = \exp(t\mathcal{L}_{A^{(k)}})$.

As shown in [43], and presented in Appendix 3.9.1, as a result of the Suzuki-Lie-Trotter procedure used for the recombination of linear combinations, the above algorithm simulates the Markovian semigroup generated by (3.100), within precision ϵ, using $\text{poly}\big(||\mathcal{L}||_{(1\to 1)}, t, 1/\epsilon, m\big)$ applications of "standard resources", i.e. implementations of quantum channels from the semigroups generated by elements of the universal set and unitary operations on the system. More precisely, the algorithm requires at most

$$N = \frac{8}{3}(2m-1)metL_1 e^{2\sqrt{\frac{1}{2}\ln(25/3)\ln(4emtL_2/\epsilon)}}, \tag{3.105}$$

implementations of channels $T_k(\tilde{t})$, each of which, as per Eq. (3.104), requires 3 "standard resources", namely two unitary operations and one quantum channel from a semigroup generated by an element of the universal set.

By comparison with our definition of *efficient* simulation in Section 4.2, we therefore see that this algorithm will be efficient, with respect to this universal set, for any class of Markovian semigroups for which m, the number of non-zero eigenvalues of the GKS matrix A, is proportional to $\ln(d)$, or alternatively, if we are within a many-body context, to the number of subsystems. As $A \in \mathcal{M}_{d^2-1}(\mathbb{C})$, we see that in the general case $m = d^2 - 1$ and the algorithm will not be efficient - however by comparing the GKSL form of Eq. (3.2) with the diagonal form of Eq. (3.3) we see that the algorithm will be efficient, with respect to this universal set, for any system for which the number

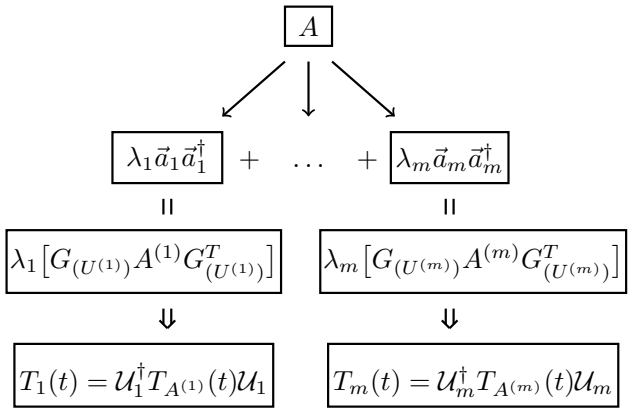

Figure 3.1: Any GKS matrix $A \geq 0$ can be decomposed into the linear combination of rank 1 GKS matrices $\vec{a}_i\vec{a}_i^\dagger$. The semigroups whose generator is specified by these matrices can be further decomposed into the unitary conjugation of semigroups whose generator is specified by an element of the universal set $A^{(i)}(\theta_i, \vec{\alpha}_i^R, \vec{\alpha}_i^I)$. As a result any quantum channel from the original semigroup can be implemented through the linear combination and unitary conjugation of channels from the semigroups whose generators belong to the universal set.

of distinct physical dissipation processes with non-zero rates (the number of distinct Lindblad operators) scales polynomially with the number of subsystems.

3.7 Worked example

As an illustration of the above algorithm we consider as an example a three level atom in the Λ configuration (see Fig. 3.2), experiencing effective dissipation described by the Lindblad master equation

$$\mathcal{L}(\rho) = \sum_{i=1}^{2} \gamma_i \left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\}_+ \right), \tag{3.106}$$

where,

$$L_1 = \cos\phi|1\rangle\langle e| + e^{i\eta}\sin\phi|2\rangle\langle e|, \tag{3.107}$$

$$L_2 = \cos\alpha|1\rangle\langle 2| + \sin\alpha|2\rangle\langle 1|. \tag{3.108}$$

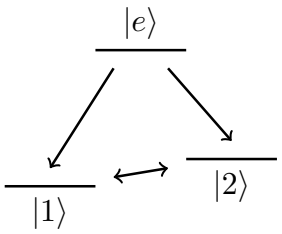

Figure 3.2: Illustration of three level Λ atom experiencing effective collective spontaneous emission and external incoherent driving.

We begin by transforming into the GKS form,

$$\mathcal{L}_A(\rho) = \sum_{l,k=1}^{8} A_{l,k}\left(F_l \rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}_+\right), \tag{3.109}$$

where $\{F_i\}|_{i=1}^8$ is a Hermitian basis for the traceless matrices in $\mathcal{M}_3(\mathbb{C})$, defined via

$$\{F_i\}|_{i=1}^2 \equiv \{d^{(l)}\}|_{l=1}^2 \tag{3.110}$$

$$\{F_i\}|_{i=3}^5 \equiv \{\sigma_x^{(j,k)}\}_{j=1}^2|_{j<k\leq 3} \tag{3.111}$$

$$\{F_i\}|_{i=6}^8 \equiv \{\sigma_y^{(j,k)}\}_{j=1}^2|_{j<k\leq 3}. \tag{3.112}$$

Setting $\phi = \eta = \alpha = \pi/3$, we find that with respect to this basis

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{3,3} & a_{3,4} & 0 & ia_{3,3} & a_{3,7} & 0 \\ 0 & 0 & \overline{a_{3,4}} & 3a_{3,3} & 0 & a_{4,6} & 3ia_{3,3} & 0 \\ 0 & 0 & 0 & 0 & a_{5,5} & 0 & 0 & a_{5,8} \\ 0 & 0 & -ia_{3,3} & \overline{a_{4,6}} & 0 & a_{3,3} & a_{3,4} & 0 \\ 0 & 0 & \overline{a_{3,7}} & -3ia_{3,3} & 0 & \overline{a_{3,4}} & 3a_{3,3} & 0 \\ 0 & 0 & 0 & 0 & \overline{a_{5,8}} & 0 & 0 & a_{8,8} \end{pmatrix}, \tag{3.113}$$

where the overbar is used to denote the complex conjugate, and

$$a_{3,3} = \frac{\gamma_1}{8} \tag{3.114}$$

$$a_{3,4} = \frac{\sqrt{3} - 3i}{16}\gamma_1 \tag{3.115}$$

$$a_{3,7} = \frac{3 + i\sqrt{3}}{16}\gamma_1 \tag{3.116}$$

$$a_{4,6} = \frac{-3 + i\sqrt{3}}{16}\gamma_1 \tag{3.117}$$

$$a_{5,5} = \frac{2 + \sqrt{3}}{4}\gamma_2 \tag{3.118}$$

$$a_{5,8} = \frac{i\gamma_2}{4} \tag{3.119}$$

$$a_{8,8} = \frac{2 - \sqrt{3}}{4}\gamma_2. \tag{3.120}$$

The next step is to decompose A into the linear combination of rank 1 generators through the spectral decomposition. Constructing this decomposition we obtain

$$A = \sum_{k=1}^{2} \lambda_k \vec{a}_k \vec{a}_k^\dagger, \tag{3.121}$$

where $\lambda_i = \gamma_i$, and

$$\vec{a}_1 = \frac{\sqrt{3}}{2\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \frac{1}{2} + \frac{i}{2\sqrt{3}} \\ i \\ 0 \\ -\frac{1}{2}i + \frac{1}{2\sqrt{3}} \\ 1 \\ 0 \end{pmatrix}, \qquad \vec{a}_2 = \frac{1}{\sqrt{1 + \left(2 + \sqrt{3}\right)^2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ (2 + \sqrt{3})i \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{3.122}$$

At this stage each constituent generator $\vec{a}_i \vec{a}_i^\dagger$ of the linear combination needs to be decomposed into the unitary conjugation of a semigroup from the universal set. We focus first on decomposing the semigroup generated by $\vec{a}_1 \vec{a}_1^\dagger$. The first step in this regard is to identify the phase ψ_1 such that

$$e^{i\psi_1}\vec{a}_1 = \cos(\theta_1)\hat{a}_1^R + i\sin(\theta_1)\hat{a}_1^I, \tag{3.123}$$

for some $\hat{a}_1^R$ and $\hat{a}_1^I$ such that $\hat{a}_1^R \cdot \hat{a}_1^I = 0$, $|\hat{a}_1^R| = |\hat{a}_1^I| = 1$ and $\theta_1 \in [0, \pi/4]$. For $\vec{a}_1$ as per (3.122) no such phase transformation is necessary, (i.e. we use $\psi_1 = 0$) and we see that

$$\vec{a}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ \frac{\sqrt{3}}{4} \\ 0 \\ 0 \\ \frac{1}{4} \\ \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} i \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \\ \frac{\sqrt{3}}{2} \\ 0 \\ -\frac{\sqrt{3}}{4} \\ 0 \\ 0 \end{pmatrix} \tag{3.124}$$

$$= \cos(\theta_1)\hat{a}_1^R + \sin(\theta_1)\hat{a}_1^I, \tag{3.125}$$

with $\theta_1 = \pi/4$. The next step is to identify $U_1^{(1)}$ and $U_2^{(1)}$ such that

$$\tilde{a}_1^R \equiv f\big(U_2^{(1)} U_1^{(1)} f^{-1}[\hat{a}_1^R] U_1^{(1)\dagger} U_2^{(1)\dagger}\big), \tag{3.126}$$

$$\tilde{a}_1^I \equiv f\big(U_2^{(1)} U_1^{(1)} f^{-1}[\hat{a}_1^I] U_1^{(1)\dagger} U_2^{(1)\dagger}\big), \tag{3.127}$$

have the form given in (3.20), where $f : \mathrm{su}(d) \to \mathbb{R}^8$ is the natural isomorphism defined via $f(iF_j) = |j\rangle$, where $\{iF_j\}|_{j=1}^8$ and $\{|j\rangle\}|_{j=1}^8$ are the standard bases for $\mathrm{su}(d)$ and $\mathbb{R}^8$ respectively. As per the proof of Theorem 3.2, $U_1^{(1)}$ is the matrix which diagonalises $\hat{A}_1^R \equiv f^{-1}(\hat{a}_1^R)$. For $\hat{a}_1^R$ as per (3.124) we find that

$$\hat{A}_1^R = \frac{\sqrt{3}}{2\sqrt{2}} \begin{pmatrix} 0 & \frac{1}{6}\left(3i + \sqrt{3}\right) & 1 \\ \frac{1}{6}\left(3i - \sqrt{3}\right) & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \tag{3.128}$$

and

$$U_1^{(1)} = \frac{\sqrt{3}}{2\sqrt{2}} \begin{pmatrix} \frac{2i}{\sqrt{3}} & \frac{1}{6}\left(3i + \sqrt{3}\right) & 1 \\ -\frac{2i}{\sqrt{3}} & \frac{1}{6}\left(3i + \sqrt{3}\right) & 1 \\ 0 & \sqrt{2}\left(-\frac{1}{2} - \frac{i\sqrt{3}}{2}\right) & \sqrt{\frac{2}{3}} \end{pmatrix} \tag{3.129}$$

such that

$$\tilde{A}_{d,1}^R \equiv U_1^{(1)} \hat{A}_1^R U_1^{(1)\dagger} = \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.130}$$

and

$$A_1^I \equiv U_1^{(1)} \hat{A}_1^I U_1^{(1)\dagger} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.131}$$

At this stage one would typically construct diagonal $U_2^{(1)}$ to eliminate 2 (i.e. $d-1$ with $d=3$) components of $f(\tilde{A}_1^I)$ while leaving $f(\tilde{A}_{d,1}^R)$ unchanged. However, in this case we see that

$$f(\tilde{A}_{d,1}^R) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad f(\tilde{A}_1^I) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \tag{3.132}$$

so that if we define $\tilde{a}_1^R \equiv f(\tilde{A}_{d,1}^R)$ and $\tilde{a}_1^I \equiv f(\tilde{A}_1^I)$ then a second unitary transformation is not necessary, as $\tilde{a}_1^R$ and $\tilde{a}_1^I$ already have the desired form. So, following the proof by defining $U^{(1)} = U_1^{(1)\dagger}$ and $G_{(U^{(1)})} = \hat{\mathrm{Ad}}(U^{(1)})$, we now have that

$$\vec{a}_1 \vec{a}_1^\dagger = G_{(U^{(1)})}\big[A^{(1)}(\theta_1, \vec{\alpha}_1^R, \vec{\alpha}_1^I)\big] G_{(U^{(1)})}^T, \tag{3.133}$$

where $A^{(1)}(\theta_1, \vec{\alpha}_1^R, \vec{\alpha}_1^I$ is an element of the universal set of semigroup generators, with $\theta_1 = \pi/4$, $\vec{\alpha}_1^R = 0$ and

$$\vec{\alpha}_1^I = \frac{\pi}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 3 \end{pmatrix}. \tag{3.134}$$

Furthermore, from Theorem 3.1 and (3.133), one has that for any channel $T_1(t) = \exp(t\mathcal{L}_{\vec{a}_1\vec{a}_1^\dagger})$ from the semigroup generated by $\vec{a}_1\vec{a}_1^\dagger$,

$$T_1(t)(\rho) = U^{(1)\dagger}\Big(T_{A^{(1)}}(t)\big[U^{(1)}\rho U^{(1)\dagger}\big]\Big)U^{(1)}, \tag{3.135}$$

where $T_{A^{(k)}}(t) = \exp(t\mathcal{L}_{A^{(k)}})$.

We can now proceed to decompose the semigroup generated by $\vec{a}_2\vec{a}_2^\dagger$, the second

component of the linear decomposition. We follow the same procedure, however in this case if we simply rewrite (3.122) as

$$\vec{a}_2 = \vec{a}_2^R + i\vec{a}_2^I \tag{3.136}$$

then we see that although $\vec{a}_2^R \cdot \vec{a}_2^I = 0$, we have $|\vec{a}_2^I| > |\vec{a}_2^R|$, and as such a non-trivial phase transformation is necessary in order to be able to write

$$e^{i\psi_2}\vec{a}_2 = \cos(\theta_2)\hat{a}_2^R + i\sin(\theta_2)\hat{a}_2^I, \tag{3.137}$$

for some $\hat{a}_2^R$ and $\hat{a}_2^I$ such that $\hat{a}_2^R \cdot \hat{a}_2^I = 0$, $|\hat{a}_2^R| = |\hat{a}_2^I| = 1$ and $\theta_2 \in [0, \pi/4]$. As $\vec{a}_2^R \cdot \vec{a}_2^I = 0$ we see that a phase transformation via $\psi_2 = \pi/2$ is sufficient, and after such a transformation we obtain an expression in the form (3.137) with

$$\theta_2 = \arccos\Big(\frac{2+\sqrt{3}}{\sqrt{1+\big(2+\sqrt{3}\big)^2}}\Big), \tag{3.138}$$

and

$$\hat{a}_2^R = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \hat{a}_2^I = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{3.139}$$

Once again, the next step is to find the unitary matrix $U_1^{(2)}$ which diagonalises $\hat{A}_2^R \equiv f^{-1}(\hat{a}_2^R)$. In this case we find

$$\hat{A}_2^R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} \\ 0 & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix}, \tag{3.140}$$

and

$$U_1^{(2)} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix}, \tag{3.141}$$

such that

$$\tilde{A}^R_{d,2} \equiv U_1^{(2)} \hat{A}^R_2 U_1^{(2)\dagger} = \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.142}$$

and

$$A^I_2 \equiv U_1^{(2)} \hat{A}^I_2 U_1^{(2)\dagger} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.143}$$

From (3.142) and (3.143) we see that $\tilde{A}^R_{d,2} = \tilde{A}^R_{d,1}$ and $\tilde{A}^I_2 = \tilde{A}^I_1$, and therefore its clear that once again no second unitary transformation is necessary, and that

$$\vec{a}_2 \vec{a}_2^\dagger = G_{(U^{(2)})}\big[A^{(2)}(\theta_2, \vec{\alpha}^R_2, \vec{\alpha}^I_2)\big] G^T_{(U^{(2)})}, \tag{3.144}$$

where $\vec{\alpha}^R_2 = \vec{\alpha}^R_1$, $\vec{\alpha}^I_2 = \vec{\alpha}^I_1$ and we have defined $U^{(2)} = U_1^{(2)\dagger}$ and $G_{(U^{(2)})} = \hat{\mathrm{Ad}}(U^{(2)})$. Finally, for any channel $T_2(t) = \exp(t\mathcal{L}_{\vec{a}_2\vec{a}_2^\dagger})$ from the semigroup generated by $\vec{a}_2\vec{a}_2^\dagger$,

$$T_2(t)(\rho) = U^{(2)\dagger}\Big(T_{A^{(2)}}(t)\big[U^{(2)}\rho U^{(2)\dagger}\big]\Big)U^{(2)}, \tag{3.145}$$

where $T_{A^{(2)}}(t) = \exp(t\mathcal{L}_{A^{(2)}})$.

At this stage, given $\epsilon > 0$, $t > 0$ and $\rho(0)$, in order to efficiently implement $T(t) = e^{t\mathcal{L}}$ one constructs $S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, t/r)$ as per (3.149), with k given by (3.155). One then implements S_{2k} rL_1 times, with r given by (3.154), and each call to $T_k(\tilde{t})$ is achieved using the unitary conjugation of some channel from the universal set, as per (3.135) and (3.145), where $\tilde{t}$ incorporates γ_k.

3.8 Conclusion

Utilising the composition framework of linear combination and unitary conjugation we have constructed a universal set of generators for the simulation of Markovian semigroup dynamics. More precisely, we have constructed a $d^2 - 3$ parameter family of semigroup generators, such that any Markovian semigroup describing the dynamics of a d dimensional Markovian open quantum system can be simulated through the implementation of unitary operations on the system and quantum channels from the semigroups generated by the $d^2 - 3$ parameter family of generators. Furthermore, assuming the ability to implement all operations from the universal set, the construction of such a universal set

implies a natural methodology for the simulation of Markovian open quantum systems: Given such a system, one utilises the construction of Theorem 3.2 to decompose the generator of the system into the linear combination and unitary conjugation of generators from the universal set, before utilising Suzuki-Lie-Trotter techniques [43, 58] to simulate the original system through simulations of the constituent semigroups. This approach will provide a method for the *efficient* simulation, with respect to this universal set, of any Markovian open quantum system for which the number of distinct physical dissipation processes with non-zero rates (the number of Lindblad operators) scales polynomially with the number of subsystems.

Given such a methodology, it is clear that in order to use this approach for the simulation of arbitrary Markovian open quantum systems one need only to focus on explicitly constructing methods, and developing the experimental capability, for efficiently simulating those systems whose generators are specified by GKS matrices belonging to the universal set of Theorem 3.2. These generators provide a significant simplification from the general case, and in principle, these systems could be simulated using any of the previous methods [37–39, 45–49] for the simulation of Markovian open quantum systems. Another appealing approach would be to investigate the possibility of utilising the inherent dissipation and decoherence within currently available controllable quantum devices for the implementation of non-unitary processes from the universal set, therefore developing the potential of quantum simulators other than universal quantum computers. One other possibility, already explored in detail for the single qubit case [43], would be to explicitly construct parametrised descriptions of the quantum channels appearing in the semigroup generated by an arbitrary element of the universal set. Given such an explicit parametrised family of quantum channels, the methods of [41] could be used to implement any such channel for any given time, on a minimal dilation space, through the simulation of constituent extreme channels.

Given these results, a natural open question concerns the extension of this approach for more general open quantum systems, such as those described by time-dependent generators [36]. In order to extend this approach one could investigate the possibility of utilising more general composition frameworks which are not constrained to preserve Markovianity, possibly including feedback [44] or probabilistic implementations of quantum channels [40, 41].

3.9 Appendix

3.9.1 Simulation of linear combinations

Given the generator of a Markovian semigroup, $\mathcal{L} = \sum_{j=1}^{m} \mathcal{L}_j$, we want to show that for any $t > 0$ it is possible to implement $T(t) = e^{t\mathcal{L}}$, up to arbitrary accuracy $\epsilon > 0$, using only $\text{poly}\big(||\mathcal{L}||_{(1\to1)}, t, 1/\epsilon, m\big)$ number of implementations of $T^{(j)}(t') = e^{t'\mathcal{L}_j}$. Using Suzuki-Lie-Trotter techniques [55–57] the analogous problem for linear combinations of Hamiltonians has been studied extensively [21, 24, 58, 59], and generalisations to the context of open quantum systems have been considered before for both the case of time-dependent [36] and time-independent [43] generators. Here we present a direct generalisation of the work in [58] to the super-operator setting, first presented in [43], which provides the best current bounds on the number of implementations of $T^{(j)}(t') = e^{t'\mathcal{L}_j}$ required, within the context of time-independent generators $\mathcal{L}$.

We begin by assuming that

$$||\mathcal{L}_1||_{(1\to1)} \geq ||\mathcal{L}_2||_{(1\to1)} \geq \cdots \geq ||\mathcal{L}_m||_{(1\to1)} \tag{3.146}$$

and defining the normalised component generators $\hat{\mathcal{L}}_j = \mathcal{L}_j/L_1$, where we have defined $L_1 := ||\mathcal{L}_1||_{(1\to1)}$. We then follow [58] and define the basic Lie-Trotter product formula [55] as,

$$S_2(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda) = \prod_{j=1}^{m} e^{(\frac{\lambda}{2})\hat{\mathcal{L}}_j} \prod_{j'=m}^{1} e^{(\frac{\lambda}{2})\hat{\mathcal{L}}_{j'}} \tag{3.147}$$

$$= \prod_{j=1}^{m} T^{(j)}(t_\lambda) \prod_{j'=m}^{1} T^{(j')}(t_\lambda), \tag{3.148}$$

where $t_\lambda = \lambda/(2L_1)$. Suzuki's higher order integrators [56,57] are then defined using the recursion relation

$$S_{2k}(\lambda) = [S_{2k-2}(p_k\lambda)]^2[S_{2k-2}((1-4p_k)\lambda)][S_{2k-2}(p_k\lambda)]^2, \tag{3.149}$$

where $p_k = (4-4^{1/(2k-1)})^{-1}$ for $k > 1$ and for notational convenience we have used $S_{2k}(\lambda)$ and $S_{2k-2}(\lambda)$ to denote $S_{2k}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda)$ and $S_{2k-2}(\hat{\mathcal{L}}_1, \ldots, \hat{\mathcal{L}}_m, \lambda)$ respectively. Note that $S_{2k}(\lambda)$ consists of a product of

$$2(m-1)5^{k-1} + 1 \tag{3.150}$$

exponentials, so that we can define

$$N_{\text{exp}} = [2(m-1)5^{k-1}+1]x \tag{3.151}$$

as the number of exponentials, and hence channels $T^{(j)}(t')$, appearing in the expression $[S_{2k}(t/r)]^x$. The following theorem [43], a direct generalization of the work in [58] to the superoperator setting, then gives the desired result

Theorem 3.3. *Let $1 \geq \epsilon > 0$ be such that $4met||\mathcal{L}_2||_{1\to 1} \geq \epsilon$, then for any $k \in \mathbb{N}$ there exists r such that*

$$\Big|\Big|\exp\Big(t\sum_{j=1}^{m}\mathcal{L}_j\Big) - \big[S_{2k}(\hat{\mathcal{L}}_1,\ldots,\hat{\mathcal{L}}_m,t/r)\big]^{rL_1}\Big|\Big|_{1\to 1} \leq \epsilon \tag{3.152}$$

and the number of exponentials required is bounded by

$$\mathrm{N}_{\text{exp}} \leq (2m-1)5^{k-1}\Big[L_1 t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/2k}\frac{4me}{3}\Big(\frac{5}{3}\Big)^{k-1}\Big] \tag{3.153}$$

where $L_2 := ||\mathcal{L}_2||_{1\to 1}$.

In particular, we can take

$$r = t\Big(\frac{4emtL_2}{\epsilon}\Big)^{1/(2k)}\frac{2ed_k}{2k+1}, \tag{3.154}$$

where $d_k = m(4/3)k(5/3)^{k-1}$ [43, 58]. As calculated in [58], if $\epsilon \leq mtL_2$ then the minimum value of the right hand side in (3.153) is achieved for

$$k = \text{round}\left(\sqrt{\frac{1}{2}\log_{25/3}\frac{4emtL_2}{\epsilon}}\right), \tag{3.155}$$

such that the number of exponentials required satisfies

$$N_{\text{exp}} \leq \frac{8}{3}(2m-1)metL_1 e^{2\sqrt{\frac{1}{2}\ln(25/3)\ln(4emtL_2/\epsilon)}}. \tag{3.156}$$

Furthermore, by definition of the $(1\to 1)$ norm we have that for any density matrix ρ and any superoperators P and Q,

$$||P(\rho) - Q(\rho)||_1 \leq ||P-Q||_{1\to 1} \tag{3.157}$$

and as such the results of Theorem 3.3 bound the error in the output state obtained

when approximating $T(t)$ with $[S_{2k}(t/r)]^{rL_1}$.

3.9.2 Properties of the adjoint representation

We summarise here properties and characterisations of the adjoint representation of $\mathrm{SU}(d)$, in order to set the notation used for a rigorous description of the effect of unitary conjugation and to provide the fundamental results used in the proof of our main result. For more detail, and proofs of the statements which follow, the interested reader is referred to [60, 61].

For any Lie group G, with Lie algebra $\mathfrak{g}$, we define the conjugation map

$$\psi_g : G \to G \tag{3.158}$$

via

$$\psi_g(h) = ghg^{-1} \tag{3.159}$$

$\forall g, h \in G$. The adjoint representation of G,

$$\mathrm{Ad} : G \to \mathrm{GL}(\mathfrak{g}), \tag{3.160}$$

is then defined via

$$\mathrm{Ad}(g) := \mathrm{d}\psi_g\big|_e : \mathfrak{g} \to \mathfrak{g}, \tag{3.161}$$

where $\mathrm{d}\psi_g\big|_e$ is the differential of ψ_g at the identity element of G. The adjoint representation of $\mathfrak{g}$,

$$\mathrm{ad} : \mathfrak{g} \to \mathrm{End}(\mathfrak{g}) \simeq \mathfrak{gl}(\mathfrak{g}), \tag{3.162}$$

is then induced from Ad and defined via,

$$\mathrm{ad}(X) = \mathrm{d}(\mathrm{Ad})\big|_e(X) : \mathfrak{g} \to \mathfrak{g} \tag{3.163}$$

$\forall X \in \mathfrak{g}$. We then define $\mathrm{Int}(\mathfrak{g}) = \mathrm{Im}(\mathrm{Ad}) \subseteq \mathrm{GL}(\mathfrak{g})$, the image of Ad, and $\mathfrak{Int}(\mathfrak{g}) = \mathrm{Im}(\mathrm{ad}) \subseteq \mathfrak{gl}(\mathfrak{g})$, the image of ad. One can show that Ad is a Lie group homomorphism, ad a Lie algebra homomorphism, and that $\mathrm{Int}(\mathfrak{g})$ is a Lie group with Lie algebra $\mathfrak{Int}(\mathfrak{g})$.

As we will be concerned with $\mathrm{SU}(d)$, we assume here that $\mathfrak{g} \simeq \mathbb{R}^n$ is a real vector space (where for $\mathfrak{g} = \mathrm{su}(d)$ we have that $n = d^2 - 1$). Under this assumption, let $\{X_i\}|_{i=1}^n$ be a basis for $\mathfrak{g}$, with structure constant

$$[X_i, X_j] = f_{ijk} X_k, \tag{3.164}$$

where we have utilised the summation notation for repeated indices. Furthermore, for arbitrary $X \in \mathfrak{g}$, let $X = x_i X_i$, so that by identifying basis elements we can define the natural linear isomorphism

$$f : \mathfrak{g} \to \mathbb{R}^n, \tag{3.165}$$

such that $f(X) = \vec{x}$. Given this, it is possible to show that $\forall X, Y \in \mathfrak{g}$,

$$\mathrm{ad}(X)(Y) = [X, Y], \tag{3.166}$$

such that via linearity of the Lie bracket

$$\mathrm{ad}(X)(Y) = \big[x_i \mathrm{ad}(X_i)\big](Y). \tag{3.167}$$

Furthermore, if $\ker(\mathrm{ad}) = 0$, which is indeed the case for $\mathfrak{g} = \mathrm{su}(d)$, then $\mathrm{ad} : \mathfrak{g} \to \mathfrak{Int}(\mathfrak{g})$ is also a linear isomorphism, such that $\{\mathrm{ad}(X_i)\}|_{i=1}^n$ is a basis for the Lie algebra $\mathfrak{Int}(\mathfrak{g})$. Using the structure constants, for any $X \in \mathfrak{g}$ we can then define $\hat{\mathrm{ad}}(X) \in \mathcal{M}_n(\mathbb{C})$, the matrix representation of $\mathrm{ad}(X)$, such that $\forall Y \in \mathfrak{g}$

$$\mathrm{ad}(X)(Y) = f^{-1}\big(\hat{\mathrm{ad}}(X) f(Y)\big), \tag{3.168}$$

via $\hat{\mathrm{ad}}(X) = x_i \hat{\mathrm{ad}}(X_i)$, where the matrix elements of $\hat{\mathrm{ad}}(X_i)$ are given by

$$[\hat{\mathrm{ad}}(X_i)]_{jk} = f_{ijk}. \tag{3.169}$$

In addition, one can show that $\forall X \in \mathfrak{g}$ the Ad map satisfies

$$\mathrm{Ad}\big(\exp(X)\big) = \exp\big(\mathrm{ad}(X)\big), \tag{3.170}$$

and that for connected matrix groups G (such as $\mathrm{SU}(d)$)

$$\mathrm{Ad}(g)(Y) = gYg^{-1}, \tag{3.171}$$

$\forall g \in G$ and $\forall Y \in \mathfrak{g}$, such that for any $g = \exp(X) \in G$ we have the equivalence

$$\begin{aligned} \mathrm{Ad}(g)(Y) &= f^{-1}\big(e^{\hat{\mathrm{ad}}(X)} f(Y)\big) \\ &= f^{-1}\big(\hat{\mathrm{Ad}}(g) f(Y)\big) \\ &= gYg^{-1}, \end{aligned} \tag{3.172}$$

where $\hat{\mathrm{Ad}}(g) \in \mathcal{M}_n(\mathbb{C})$ is the matrix representation of $\mathrm{Ad}(g)$.

Bibliography

[1] R. Sweke, I. Sinayskiy, D. Bernard, and F. Petruccione. Universal simulation of Markovian open quantum systems. *Phys. Rev. A*, 94:062308, 2016.

[2] H. P. Breuer and F. Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press, 2002.

[3] A. J. Daley. Quantum trajectories and open many-body quantum systems. *Adv. Phys.*, 63:77, 2014.

[4] M. Žnidarič, T. Prosen, G. Benenti, G. Casati, and D. Rossini. Thermalization and ergodicity in one-dimensional many-body open quantum systems. *Phys. Rev. E*, 81:051135, 2010.

[5] M. J. Kastoryano and F. G. S. L Brandao. Quantum Gibbs Samplers: the commuting case. *Comm. Math. Phys.*, 344:915–957, 2016.

[6] I. Pizorn. One-dimensional Bose-Hubbard model far from equilibrium. *Phys. Rev. A*, 88:043635, 2013.

[7] T. Prosen and M. Žnidarič. Matrix product simulations of non-equilibrium steady states of quantum spin chains. *J. Stat. Mech.*, 02:02035, 2009.

[8] T. Prosen. Open XXZ spin chain: Nonequilibrium steady state and a strict bound on ballistic transport. *Phys. Rev. Lett.*, 106:217206, 2011.

[9] G. Benenti, G. Casati, T. Prosen, D. Rossini, and M. Žnidarič. Charge and spin transport in strongly correlated one-dimensional quantum systems driven far from equilibrium. *Phys. Rev. B*, 80:035110, 2009.

[10] T. Prosen and M. Žnidarič. Diffusive high-temperature transport in the one-dimensional Hubbard model. *Phys. Rev. B*, 86:125118, 2012.

[11] A. Marais, I. Sinayskiy, A. Kay, F. Petruccione, and A. Ekert. Decoherence-assisted transport in quantum networks. *New J. Phys.*, 15:013038, 2013.

[12] I. Sinayskiy, A. Marais, F. Petruccione, and A. Ekert. Decoherence-assisted transport in a dimer system. *Phys. Rev. Lett.*, 108:020602, 2012.

[13] R. Dorner, J. Goold, and V. Vedral. Towards quantum simulations of biological information flow. *Interface Focus*, 2:522, 2012.

[14] F. Verstraete, M. M. Wolf, and J. I. Cirac. Quantum computation and quantum-state engineering driven by dissipation. *Nature Physics*, 5:633, 2009.

[15] I. Sinayskiy and F. Petruccione. Efficiency of open quantum walk implementation of dissipative quantum computing algorithms. *Quant. Inf. Proc.*, 11:1301, 2012.

[16] J. C. Budich, P. Zoller, and S. Diehl. Dissipative preparation of Chern insulators. *Phys. Rev. A*, 91:042117, 2015.

[17] S. Diehl, E. Rico, M. A. Baranov, and P. Zoller. Topology by dissipation in atomic quantum wires. *Nature Physics*, 7:971, 2011.

[18] C. E. Bardyn, M. A. Baranov, C. V. Kraus, E. Rico, A. Imamoğlu, P. Zoller, and S. Diehl. Topology by dissipation. *New J. Phys.*, 15:085001, 2013.

[19] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller. Preparation of entangled states by quantum Markov processes. *Phys. Rev. A*, 78:042307, 2008.

[20] S. Diehl, A. Micheli, A. Kantian, B. Kraus, H.P. Büchler, and P. Zoller. Quantum states and phases in driven open quantum systems with cold atoms. *Nature Physics*, 4:878, 2008.

[21] B. C. Sanders. Efficient algorithms for universal quantum simulation. In G. W. Dueck and D. M. Miller, editors, *Reversible Computation: 5th International Conference, RC 2013, Victoria, BC, Canada, July 4-5, 2013. Proceedings*, pages 1–10. Springer, 2013.

[22] K. L. Brown, W. J. Munro, and V. M. Kendon. Using quantum computers for quantum simulation. *Entropy*, 12:2268, 2010.

[23] I. M. Georgescu, S. Ashhab, and F. Nori. Quantum simulation. *Rev. Mod. Phys.*, 86:153, 2014.

[24] D. W. Berry, A. M. Childs, and R. Kothari. Hamiltonian simulation with nearly optimal dependence on all parameters. *Proceedings of the 56th IEEE Symposium on Foundations of Computer Science (FOCS 2015)*, pages 792–809, 2015.

[25] M. Hillery, M. Ziman, and V. Bužek. Implementation of quantum maps by programmable quantum processors. *Phys. Rev. A*, 66:042302, 2002.

[26] M. Koniorczyk, V. Bužek, P. Adam, and A. Lázló. Simulation of Markovian quantum dynamics on quantum logic networks. arXiv:quant-ph/0205008, 2005.

[27] T. Rybár, S. N. Filippov, M. Ziman, and V. Bužek. Simulation of indivisible qubit channels in collision models. *J. Phys. B: At. Mol. Opt. Phys.*, 45:154006, 2012.

[28] S. Lloyd. Universal quantum simulators. *Science*, 273:1073, 1996.

[29] B. M. Terhal, I. L. Chuang, D. P. DiVincenzo, M. Grassl, and J. A. Smolin. Simulating quantum operations with mixed environments. *Phys. Rev. A*, 60:881, 1999.

[30] B. M. Terhal and D. P. DiVincenzo. Problem of equilibration and the computation of correlation functions on a quantum computer. *Phys. Rev. A*, 61:022301, 2000.

[31] D. Bacon, A. M. Childs, I. L. Chuang, J. Kempe, D. W. Leung, and X. Zhou. Universal simulation of Markovian quantum dynamics. *Phys. Rev. A*, 64:062302, 2001.

[32] K. Temme, T. J. Osborne, K. G. Vollbrecht, D. Poulin, and F. Verstraete. Quantum Metropolis Sampling. *Nature*, 471:87, 2011.

[33] D. Poulin and P. Wocjan. Sampling from the thermal quantum Gibbs state and evaluating partition functions with a quantum computer. *Phys. Rev. Lett.*, 103:220502, 2009.

[34] C. Chiang and P. Wocjan. Quantum algorithm for preparing thermal Gibbs states - detailed analysis. *NATO Science for Peace and Security Series D: Information and Communication Security*, 26:138–147, 2010.

[35] M. Yung and A. Aspuru-Guzik. A quantum quantum Metropolis algorithm. *Proc. Natl. Acad. Sci. USA*, 109:754, 2012.

[36] M. Kliesch, T. Barthel, C. Gogolin, M. J. Kastoryano, and J. Eisert. Dissipative Quantum Church-Turing Theorem. *Phys. Rev. Lett.*, 107:120501, 2011.

[37] T. Barthel and M. Kliesch. Quasilocality and efficient simulation of Markovian quantum dynamics. *Phys. Rev. Lett.*, 108:230504, 2012.

[38] D. G. Tempel and A. Aspuru-Guzik. The Kitaev-Feynman clock for open quantum systems. *New J. Phys.*, 16:113066, 2014.

[39] R. Di Candia, J. S. Pedernales, A. del Campo, E. Solano, and J. Casanova. Quantum simulation of dissipative processes without reservoir engineering. *Sci. Rep.*, 5:9981, 2015.

[40] D. S. Wang, D. W. Berry, M. C. de Oliveira, and B. C. Sanders. Solovay-Kitaev decomposition strategy for single-qubit channels. *Phys. Rev. Lett.*, 111:130504, 2013.

[41] D. S. Wang and B.C. Sanders. Quantum circuit design for accurate simulation of qudit channels. *New J. Phys.*, 17:043004, 2015.

[42] H. Wang, S. Ashhab, and F. Nori. Quantum algorithm for simulating the dynamics of an open quantum system. *Phys. Rev. A*, 83:062317, 2011.

[43] R. Sweke, I. Sinayskiy, and F. Petruccione. Simulation of single qubit open quantum systems. *Phys. Rev. A*, 90:022331, 2014.

[44] S. Lloyd and L. Viola. Engineering quantum dynamics. *Phys. Rev. A (R)*, 65:010101, 2001.

[45] M. Müller, K. Hammerer, Y. L. Zhou, C. F. Roos, and P. Zoller. Simulating open quantum systems: from many-body interactions to stabilizer pumping. *New J. Phys.*, 13:085007, 2011.

[46] P. Schindler, M. Müller, D. Nigg, J. T. Barreiro, E. A. Martinez, M. Hennrich, T. Monz, S. Diehl, P. Zoller, and R. Blatt. Quantum simulation of dynamical maps with trapped ions. *Nature Physics*, 9:361, 2013.

[47] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C.F. Roos, P. Zoller, and R. Blatt. An open-system quantum simulator with trapped ions. *Nature*, 470:486, 2011.

[48] H. Weimer, M. Müller, H. P. Büchler, and I. Lesanovsky. Digital quantum simulation with Rydberg atoms. *Quant. Inf. Proc.*, 10:885, 2011.

[49] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H. P. Büchler. A Rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[50] C. M. Herdman, K. C. Young, V. W. Scarola, M. Sarovar, and K. B. Whaley. Stroboscopic generation of topological protection. *Phys. Rev. Lett.*, 104:230501, 2010.

[51] K. C. Young, M. Sarovar, J. Aytac, C. M. Herdman, and K. B. Whaley. Finite temperature quantum simulation of stabilizer Hamiltonians. *J. Phys. B: At. Mol. Opt. Phys.*, 45:154012, 2012.

[52] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 2000.

[53] W. F. Stinespring. Positive functions on C^*-algebras. *Proc. Am. Math. Soc.*, 6:211, 1955.

[54] J. Watrous. Notes on super-operator norms induced by Schatten norms. *Quantum Information and Computation*, 5:58, 2005.

[55] H. F. Trotter. On the product of semi-groups of operators. *Proc. Amer. Math. Soc.*, 10:545, 1959.

[56] M. Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Phys. Lett. A*, 146:319, 1990.

[57] M. Suzuki. General theory of fractal path integrals with applications to manybody theories and statistical physics. *J. Math. Phys.*, 32:400, 1991.

[58] A. Papageorgiou and C. Zhang. On the efficiency of quantum algorithms for Hamiltonian simulation. *Quant. Inf. Proc.*, 11:541, 2012.

[59] N. Wiebe, D. Berry, P. Høyer, and B. C. Sanders. Higher order decompositions of ordered operator exponentials. *J. Phys. A: Math. Theor.*, 43:065203, 2010.

[60] W. Fulton and J. Harris. *Representation Theory. A First Course*. Springer-Verlag, 1991.

[61] J. M. Lee. *Introduction to Smooth Manifolds*. Springer-Verlag, 2013.

Chapter 4

Digital quantum simulation of many-body non-Markovian dynamics

We present an algorithmic method for the digital quantum simulation of many-body locally-indivisible non-Markovian open quantum systems. It consists of two parts: Firstly, a Suzuki-Lie-Trotter decomposition of the global system propagator into the product of subsystem propagators, which may not be quantum channels, and secondly, an algorithmic procedure for the implementation of the subsystem propagators through unitary operations and measurements on a dilated space. By providing rigorous error bounds for the relevant Suzuki-Lie-Trotter decomposition, we are able to analyse the efficiency of the method, and connect it with an appropriate measure of the local indivisibility of the system. In light of our analysis, the proposed method is expected to be experimentally achievable for a variety of interesting cases.

This chapter has been been previously published in [1].

4.1 Introduction

All quantum systems are invariably in contact with an environment to some extent. Therefore, the development of tools for the study of such open quantum systems, undergoing non-unitary dynamics as a result of system-environment interactions, is of importance for understanding a rich variety of phenomena [2, 3]. Historically, effort has been focused on studying Markovian open quantum systems, whose dynamics is described by master equations in the Gorini, Kossakowski, Sudarshan and Lindblad (GKSL) form [2–4]. However, recently there has been an explosion of interest in open quantum systems beyond the Markovian regime, in which, since the typical assumptions made in deriving GKSL master equations are no longer valid, more complex, history-dependent, descriptions of the system dynamics are necessary [5–7].

In particular, the study of non-Markovian open quantum systems promises to allow us to better understand the nature of dissipation and decoherence [2–12], thermalisation and equilibration [13,14], non-equilibrium phase transitions [15,16] and transport phenomena in strongly correlated [17–19] and biological systems [20–26]. Furthermore, within the Markovian context, it has been shown that dissipation and decoherence, traditional enemies of quantum information processing, can be exploited as a resource for quantum computation [27–29], the preparation of topological phases [30–32] and the preparation of entangled states [33, 34]. In this sense, it is desirable to understand the extent to which these protocols are robust against relaxation of the strict assumptions involved in this setting.

Simulations on controllable quantum devices promise to be one of the most effective tools for the study of open quantum systems. While a plethora of methods have been developed for the simulation of Markovian open quantum systems, on a wide variety of quantum devices [35–50], there have only recently begun to emerge proposals for either classical [51–54] or quantum [29, 55–57] simulation of non-Markovian open quantum systems. If one has knowledge of certain properties of the environment, then one of the most natural approaches is through methods of embedding non-Markovian open quantum systems in larger Markovian systems [7, 58–60], which can then be simulated through any of the available methods. However, inspired by the recent success of digital quantum simulations in a variety of contexts [61–63], largely based on "Trotterization" of the system's dynamics [64–66], one may wonder about the applicability of these digital methods to a class of many-body non-Markovian dynamics, to which they appear well suited.

In this work, we present a method for the digital quantum simulation of many-body

k-local, locally-indivisible non-Markovian open quantum systems, rigorously defined in Section 4.2. The first part of this method, described in Section 4.3, consists in a Suzuki-Lie-Trotter (SLT) decomposition [64–67] of the global system propagator into the product of local propagators, which due to the local-indivisibility of the system, may not be quantum channels. Generalising the work of Ref. [35] to this context, we provide a rigorous error bound for such an SLT decomposition, allowing us to study the efficiency of the digital method. Importantly, as discussed in Section 4.3, we cannot expect to obtain an efficient method for an arbitrary non-Markovian open quantum system, and as such the primary aim of this analysis is to understand how the efficiency of the method depends on appropriate measures of the indivisibility of the system of interest.

The second part of the method consists in an algorithmic procedure for the implementation of Hermiticity- and trace-preserving maps which are not quantum channels. Specifically, inspired by the notion of quantum instruments [68, 69], we show in Section 4.4 how any such map may be algorithmically implemented through unitary operations and measurements on a dilated space. In Section 4.5, we then combine the results of Sections 4.3 and 4.4 to provide a complete method for the digital algorithmic simulation of k-local, locally-indivisible, non-Markovian open quantum systems. Furthermore, we provide in Section 4.5 a detailed analysis of the efficiency of this method, which then allows for an assessment of whether a particular system may be feasibly simulated, given a specified set of resources. In light of this analysis, it is expected that the proposed method should be experimentally achievable for a variety of interesting cases, in particular those which are weakly indivisible with respect to the measures we define. Finally, in Section 4.6 we summarise our results and present an outlook on future directions.

4.2 Setting

We consider finite lattices Λ, consisting of N lattice sites so that $|\Lambda| = N$. With each $x \in \Lambda$ there exists an associated finite Hilbert space $\mathcal{H}_x \simeq \mathbb{C}^{d_x}$, and we define $\mathcal{H}_X = \bigotimes_{x\in X} \mathcal{H}_x$ for all subsets $X \subset \Lambda$, and $\mathcal{H} \equiv \mathcal{H}_\Lambda$. For simplicity, we assume that $d_x = d$ for all $x \in \Lambda$. We denote the space of all bounded linear operators $A : \mathcal{H} \to \mathcal{H}$ as $\mathcal{B}(\mathcal{H})$, and given $A \in \mathcal{B}(\mathcal{H})$, we define the support of A, denoted $\mathrm{supp}(A)$, as the smallest subset $X \subset \Lambda$ for which there exists a non-trivial $A_X \in \mathcal{B}(\mathcal{H}_X)$ such that $A = A_X \otimes \mathbb{1}_{\Lambda/X}$. For any $X \subset \Lambda$, $\mathcal{B}_X(\mathcal{H}) \equiv \{A \in \mathcal{B}(\mathcal{H}) | \mathrm{supp}(A) \subset X\}$ denotes the space of all bounded linear operators on $\mathcal{H}$ with support contained in X. Given a Liouvillian $\mathcal{L} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}) \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, the support of $\mathcal{L}$ is given by $\mathrm{supp}(\mathcal{L}) \equiv \bigcup\{X \subset \Lambda | \mathcal{B}_{\Lambda/X}(\mathcal{H}) \subset \ker(\mathcal{L})\}$, which is the set of sites on which $\mathcal{L}$ generates a non-trivial time evolution, and $\mathbb{L}_X = \{\mathcal{L} \in$

$\mathcal{B}(\mathcal{B}(\mathcal{H}))|\text{supp}(\mathcal{L}) \subset X\}$ is the set of Liouvillians with support in X

We are interested in k-local open many-body quantum systems described by time-local master equations. These are systems whose dynamics satisfies

$$\frac{d}{dt}\rho(t) = \mathcal{L}(t)[\rho(t)] = \sum_{Z\subset\Lambda} \mathcal{L}_Z(t)[\rho(t)], \tag{4.1}$$

for some piece-wise continuous time-local Liouvillian $\mathcal{L} : \mathbb{R}^+ \to \mathcal{B}(\mathcal{B}(\mathcal{H}))$, which can be written as the sum of strictly k-local terms $\mathcal{L}_Z : \mathbb{R}^+ \to \mathbb{L}_Z$, with $Z \subset \Lambda$. Here, strict k-locality means that $|Z| \leq k$ for all $\mathcal{L}_Z$ such that $\mathcal{L}_Z(t) \neq 0$ for all t - i.e. each $\mathcal{L}_Z$ term of the Liouvillian acts non-trivially on at most k subsystems. Given a system defined by Eq. (4.1), we denote by $K = |\{\mathcal{L}_Z(t)|\mathcal{L}_Z(t) \neq 0\}| \leq N^k$, the number of strictly k-local terms in the decomposition of $\mathcal{L}$. Labelling the K non-trivial strictly k-local Liouvillians then allows us to redefine Eq. (4.1) as

$$\frac{d}{dt}\rho(t) = \mathcal{L}(t)[\rho(t)] = \sum_{i=1}^{K} \mathcal{L}_i(t)[\rho(t)]. \tag{4.2}$$

We then define the system propagators as the family of superoperators $\{T_{\mathcal{L}}(t,s)\}$ satisfying $\rho(t) = T_{\mathcal{L}}(t,s)\rho(s)$, for all $t \geq s \geq 0$. These propagators uniquely solve the initial value problem

$$\frac{d}{dt}T_{\mathcal{L}}(t,s) = \mathcal{L}(t)T_{\mathcal{L}}(t,s), \qquad T_{\mathcal{L}}(s,s) = \mathbb{1}. \tag{4.3}$$

In addition, for each $i \in [1,K]$, we define the *local* propagators $\{T_{\mathcal{L}_i}(t,s)\}$ as the family of superoperators which uniquely solve the initial value problem

$$\frac{d}{dt}T_{\mathcal{L}_i}(t,s) = \mathcal{L}_i(t)T_{\mathcal{L}_i}(t,s), \qquad T_{\mathcal{L}_i}(s,s) = \mathbb{1}. \tag{4.4}$$

In Ref. [35], the digital simulation of such systems has been considered, but in the case of Markovian many-body open quantum systems, where each strictly k-local Liouvillian can be written in the GKSL form [2–4]. More specifically, where

$$\mathcal{L}_i(t)[\cdot] = -i[H_i(t), \cdot] + \sum_{j=1}^{d^k} \gamma_{i,j}(t)\mathcal{D}(L_{i,j}(t))[\cdot], \tag{4.5}$$

with

$$\mathcal{D}(L_{i,j}(t))[\cdot] = L_{i,j}(t) \cdot L_{i,j}(t)^\dagger - \frac{1}{2}\{L_{i,j}(t)^\dagger L_{i,j}(t), \cdot\}_+$$

and with $\gamma_{i,j}(t) \geq 0$, for all $i \in [1, K]$, $j \in [1, d^k]$ and $t \in \mathbb{R}^+$. In this case, the system is called *locally divisible*, meaning that, for all $i \in [1, K]$, and for all $0 \leq s \leq t \in \mathbb{R}^+$, the local propagator $T_{\mathcal{L}_i}(t, s)$ is a quantum channel (completely positive trace preserving map) [4, 6]. In this work, we aim to go beyond this case and consider *locally indivisible* dynamics described by time-local master equations, i.e. dynamics generated by a k-local Liouvillian as in Eq. (4.1), but for which $T_{\mathcal{L}_i}(t, s)$ may not be a quantum channel for all $i \in [1, K]$ and for all $0 \leq s \leq t \in \mathbb{R}^+$. Time-local master equations of this type are capable of describing many non-Markovian systems [5–7], and the simplest example of such a process is given by a system whose dynamics is described by Eq. (4.5), but with dissipation rates $\gamma_{i,j}(t)$ which are not necessarily positive for all i, j and t [2,4]. We also note that we do not attempt to address here the question of which k-local Liouvillians generate legitimate completely positive dynamics, as the simulation method given here is valid even in the case when the global dynamics is not completely positive.

In order to quantify errors made within the presented simulation scheme, we utilise the $(1 \to 1)$-norm for super-operators, where in general the $(p \to q)$-norm of a super-operator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$ is defined as [68]

$$||T||_{p\to q} := \sup_{||A||_p=1} ||T(A)||_q. \tag{4.6}$$

The $(p \to q)$-norm defined above is induced from the Schatten p-norm of an operator, defined as $||A||_p := \big(\mathrm{tr}(|A|^p)\big)^{\frac{1}{p}}$, for all $A \in \mathcal{B}(\mathcal{H})$. Notice that the definition corresponds up to a factor of $1/2$ with the trace distance, $\mathrm{dist}(\rho, \sigma) := \sup_{0\leq A\leq 1} \mathrm{tr}\big(A(\rho - \sigma)\big)$, arising from a physical motivation of operational distinguishability of quantum states [69], which is relevant when working in the Schrödinger picture.

4.3 Trotter decomposition of locally indivisible dynamics

In line with conventional digital quantum simulation techniques [61–63], our strategy for the simulation of locally indivisible dynamics will be to implement $T_{\mathcal{L}}(t, 0)$ through stroboscopic implementations of small time slices of the strictly k-local propagators, formalised via a Suzuki-Lie-Trotter (SLT) decomposition of $T_{\mathcal{L}}(t, 0)$ [64–66]. In order to evaluate the performance of this strategy, it is necessary to obtain error bounds on the relevant SLT decomposition. To this end, we aim to generalise the results obtained in Ref. [35] to the case of locally indivisible systems. It is essential to note that we *cannot* expect to obtain an efficient simulation method for arbitrary non-Markovian systems [35]. This is largely due to the fact that in many non-Markovian situations, in which the system

of interest is strongly coupled to an environment, the dominant contribution to the dynamics arises from the total system plus environment combination, and it is therefore unrealistic to expect efficient scaling with respect to the size of only the measured system of interest. As an illustration, if efficient simulation of arbitrary non-Markovian dynamics were possible, then one could in principle imagine efficiently simulating an extremely complicated process or computation occurring in the environment, whose results can flow back into the system of interest due to the non-Markovian character of the environment.

In light of these considerations, the primary goal of our analysis will be to provide an error bound for a relevant SLT decomposition. This will allow us to understand how the efficiency of the SLT-based digital simulation method depends on various "measures of local indivisibility" of the simulated system. Then, given a particular locally indivisible non-Markovian system, this would permit an experimentalist the ability to determine whether the resources required for such a simulation are practically feasible.

To this end, given a super-operator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, let us define the check function

$$\mathrm{Ch}\big(T\big) = \begin{cases} 0, & \text{if } T \text{ is a quantum channel,} \\ 1, & \text{otherwise.} \end{cases}$$

Note that, given a particular super-operator $T \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, the value of Ch(T) can in principle be determined through construction and analysis of the Choi-Jamiolkowski state [69]. This procedure will be practical provided that the dimension of the Hilbert space $\mathcal{H}$ is relatively small. Now, given a k-local system specified by a Liouvillian $\mathcal{L}$, as in Eqs. (4.1) and (4.2), let us consider a fixed final time $t \geq 0$ and divide the time interval $[0, t]$ into m subintervals of length $\Delta t \equiv t/m$, as required by any SLT scheme. Given these values of t and m, let us then define $T_i^j \equiv T^j_{\mathcal{L}_i}(tj/m, t(j-1)/m)$ for $i \in [1, K]$ and $j \in [1, m]$. This leads to the following "measures of local indivisibility",

$$\tilde{N}_i^m = \sum_{j=1}^{m} \mathrm{Ch}\Big(T_i^j\Big) \leq m, \tag{4.7}$$

$$\hat{N}_j^m = \sum_{i=1}^{K} \mathrm{Ch}\Big(T_i^j\Big) \leq K. \tag{4.8}$$

These quantities are defined such that $\tilde{N}_i^m$ measures the number of time intervals in the SLT scheme for which the propagator T_i^j is not a quantum channel, while $\hat{N}_j^m$ measures the number of local propagators which are not quantum channels during some given time interval $[tj/m, t(j-1)/m]$. Note that, as a consequence of strict k-locality, it will

generally be possible to calculate these measures on a conventional computer for realistic systems in which k is small and independent of the total system size N. Given these quantities, we then define

$$\tilde{N}^m = \max_{1\leq i\leq K} \left[\tilde{N}_i^m\right] \leq m, \tag{4.9}$$

$$\hat{N}^m = \max_{1\leq j\leq m} \left[\hat{N}_j^m\right] \leq K. \tag{4.10}$$

Clearly, for locally divisible dynamics $\tilde{N}^m = \hat{N}^m = 0$. Note that all quantities defined so far depend implicitly on the discretisation factor m, and that naively it is possible to bound $\tilde{N}^m$ from above by m, which occurs in the worst case scenario when all local propagators are not quantum channels - i.e. when the system is locally "totally indivisible". However, it is desirable to find a tighter upper bound than this and, to this end, we define

$$t_i^{\mathrm{ID}} = \lim_{m\to\infty} \tilde{N}_i^m \Delta t = \lim_{m\to\infty} \frac{\tilde{N}_i^m t}{m} \leq t, \tag{4.11}$$

and $t^{\mathrm{ID}} = \max_{1\leq i\leq K} t_i^{\mathrm{ID}}$. Furthermore, let us define C_i^m, the number of "disjoint indivisible intervals due to $\mathcal{L}_i$", via $C_i^m = \sum_{j=1}^{m-1} \mathrm{Seq}\big(T_i^j, T_i^{j+1}\big)$, where

$$\mathrm{Seq}\big(T_i^j, T_i^{j+1}\big) = \begin{cases} 1 & \mathrm{Ch}(T^j) = 0 \wedge \mathrm{Ch}(T^{j+1}) = 1 \\ 0 & \text{otherwise.} \end{cases}$$

In addition, let us define $C_i = \lim_{m\to\infty} C_i^m$, and $\tilde{C} = 2\max_{1\leq i\leq K} C_i$, so that, at this stage, it is possible to see that

$$\tilde{N}^m \leq \min\Big(\frac{t^{\mathrm{ID}}}{\Delta t} + \tilde{C}, m\Big). \tag{4.12}$$

Finally, we do not want to specify a priori that our local equations of motion are in a specific form, so we specify the local quantity

$$\beta = \sup_{0\leq s\leq t} \Big(\max_{1\leq i\leq K} \big(||\mathcal{L}_i(s)||_{1\to 1}\big)\Big), \tag{4.13}$$

which allows us to state the following theorem:

Theorem 4.1. *Given a system whose dynamics is described by Eqs.* (4.1) *and* (4.2)*, the error of a first order SLT decomposition of a time evolution up to time* t *in* m *steps*

is bounded by,

$$\left|\left|T_{\mathcal{L}}(t,0)-\prod_{j=1}^{m}\prod_{i=1}^{K}T_i^j\right|\right|_{1\to 1}\leq E(m,K,\beta,t,\tilde{N}^m,\hat{N}^m),$$

where

$$\begin{aligned}E&=\frac{K^2\beta^2t^2}{m}e^{(3+K(2+\tilde{N}^m)+K\min[m,K\tilde{N}^m]+\hat{N}^m)\beta(t/m)}\\&\leq\frac{K^2\beta^2t^2}{m}e^{(3+[3+\tilde{C}]K+\tilde{C}K^2)\beta(t/m)}e^{(K+K^2)t^{\mathrm{ID}}\beta}.\end{aligned}\tag{4.14}$$

The proof of Theorem 4.1 can be found in Appendix 4.7.1. Note that we also have the following important corollary:

Corollary 4.1. *Given*

$$0\leq\epsilon\leq\frac{(2K^2\beta t\ln(2)e^{(K+K^2)t^{\mathrm{ID}}\beta})}{(3+[3+\tilde{C}K+\tilde{C}K^2])},\tag{4.15}$$

then

$$\left|\left|T_{\mathcal{L}}(t,0)-\prod_{j=1}^{m}\prod_{i=1}^{K}T_i^j\right|\right|_{1\to 1}\leq\epsilon,\tag{4.16}$$

provided $m\geq 2K\beta^2t^2e^{(K+K^2)t^{\mathrm{ID}}\beta}/\epsilon$.

From Corollary 4.1 (also proven in Appendix 4.7.1), it is clear that, as expected, in the case of locally indivisible dynamics, the number of strictly k-local propagators scales exponentially in K, and therefore potentially exponentially in N because of the the relationship $K\leq N^k$, which is not necessarily saturated. However, note that, when the dynamics is locally divisible, we have that $t^{\mathrm{ID}}=0$. Therefore, the number of local propagators scales polynomially in N, reproducing the results of Ref. [35]. We also note that it is possible to replace the strictly k-local propagators T_i^j, with the strictly k-local propagators $T_i^{j,\mathrm{avg}}=\exp(\Delta t\mathcal{L}_i^{j,\mathrm{avg}})$ of the *averaged* Liouvillians,

$$\mathcal{L}_i^{j,\mathrm{avg}}=\frac{m}{t}\int_{t(j-1)/m}^{tj/m}\mathcal{L}_i(s)ds,\tag{4.17}$$

without changing the scaling of the SLT error [35]. Furthermore, when the Liouvillian is in GKSL form given in Eq. (4.5), but possibly with negative dissipation rates at certain

time, the SLT error can be expressed in terms of

$$\tilde{\beta} = \sup_{0\leq s\leq t} \Big(\max_{1\leq i\leq K} \big(\max_{1\leq j\leq d^k} \big(||L_{i,j}(s)||_\infty \big) \Big), \tag{4.18}$$

the largest operator norm of the Lindblad operators [35].

At this stage, the strategy in the locally divisible case is clear, as each strictly k-local propagator, which is a quantum channel, can be implemented through a unitary Stinespring dilation requiring an ancilla space whose dimension depends only on k and d [35,68,69]. However, in the locally indivisible case, *not all* local propagators are quantum channels (or even positive maps) and therefore, any realisation of an SLT scheme, such as the one provided by Theorem 4.1, requires a method for the implementation of non-positive maps.

4.4 Algorithmic implementation of non-positive maps

In this section, we construct a method to implement the strictly k-local propagators emerging from the SLT decomposition given in Theorem 4.1, which are *not* quantum channels. In particular we restrict ourselves to Hermiticity- and trace preserving (HPTP), but not necessarily positive maps. Such maps would for instance arise in the case of a k-local system specified by a Liouvillian in GKSL form, but with negative dissipation rates for certain time intervals. As mentioned briefly in Section 4.3, we stress that, due to *strict* k-locality of these propagators, the support of these maps for realistic many-body systems will be sufficiently small, so that it is possible to obtain their spectrum either analytically or numerically.

Given an HPTP map $T : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, there always exists completely positive, but not necessarily trace preserving (CPnTP), maps $T^{(0)}$ and $T^{(1)}$ such that $T = T^{(0)} - T^{(1)}$. This can be proven via the spectral decomposition of the associated Choi-Jamiolkowski state [68]. As a result, we see that, if one can implement the CPnTP maps $T^{(0)}$ and $T^{(1)}$, then one can implement T algorithmically. Specifically, given any initial state $\rho \in \mathcal{B}(\mathcal{H})$ and any observable $A \in \mathcal{B}(\mathcal{H})$, and defining $\rho' = T(\rho)$, we have

$$\begin{aligned}
\langle A \rangle_{\rho'} &\equiv \mathrm{tr}[A\rho'] \\
&= \mathrm{tr}[AT^{(0)}(\rho)] - \mathrm{tr}[AT^{(1)}(\rho)] \\
&= \mathrm{tr}[A\rho'_{(0)}] - \mathrm{tr}[A\rho'_{(1)}] \\
&= \langle A \rangle_{\rho'_{(0)}} - \langle A \rangle_{\rho'_{(1)}},
\end{aligned}$$

i.e. expectation values of the desired state ρ' can be algorithmically reconstructed from the expectation values of the outputs $\rho'_{(0)}$ and $\rho'_{(1)}$ of CPnTP maps $T^{(0)}$ and $T^{(1)}$. In light of this, we are able to restrict our attention to constructing a method for the implementation of CPnTP maps.

To this end, let us consider a CPnTP map $T^{(x)} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$, with $\mathcal{H}_S \simeq \mathbb{C}^d$, and Kraus representation $\{K_x^{(i)}\}|_{i=1}^{d_x}$, where $d_x \leq d^2$. Furthermore, let us define the "gauge" G_x via

$$G_x = \sum_{i=1}^{d_x} (K_x^{(i)})^\dagger K_x^{(i)}. \tag{4.19}$$

As $T^{(x)}$ is not trace preserving, we know that $G_x \neq \mathbb{1}$. At this stage, we can identify two cases: case 1 is when the gauge G_x is sub-normalised, $\mathbb{1} - G_x \geq 0$, and case 2 is when the gauge G_x is not sub-normalised. More specifically, let us define $g_x = \max\big[\text{spec}(G_x)\big]$. From the structure of G_x (Hermitian and positive semi-definite), we know that that $g_x \geq 0$. Then, we are in case 1 when $g_x \leq 1$, and in case 2 otherwise. If we are in case 2, then we can define the "renormalised" map $\hat{T}^{(x)}$ via Kraus operators $\{\hat{K}_x^{(i)}\}|_{i=1}^{d_x}$, where $\hat{K}_x^{(i)} = (1/\sqrt{g_x})K_x^{(i)}$. Let us denote the gauge of $\hat{T}^{(x)}$ as $\hat{G}_x$, and note that

$$\hat{G}_x = \frac{1}{g_x} G_x, \tag{4.20}$$

so that $\hat{G}_x$ is sub-normalised by construction. Furthermore, note that for all $\rho \in \mathcal{B}(\mathcal{H}_S)$, we have that

$$T^{(x)}(\rho) = g_x \hat{T}^{(x)}(\rho), \tag{4.21}$$

so that, if we can implement $\hat{T}^{(x)}$, then $T^{(x)}$ can be implemented algorithmically.

Given this setup, the problem considered here is the following:

Problem: *Given a CPnTP map $T^{(x)} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$, with $\mathcal{H}_S \simeq \mathbb{C}^d$, and an observable $A \in \mathcal{B}(\mathcal{H}_S)$, and given multiple copies of $\rho \in \mathcal{B}(\mathcal{H}_S)$ (i.e. from some standard preparation procedure or preliminary circuit), describe an algorithmic procedure which yields $\langle A \rangle_{\rho'_{(x)}}$, where*

$$\langle A \rangle_{\rho'_{(x)}} = \text{Tr}[A\rho'_{(x)}], \tag{4.22}$$

with $\rho'_{(x)} = T^{(x)}(\rho)$.

If we first restrict ourselves to case 1, then the protocol described below, inspired by the notion of quantum instruments [68, 69], provides a solution to the problem.

Step 1: Construct $K_x^{(\infty)}$ such that

$$G_x + (K_x^{(\infty)})^\dagger K_x^{(\infty)} = \mathbb{1} \tag{4.23}$$

Note that the existence of $K_x^{(\infty)}$ is guaranteed by virtue of the assumed sub-normalisation of G_x. Furthermore, note that through the inclusion of the additional Kraus operator $K_x^{(\infty)}$, we can extend $T^{(x)}$ to a map $T_e^{(x)}$ which is both completely positive *and* trace preserving.

Step 2: Construct the unitary operator $U_x \in \mathcal{B}(\mathbb{C}^{d_x+1} \otimes \mathcal{H}_S)$ via

$$U_x = \begin{pmatrix} K_x^{(1)} & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ K_x^{(d_x)} & \vdots & \vdots & \vdots \\ K_x^{(\infty)} & \vdots & \vdots & \vdots \end{pmatrix}. \tag{4.24}$$

Note that U_x is precisely the Stinespring dilation of $T_e^{(x)}$, the trace preserving extension of $T^{(x)}$, with dilation space $\mathcal{H}_{E_x} \simeq \mathbb{C}^{d_x+1}$.

Step 3: Define the set of projectors $P^{(x)} = \{P_1^{(x)}, P_2^{(x)}\}$ via

$$P_1^{(x)} = \sum_{j=1}^{d_x} \sum_{k=1}^{d} |j,k\rangle\langle j,k| \tag{4.25}$$

$$P_2^{(x)} = \sum_{k=1}^{d} |d_x+1,k\rangle\langle d_x+1,k| \tag{4.26}$$

where $\{|j,k\rangle\}|_{j=1}^{d_x+1}|_{k=1}^{d}$ is the basis for $\mathcal{H}_{E_x} \otimes \mathcal{H}_S$ in which U_x is given.

Step 4: Note now that, if one starts with the state $|1\rangle\langle 1| \otimes \rho$, applies the unitary U_x, and then performs the measurement defined by $P^{(x)}$, then the probability of obtaining "measurement outcome 1" is given by

$$\Pr_x(1) \equiv \mathrm{Tr}[P_1^{(x)} U_x(|1\rangle\langle 1| \otimes \rho) U_x^\dagger P_1^{(x)}], \tag{4.27}$$

in which case the reduced state of the system is

$$\rho' = \mathrm{Tr}_{E_x}\left[\frac{P_1^{(x)} U_x(|1\rangle\langle 1| \otimes \rho) U_x^\dagger P_1^{(x)}}{\mathrm{Tr}[P_1^{(x)} U_x(|1\rangle\langle 1| \otimes \rho) U_x^\dagger P_1^{(x)}]}\right]. \tag{4.28}$$

Furthermore, note that by construction

$$T^{(x)}(\rho) = \mathrm{Tr}_{E_x}\big[P_1^{(x)} U_x(|1\rangle\langle 1| \otimes \rho) U_x^\dagger P_1^{(x)}\big], \tag{4.29}$$

so that we can rewrite Eq. (4.28), with the help of Eqs. (4.27) and (4.29), as

$$\rho' = \frac{T^{(x)}(\rho)}{\mathrm{Pr}_x(1)}, \tag{4.30}$$

or alternatively

$$\rho'_{(x)} = \mathrm{Pr}_x(1)\rho'. \tag{4.31}$$

Step 5 (case 1): Finally, note that via Eq. (4.31)

$$\begin{aligned} \langle A\rangle_{\rho'_{(x)}} &= \mathrm{Tr}[A\rho'_{(x)}] \\ &= \mathrm{Pr}_x(1)\mathrm{Tr}[A\rho'] \\ &= \mathrm{Pr}_x(1)\langle A\rangle_{\rho'}. \end{aligned} \tag{4.32}$$

Now, $\langle A\rangle_{\rho'}$ can be obtained from the state ρ', which in turn can be produced through unitary evolution of a dilated system via U_x, followed by the measurement $P^{(x)}$, and postselecting on "measurement outcome 1". Furthermore, the constant $\mathrm{Pr}_x(1)$ can be asymptotically obtained through repetitions of the process of unitary evolution and measurement (with the same initial state each time), by recording the proportion of "measurement outcome 1" to "measurement outcome 2". To sum up, through unitary evolutions and measurements of a dilated system, it is possible to obtain algorithmically the desired value of $\langle A\rangle_{\rho'}$, provided the assumption of sub-normalisation holds.

Now, let us consider the case when sub-normalisation is not satisfied, i.e. case 2. In this case, we can repeat steps 1 through 4, not for the map $T^{(x)}$, but for the "renormalised" map $\hat{T}^{(x)}$. Finally, we slightly modify step 5, where the hats now just indicate the relevant object defined from $\hat{T}^{(x)}$, as opposed to $T^{(x)}$:

Step 5 (case 2): Note that

$$\begin{aligned} \langle A\rangle_{\rho'_{(x)}} &= \mathrm{Tr}[A g_x \hat{T}^{(x)}(\rho)] \\ &= g_x \mathrm{Pr}_x(1)\mathrm{Tr}[A\hat{\rho}'] \\ &= g_x \hat{\mathrm{Pr}}_x(1)\langle A\rangle_{\hat{\rho}'}. \end{aligned} \tag{4.33}$$

Now, $\langle A\rangle_{\hat{\rho}'}$ can be obtained from the state $\hat{\rho}'$ which, again, can be produced through

unitary evolution of a dilated system via $\hat{U}_x$, followed by the measurement $P^{(x)}$. Again, the constant $\hat{\Pr}_x(1)$ can be obtained asymptotically through repetitions of the process of unitary evolution and measurement.

Clearly, for this protocol to work, it is necessary to obtain the value of the constant $\Pr_x(1)$. In a practical setting, it is necessary to construct some estimator $\Pr_x^{N_T}(1)$ for $\Pr_x(1)$ from a finite number of measurements N_T. The error in approximating the desired output state $\rho'_{(x)} = \Pr_x(1)\rho'$ with $\tilde{\rho}'_{(x)} = \Pr_x^{N_T}(1)\rho'$ is then given by

$$||\rho'_{(x)} - \tilde{\rho}'_{(x)}|| = |\Pr_x(1) - \Pr_x^{N_T}(1)|||\rho'|| \tag{4.34}$$

$$= |\Pr_x(1) - \Pr_x^{N_T}(1)|. \tag{4.35}$$

Therefore, given some error threshold $\epsilon \geq 0$, it is necessary to determine the minimum number of repetitions of the process of unitary evolution and measurement which are necessary to construct an estimator $\Pr_x^{N_T}(1)$ such that $|\Pr_x(1) - \Pr_x^{N_T}(1)| \leq \epsilon$. Given that the measurement P only has two possible outcomes, this is essentially the problem of constructing a binomial proportion confidence interval.

As discussed in Refs. [70,71], in order to construct an interval with reliable properties for a potentially small number of trials, or a value of $\Pr_x(1)$ which is potentially close to either 0 or 1, it is necessary to use the Wilson score interval [72]. Formally, let us denote the number trials in which measurement outcome 1 is observed as N_1, and define the proportion $\hat{p} = N_1/N_T$. Furthermore, the maximum error associated with our estimator will be associated with some confidence level, given by the z-value of a standard normal distribution, and denoted here as z. The Wilson score interval then prescribes that the best estimate $\Pr_x^{N_T}(1)$ is given by

$$\Pr_x^{N_T}(1) = \frac{\hat{p} + \frac{1}{2N_T}z^2}{1 + \frac{1}{N_T}z^2}, \tag{4.36}$$

with a confidence interval $[\Pr_x^{N_T}(1) - E_z, \Pr_x^{N_T}(1) + E_z]$, where

$$E_z = \frac{z\sqrt{\frac{1}{N_T}\hat{p}(1-\hat{p}) + \frac{1}{4N_T^2}z^2}}{1 + \frac{1}{N_T}z^2}. \tag{4.37}$$

As an example, given a z-value $z = 4.42$, associated with a 99.99% confidence [70], this means that we will have

$$|\Pr_x(1) - \Pr_x^{N_T}(1)| \leq E_z \tag{4.38}$$

99.99% of the times in which such an estimator is constructed. Therefore, given a maximum error tolerance of $\epsilon \geq 0$, one can show, by noting that the right hand side of Eq. (4.37) is maximized for $\hat{p} = 1/2$, that

$$|\mathrm{Pr}_x(1) - \mathrm{Pr}_x^{N_T}(1)| \leq \epsilon, \tag{4.39}$$

with the confidence level associated with z, provided that

$$\frac{N_T^2}{N_T + z^2} \geq \frac{z^2}{4\epsilon^2}. \tag{4.40}$$

Note, from Eqs. (4.36), (4.37) and (4.40), that in the large N_T limit the best estimate is given by $\mathrm{Pr}_x^{N_T}(1) = \hat{p}$, and the condition given by Eq. (4.40) becomes

$$N_T \geq \frac{z^2}{4\epsilon^2}, \tag{4.41}$$

which is what one would expect from using the more intuitive Wald confidence interval [70, 71].

At this stage, we have therefore obtained a complete algorithmic procedure for the approximate implementation of an arbitrary HPTP super-operator. In the following section, we proceed to combine this technique with the results of Section 4.3, in order to formulate a complete procedure for the simulation of k-local locally indivisible dynamics.

4.5 Algorithmic digital simulation of locally indivisible dynamics

In this section, we present an algorithmic digital method for the implementation of

$$\tilde{T} \equiv \prod_{j=1}^{m} \prod_{i=1}^{K} T_i^j, \tag{4.42}$$

with m fixed by Corollary 4.1. In order to develop a concise notation, let us define a multi-index $\gamma = (j, i) \in [1, mK]$, such that $\tilde{T}$ can be rewritten as

$$\tilde{T} = \prod_{\gamma=1}^{mK} T^{\gamma}. \tag{4.43}$$

We stress that the γ indexes the strictly k-local propagators in the SLT decomposition, and does not indicate an exponent. Given this notation, we will then say that T_i^j is the nth non-CP map if T_i^j is non-CP (i.e. $\mathrm{Ch}(T_i^j) = 1$) and $\sum_{\gamma=1}^{(j,i)} \mathrm{Ch}(T^\gamma) = n$. Furthermore, if T^γ is non-CP, but HPTP, as we are assuming all non-CP strictly k-local propagators are, then we denote the decomposition of T^γ into the difference of CPnTP maps, as shown in Section 4.4, via $T^\gamma = T^{\gamma,0} - T^{\gamma,1}$. In addition, it will be useful for us to define $\beta(x,n)$ as the nth element of the binary representation of non-negative integer x, and

$$f_x(T^\gamma) = \begin{cases} T^\gamma, & \text{if } \mathrm{Ch}(T^\gamma) = 0, \\ T^{\gamma,\beta(x,n)}, & \text{if } T^\gamma \text{ is the } n\text{'th non-CP map.} \end{cases}$$

Defining the total number of non-CP maps appearing in the decomposition of $\tilde{T}$ as $\tilde{N}^m_{\mathrm{TOT}} = \sum_{i=1}^K \tilde{N}^m_i$, allows us to define the rth circuit, denoted C_r and consisting only of quantum channels and CPnTP maps, as

$$C_r = \prod_{\gamma=1}^{mK} f_r(T^\gamma), \tag{4.44}$$

where $r \in [0, 2^{\tilde{N}^m_{\mathrm{TOT}}} - 1]$. Finally, defining the parity function $\mathcal{P}$ as

$$\mathcal{P}(r) = \begin{cases} 1, & \text{if the binary representation of} \\ & \quad r \text{ has an odd number of 1's,} \\ 0, & \text{otherwise.} \end{cases}$$

allows us to obtain the expression

$$\tilde{T} = \sum_{r=0}^{2^{\tilde{N}^m_{\mathrm{TOT}}}-1} (-1)^{\mathcal{P}(r)} C_r. \tag{4.45}$$

In essence, Eq. (4.45) shows how $\tilde{T}$ can be implemented algorithmically through the implementation of circuits consisting only of quantum channels and CPnTP maps. In other words, given an initial state $\rho(0)$ and an observable A, and defining $\tilde{\rho}(t) = \tilde{T}(\rho(0))$

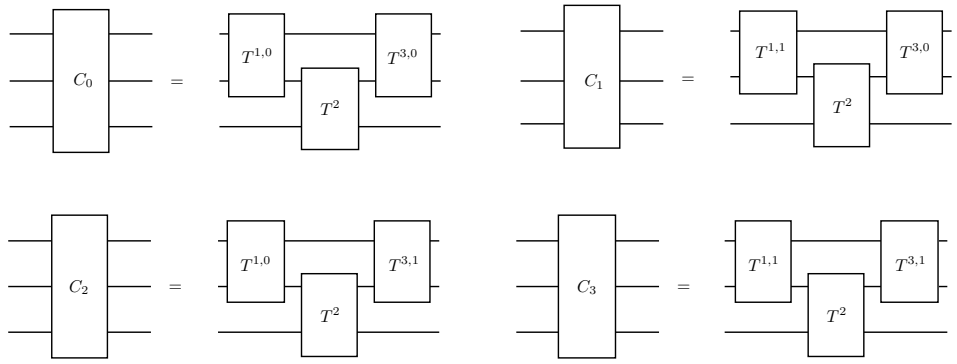

Figure 4.1: Given a 2-local global propagator $\tilde{T} = T^3T^2T^1$, with $\mathrm{Ch}(T^1) = \mathrm{Ch}(T^3) = 1$ and $\mathrm{Ch}(T^2) = 0$, this propagator can be implemented algorithmically through the implementation of the four circuits $\{C_r\}|_{r=0}^3$. Each circuit C_r consists only of quantum channels and CPnTP maps.

and $\rho^{(r)}(t) = C_r(\rho(0))$, it follows from Eq. (4.45) that

$$\begin{aligned}\langle A\rangle_{\tilde{\rho}(t)} &= \mathrm{tr}[A\tilde{\rho}(t)] \\ &= \sum_{r=0}^{2^{\tilde{N}^m_{\mathrm{TOT}}}-1} (-1)^{\mathcal{P}(r)}\mathrm{tr}[A\rho^{(r)}(t)] \\ &= \sum_{r=0}^{2^{\tilde{N}^m_{\mathrm{TOT}}}-1} (-1)^{\mathcal{P}(r)}\langle A\rangle_{\rho^{(r)}(t)},\end{aligned} \tag{4.46}$$

i.e. expectation values of the desired state $\tilde{\rho}(t)$ can be reconstructed from the expectation values of $\rho^{(r)}(t)$, the outputs of circuits C_r.

As an example, illustrated in Fig. 4.1, let us consider a two-local global propagator $\tilde{T} = T^3T^2T^1$ acting on a total system of three sites. Here, T^2 is a quantum channel acting non-trivially on sites 2 and 3, so $\mathrm{Ch}(T^2) = 0$, while T^1 and T^3, acting non-trivially on sites 1 and 2, are not quantum channels, so $\mathrm{Ch}(T^1) = \mathrm{Ch}(T^3) = 1$. In this simple situation. we have that the total number of non-CP maps is two. Therefore, given an initial state $\rho(0)$, the expectation values of the state $\tilde{\rho}(t) = \tilde{T}(\rho(0))$ can be reconstructed algorithmically, via Eq. (4.45), from the states $\rho^r(t) = C_r(\rho(0))$ for $r \in [0:3]$.

At this stage, what remains to be done is to incorporate explicitly into this algorithmic procedure for implementing $\tilde{T}$, the implementation of CPnTP maps within the circuits C_r. To this end, given a CPnTP map $T^{\gamma,i}$, with $i \in \{0,1\}$, let us denote the as-

sociated sub-normalised map as $T_s^{\gamma,i} = (1/g^{\gamma,i})T^{\gamma,i}$ and the associated CPTP extension of $T_s^{\gamma,i}$ as $T_e^{\gamma,i}$. We then denote the unitary Stinespring dilation of $T_e^{\gamma,i}$, constructed as per Eq. (4.24), as $U^{\gamma,i}$. Furthermore, given an arbitrary state ρ, we denote the output of a successful trial by

$$\begin{aligned} A^{\gamma,i}(\rho) &= \frac{\mathrm{tr}_{E^{\gamma,i}}\left[P_1^{\gamma,i}U^{\gamma,i}(|1\rangle\langle 1|\otimes\rho)(U^{\gamma,i})^\dagger P_1^{\gamma,i}\right]}{N^{\gamma,i}(\rho)} \\ &= \frac{T_s^{\gamma,i}(\rho)}{N^{\gamma,i}(\rho)} \\ &= \frac{T^{\gamma,i}(\rho)}{g^{\gamma,i}N^{\gamma,i}(\rho)}, \end{aligned} \tag{4.47}$$

where $P_1^{\gamma,i}$ is defined as per Step 3 of the procedure described in Section 4.4, and we denote the probability of measurement outcome 1 on the input state $|1\rangle\langle 1|\otimes\rho$ by $N^{\gamma,i}(\rho)$. Note at this stage, from Eq. (4.47), that

$$T^{\gamma,i}(\rho) = g^{\gamma,i}N^{\gamma,i}(\rho)A^{\gamma,i}(\rho). \tag{4.48}$$

Now, let us define

$$M_r^\gamma(\rho) = \begin{cases} T^\gamma(\rho), & \text{if } \mathrm{Ch}(T^\gamma) = 0, \\ A^{\gamma,\beta(r,n)}(\rho), & \text{if } T^\gamma \text{ is the } n\text{'th non-CP map.} \end{cases}$$

Given an initial state $\rho(0)$, then

$$\tilde{\rho}^{(r)}(j) = \prod_{\gamma=1}^{j} M_r^\gamma(\rho(0)), \tag{4.49}$$

such that

$$\rho^{(r)}(t) = C_r(\rho(0)) = \tilde{\rho}^{(r)}(mK)\Big(\prod_{\gamma=1}^{mK}\mathcal{G}_r^\gamma\mathcal{N}_r^\gamma\Big), \tag{4.50}$$

where

$$\mathcal{G}_r^\gamma = \begin{cases} 1, & \text{if } \mathrm{Ch}(T^\gamma) = 0, \\ 1, & \text{if } T^{\gamma,\beta(r,n)} \text{is sub-normalised,} \\ g^{\gamma,\beta(r,n)}, & \text{otherwise,} \end{cases}$$

and

$$\mathcal{N}_r^\gamma = \begin{cases} 1, & \text{if } \mathrm{Ch}(T^\gamma) = 0, \\ N^{\gamma,\beta(r,n)}(\tilde{\rho}^r(\gamma-1)), & \text{otherwise.} \end{cases}$$

Note that Eqs. (4.49) and (4.50) formalise the algorithmic procedure to implement the circuits C_r, by means of (a) quantum channels and (b) unitary operations and measurements on a dilated space. The quantum channels can be straightforwardly implemented via unitary Stinespring dilations [35]. At this stage, combining Eqs. (4.45), (4.49) and (4.50), we end up with the expression

$$\begin{aligned} \tilde{\rho}(t) &= \tilde{T}(\rho(0)) \\ &= \left(\sum_{r=0}^{2^{\tilde{N}_{\mathrm{TOT}}^m}-1} (-1)^{\mathcal{P}(r)} \Big[\prod_{\gamma=1}^{mK} \mathcal{G}_r^\gamma \mathcal{N}_r^\gamma \Big] \Big[\prod_{\gamma=1}^{j} M_r^\gamma \Big] \right) \rho(0). \end{aligned}$$

Via a similar analysis to Eq. (4.46), it is therefore clear that expectation values of the desired output state $\tilde{\rho}(t)$ can be algorithmically reconstructed from the expectation values of the states

$$\tilde{\rho}^{(r)}(mK) = \prod_{\gamma=1}^{mK} M_r^\gamma(\rho(0)). \tag{4.51}$$

These states can be obtained through unitary operations and measurements, involving ancillary spaces whose dimensions, independent of N, depend only on d and k. Using the same example illustrated in Fig. 4.1, this procedure of obtaining $\tilde{\rho}^{(r)}(mK)$ is shown in Figure 4.2, for the case of $r = 0$.

From Eq. (4.50), it is clear that the algorithmic reconstruction of the states $\rho^r(t)$ from the states $\tilde{\rho}^{(r)}(mK)$, requires knowledge of the constants $\mathcal{N}_r^\gamma$. However, as discussed in Section 4.4, we approximate in practice the states $\rho^r(t)$ with the states

$$\phi^{(r)}(t) = \tilde{\rho}^{(r)}(mK) \Big(\prod_{\gamma=1}^{mK} \mathcal{G}_r^\gamma \tilde{\mathcal{N}}_r^\gamma \Big), \tag{4.52}$$

where $\tilde{\mathcal{N}}_r^\gamma$ is an estimator for $\mathcal{N}_r^\gamma$, constructed from a finite number of measurements. The final output of the algorithmic procedure described here, an approximation of the desired state $\tilde{\rho}(t) = \tilde{T}(\rho(0))$, is therefore the state

$$\tilde{\phi}(t) = \sum_{r=0}^{2^{\tilde{N}_{\mathrm{TOT}}^m}-1} (-1)^{\mathcal{P}(r)} \phi^{(r)}(t). \tag{4.53}$$

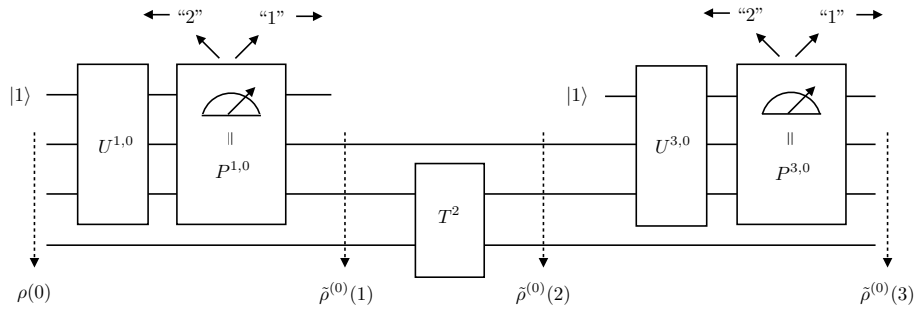

Figure 4.2: Considering the same example as shown in Figure 4.1, the circuit shown here illustrates the method, given by Eq. (4.51), for constructing $\tilde{\rho}^{(0)}(3)$, from which the state $\rho^{(0)}(t) = C_0(\rho(0))$ can be algorithmically reconstructed. Starting with the specified initial state $\rho(0)$, the first CPnTP map $T^{1,0}$ is implemented, as described in Section 4.4, through a unitary operation $U^{1,0}$ and a measurement $P^{1,0}$ on a dilated space. It is crucial to note that if measurement outcome 1 is obtained when performing the measurement, then the correct state $\tilde{\rho}^{(0)}(1)$ has been obtained and the procedure can continue, but if measurement outcome 2 is obtained then the procedure needs to be restarted. The quantum channel T^2 can then be implemented straightforwardly, via a conventional Stinespring dilation (not shown), before the second CPnTP map $T^{3,0}$ is implemented, analogously to $T^{1,0}$.

One can then show that the algorithmic error made in approximating $\tilde{\rho}(t)$ with $\tilde{\phi}(t)$ is bounded by

$$||\tilde{\rho}(t) - \tilde{\phi}(t)|| \leq 2^{\tilde{N}^m_{\mathrm{TOT}}-1} \max_r ||\rho^{(r)}(t) - \phi^{(r)}(t)||, \tag{4.54}$$

and that the error made in approximating $\rho^{(r)}(t)$ with $\phi^{(r)}(t)$ is bounded by

$$||\rho^{(r)}(t) - \phi^{(r)}(t)|| \leq G_r \tilde{N}^m_{\mathrm{TOT}} \max_{1\leq\gamma\leq mK} |\mathcal{N}^\gamma_r - \tilde{\mathcal{N}}^\gamma_r|,$$

with $G_r \equiv \prod_{\gamma=1}^{mK} \mathcal{G}^\gamma_r$. As a result, if one requires that the total algorithmic error is less than $\epsilon_A \geq 0$, one then needs to ensure that

$$\max_r \Big(\max_\gamma \big(|\mathcal{N}^\gamma_r - \tilde{\mathcal{N}}^\gamma_r| \big) \Big) \leq \frac{\epsilon_A}{G \tilde{N}^m_{\mathrm{TOT}} 2^{\tilde{N}^m_{\mathrm{TOT}}-1}}, \tag{4.55}$$

where $G \equiv \max_r \big[G_r\big]$. From Eqs. (4.40) and (4.55), it is then straightforward to calculate the number of trials necessary to obtain a sufficiently accurate estimator $\tilde{\mathcal{N}}^\gamma_r$.

At this stage, given an initial state $\rho(0)$, if the Trotterization error, given by Theorem

4.1, is less than ϵ_T, i.e. if $\left|\left|T_{\mathcal{L}}(t,0)-\tilde{T}\right|\right|_{1\to 1} \leq \epsilon_T$, and if the algorithmic error associated with implementing $\tilde{T}$ is less than ϵ_A, then the *total* error will be upper bounded by

$$||\rho(t) - \tilde{\phi}(t)|| \leq \epsilon_T + \epsilon_A. \tag{4.56}$$

Therefore, if one requires a total error less than ϵ, it suffices to choose m such that $\epsilon_T \leq \epsilon/2$, via Corollary 4.1, and the number of trials required for the construction of the estimators $\mathcal{N}_r^\gamma$, via Eqs. (4.40) and (4.55), such that $\epsilon_A \leq \epsilon/2$.

Finally, it is necessary to make some comments regarding the efficiency of the method. As discussed earlier, it is not expected to obtain an efficient method for an arbitrary locally-indivisible system. Indeed, from the analysis above one can see that the number of strictly k-local CPnTP maps which need to be implemented, given by $(2^{\tilde{N}_{\mathrm{TOT}}^M})mK$, where m is given by Corollary 4.1, depends strongly on the the indivisibility of the system as measured by $\tilde{N}_{\mathrm{TOT}}^M$ and t^{ID}. Furthermore, as a result of the algorithmic procedure for implementing the non-CP strictly k-local propagators, each circuit C_r in fact needs to be successfully implemented a number of times, given by Eqs. (4.40) and (4.55), to construct the required estimators $\tilde{\mathcal{N}}_r^\gamma$. However, as pointed out earlier, it is crucial to note that, as a result of the definition of $A^{\gamma,i}$, a *successful implementation* of the circuit C_r requires that all measurements involved in the circuit result in "measurement outcome 1". Therefore, the probability of achieving a successful implementation of circuit C_r is given by $P(C_r) = \prod_{\gamma=1}^{mK} \mathcal{N}_r^\gamma$, with

$$\Big(\max_{1\leq\gamma\leq mk}\left[\mathcal{N}_r^\gamma\right]\Big)^{\tilde{N}_{\mathrm{TOT}}^m} \geq P(C_r) \geq \Big(\min_{1\leq\gamma\leq mk}\left[\mathcal{N}_r^\gamma\right]\Big)^{\tilde{N}_{\mathrm{TOT}}^m}.$$

In practice, as $\mathcal{N}^{\gamma,i}(\rho) \equiv \mathrm{tr}(T_s^{\gamma,i})(\rho)$, the value of $\mathcal{N}_r^\gamma$ can be estimated by implementing the strictly k-local propagator $T_s^{\gamma,\mathcal{B}(r,n)}$ on a classical computer for a random selection of inputs ρ, and by taking the average value of output traces. This estimated value of $\mathcal{N}_r^\gamma$, in conjunction with the value of t^{ID} and $\tilde{N}_{\mathrm{TOT}}^m$, can then be used to decide whether the algorithmic procedure given here is plausible for the system of interest.

4.6 Conclusions and outlook

We have presented an algorithmic digital quantum simulation method for many-body locally-indivisible non-Markovian open quantum systems. The method consists of an SLT decomposition of the k-local global system propagator into the product of strictly k-local propagators, which may not be quantum channels. In this case, we also provide

an algorithmic method for the implementation of those strictly k-local propagators which are not quantum channels, through unitary operations and measurements on a dilated space. The efficiency of the method, which reduces to the method of Ref. [35] in the case of locally divisible dynamics, expectably depends on various measures of the local indivisibility of the system. For systems which are weakly indivisible, with respect to the measures defined here, this method should be achievable with current experimental setups [61, 62].

In light of these results, various natural avenues arise for the extension of this work. The first direction consists in investigating any potential improvements that could be gained from utilising higher order SLT decompositions [65, 66]. However, as discussed in Refs. [61–63], due to practical experimental constraints on gate implementation, any such analysis needs to take into account the tradeoff which arises between greater accuracy in the SLT decomposition and a larger number of required gates. The second natural direction involves investigating alternative or improved methods for the implementation of strictly k-local propagators which are not quantum channels. In particular, it would be of interest to construct methods for the simulation of maps which are not necessarily Hermiticity and trace preserving.

Finally, given the necessary inefficiency of digital methods for the simulation of non-Markovian systems, it would be of interest to investigate the potential of digital-analog approaches [73–75]. In particular, it would be of interest to investigate whether efficient simulations are possible through the utilisation of non-Markovian analog building blocks, such as recently introduced quantum memristors [29, 76], combined with digital steps. Furthermore, one should investigate whether such efficient simulations could play any role in the emerging field of quantum machine learning [77], where purely digital approaches may be restricted by fundamental obstacles.

4.7 Appendix

4.7.1 Proof of Theorem 4.1

In this appendix we will provide a proof for Theorem 4.1, and the associated Corollary 4.1, through a sequence of lemmas, following the strategy given in [35], but generalised to the case of locally indivisible dynamics where necessary. In what follows, for notational convenience, we will drop the subscript $1 \to 1$ notation from all super-operator norms, as well as the subscript 1 for operator norms. In addition, given a k-local system described

by Eqs. (4.1) and (4.2), and using the same notation as in Theorem 4.1, we will define

$$\xi \equiv \left|\left| T_{\mathcal{L}}(t,0) - \prod_{j=1}^{m}\prod_{i=1}^{K} T_i^j \right|\right|. \tag{4.57}$$

Given this notation we can then state our first lemma, which will allow us to bound the norms of both local and global propagators.

Lemma 4.1. *Given $T_{\mathcal{L}}(t,s) \in \mathcal{B}(\mathcal{B}(\mathcal{H}))$, which solves the initial value problem* (4.3) *for some piecewise continuous Liouvillian $\mathcal{L} : \mathbb{R}^+ \to \mathcal{B}(\mathcal{B}(\mathcal{H}))$ and some $0 \leq s \leq t$, then $\big(T_{\mathcal{L}}(t,s)\big)^{-1}$ exists, denoted $T_{\mathcal{L}}^{-1}(t,s)$, and we have that*

$$||T_{\mathcal{L}}(t,s)|| \leq \exp\left[\int_s^t ||\,\mathcal{L}(r)||dr\right] \tag{4.58}$$

$$\leq \exp\left[(t-s)\left(\sup_{s\leq r\leq t} ||\mathcal{L}(r)||\right)\right], \tag{4.59}$$

and

$$||T_{\mathcal{L}}^{-1}(t,s)|| \leq \exp\left[\int_s^t ||\,\mathcal{L}(r)||dr\right] \tag{4.60}$$

$$\leq \exp\left[(t-s)\left(\sup_{s\leq r\leq t} ||\mathcal{L}(r)||\right)\right], \tag{4.61}$$

Furthermore, if $T_{\mathcal{L}}(t,s)$ is a quantum channel (CPTP), then we have that $||T_{\mathcal{L}}(t,s)|| = 1$.

The proof of lemma 4.1 can be found in [35] using properties of product integrals given in [78]. We can now proceed to begin to construct a bound on ξ via the following lemma:

Lemma 4.2. *Given a k-local system, described by Eqs.* (4.1) *and* (4.2)*, we have that*

$$\xi \leq \left[\sum_{j=0}^{m-1}\left(\Big[\prod_{l=j+2}^{m} P_2^l\Big] P_1^j\right)\right]\left(\max_{1\leq j\leq m}\left|\left|T_{\mathcal{L}}^j - \prod_{i=1}^{K} T_i^j\right|\right|\right), \tag{4.62}$$

where

$$P_1^\alpha = \left|\left|\prod_{j=1}^{\alpha}\prod_{i=1}^{K} T_i^j\right|\right|, \qquad P_2^\alpha = \left|\left|\, T_{\mathcal{L}}^\alpha \,\right|\right|, \tag{4.63}$$

and $P_1^0 = 1$.

Proof. Using the same strategy as in Ref. [35], but taking note that $||T_i^j|| \neq 1$ for all i, j,

we find that

$$\xi = \Big|\Big| \prod_{j=1}^{m} T_{\mathcal{L}}^{j} - \prod_{j=1}^{m}\prod_{i=1}^{K} T_i^j \Big|\Big| \tag{4.64}$$

$$= \Big|\Big| T_{\mathcal{L}}^{m} \prod_{j=1}^{m-1} T_{\mathcal{L}}^{j} - \Big(\prod_{i=1}^{K} T_i^m\Big)\Big(\prod_{j=1}^{m-1}\prod_{i=1}^{K} T_i^j\Big) \Big|\Big|$$

$$\leq \Big|\Big| \prod_{j=1}^{m-1}\prod_{i=1}^{K} T_i^j \Big|\Big| \Big|\Big| T_{\mathcal{L}}^{m} - \prod_{i=1}^{K} T_i^m \Big|\Big| + \Big|\Big| T_{\mathcal{L}}^{m} \Big|\Big| \Big|\Big| \prod_{j=1}^{m-1} T_{\mathcal{L}}^{j} - \prod_{j=1}^{m-1}\prod_{i=1}^{K} T_i^j \Big|\Big| \tag{4.65}$$

$$\leq \sum_{j=0}^{m-1} \Big[\Big(\Big[\prod_{l=j+2}^{m} P_2^l \Big] P_1^j \Big) \Big|\Big| T_{\mathcal{L}}^{j+1} - \prod_{i=1}^{K} T_i^{j+1} \Big|\Big| \Big] \tag{4.66}$$

$$\leq \Big[\sum_{j=0}^{m-1} \Big(\Big[\prod_{l=j+2}^{m} P_2^l \Big] P_1^j \Big) \Big] \Big(\max_{1\leq j\leq m} \Big|\Big| T_{\mathcal{L}}^{j} - \prod_{i=1}^{K} T_i^j \Big|\Big| \Big).$$

In the above, (4.66) follows from (4.65) by comparing the last norm on line (4.65) with the right hand side of (4.64), and then iterating. □

We now note that

$$P_1^{\alpha} \leq \prod_{i=1}^{K}\prod_{j=1}^{m} \Big|\Big| T_i^j \Big|\Big| \tag{4.67}$$

$$\leq \prod_{i=1}^{K} \Big(\big[e^{\beta \Delta t} \big]^{\tilde{N}_i^m} \Big) \tag{4.68}$$

$$\leq e^{K\beta \tilde{N}^m \Delta t} \tag{4.69}$$

$$\leq e^{K\beta m \Delta t}, \tag{4.70}$$

and

$$\prod_{i=j+2}^{m} P_2^i \leq \prod_{i=1}^{m} \Big|\Big| T_{\mathcal{L}}^{i} \Big|\Big| \tag{4.71}$$

$$\leq \prod_{i=1}^{\min(K\tilde{N}^m, m)} e^{\beta K \Delta t} \tag{4.72}$$

$$\leq e^{K\beta[\min(K\tilde{N}^m, m)]\Delta t} \tag{4.73}$$

$$\leq e^{K\beta m \Delta t}, \tag{4.74}$$

where (4.68) follows from (4.67), and (4.72) follows from (4.71) via Lemma 4.1 and the definition of β. As a result of the above observations and the statement of Lemma 4.2 we then get the following corollary:

Corollary 4.2. *Given a k-local system, described by Eqs.* (4.1) *and* (4.2)*, we have that*

$$\xi \leq m\Big(e^{[\min(K\tilde{N}^m,m)+\tilde{N}^m]K\beta\Delta t}\Big) \Big(\max_{1\leq j\leq m}\Big|\Big|T^j_{\mathcal{L}}-\prod_{i=1}^{K}T^j_i\Big|\Big|\Big).$$

From Corollary 4.2, it is clear that, to proceed, it is necessary to bound the quantity $||T^j_{\mathcal{L}}-\prod_{i=1}^{K}T^j_i||$. Such a bound is provided by the following lemma:

Lemma 4.3. *Using the notation and setting of Sections 4.2 and 4.3 we have that*

$$||T^j_{\mathcal{L}}-\prod_{i=1}^{K}T^j_i|| \leq \Big(Ke^{\beta\hat{N}^m_j\Delta t}\Big)\Big(\max_{2\leq\phi\leq K}||T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z}-T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}||\Big).$$

Defining $\chi \equiv ||T^j_{\mathcal{L}}-\prod_{i=1}^{K}T^j_i||$ for notational convenience, the proof proceeds as follows:

Proof. Taking proper account of the presence of non-CP strictly k-local propagators, we

find that

$$\chi = ||T^j_{\mathcal{L}_K+\sum_{z=1}^{K-1}\mathcal{L}_z} - T^j_K \prod_{i=1}^{K-1} T^j_i|| \tag{4.75}$$

$$\leq ||T^j_{\mathcal{L}_K+\sum_{z=1}^{K-1}\mathcal{L}_z} - T^j_K T^j_{\sum_{z=1}^{K-1}\mathcal{L}_z} + T^j_K T^j_{\sum_{z=1}^{K-1}\mathcal{L}_z} - T^j_K \prod_{i=1}^{K-1} T^j_i|| \tag{4.76}$$

$$\leq ||T^j_{\mathcal{L}_K+\sum_{z=1}^{K-1}\mathcal{L}_z} - T^j_K T^j_{\sum_{z=1}^{K-1}\mathcal{L}_z}|| + ||T^j_K||||T^j_{\sum_{z=1}^{K-1}\mathcal{L}_z} - \prod_{i=1}^{K-1} T^j_i|| \tag{4.77}$$

$$\leq \sum_{\phi=2}^{K}\left[\left(T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}\right)\left(\prod_{i=\phi+1}^{K}||T^j_i||\right)\right] \tag{4.78}$$

$$\leq \left[\sum_{\phi=2}^{K}\left(\prod_{i=\phi+1}^{K}||T^j_i||\right)\right]\left[\max_{2\leq\phi\leq K}||T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}||\right] \tag{4.79}$$

$$\leq K\left[\prod_{i=1}^{K}||T^j_i||\right]\left[\max_{2\leq\phi\leq K}||T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}||\right] \tag{4.80}$$

$$\leq \left(Ke^{\beta\hat{N}^m_j\Delta t}\right)\left(\max_{2\leq\phi\leq K}||T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}||\right) \tag{4.81}$$

Note that line (4.78) follows from line (4.77) by comparing the last norm on line (4.77) with the norm on line (4.75) and iterating. Similarly, line (4.81) follows from line (4.80) via Lemma 4.1, the definition of $\hat{N}^m_j$ and the definition of β. □

We now focus our attention on bounding the quantity

$$\Gamma \equiv ||T^j_{\sum_{z=1}^{\phi}\mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1}\mathcal{L}_z}||, \tag{4.82}$$

To which end we use the following lemma:

Lemma 4.4. *Given two arbitrary time-dependent Liouvillians $\mathcal{K}$ and $\mathcal{L}$ the following relationship holds*

$$||T_{\mathcal{K}+\mathcal{L}}(t,s) - T_{\mathcal{K}}(t,s)T_{\mathcal{L}}(t,s)|| \leq \frac{1}{2}(t-s)^2\left[\sup_{s\leq\mu\leq r\leq t}||\big[\mathcal{K}(u),\mathcal{L}(r)\big]||\right] \times \left[e^{\left[(t-s)\left(3\sup_{s\leq\nu\leq t}||\mathcal{K}(\nu)||+2\sup_{s\leq\nu\leq t}||\mathcal{L}(\nu)||\right)\right]}\right]. \tag{4.83}$$

Proof. For notational convenience let us define

$$\zeta = ||T_{\mathcal{K}+\mathcal{L}}(t,s) - T_{\mathcal{K}}(t,s)T_{\mathcal{L}}(t,s)||. \tag{4.84}$$

As shown in Ref. [35], using the fundamental theorem of calculus allows one to obtain

$$\zeta = \Big|\Big| \int_s^t dr \int_s^r d\mu T_{\mathcal{K}}(t,s) T_{\mathcal{L}}(t,r) T_{\mathcal{K}}^{-1}(\mu,s) \big[\mathcal{L}(r), \mathcal{K}(\mu)\big] T_{\mathcal{K}}^{-1}(r,\mu) T_{\mathcal{K}+\mathcal{L}}(r,s) \Big|\Big|, \quad (4.85)$$

from which, using Lemma 4.1, submultiplicativity of the $1 \to 1$ norm and the triangle inequality, and again noting that not all propagators are necessarily quantum channels, it follows that,

$$\begin{aligned}
\zeta &\leq \int_s^t dr \int_s^r d\mu \Bigg(||\big[\mathcal{L}(r), \mathcal{K}(\mu)\big]|| \exp\Big[\Big(\int_s^t ||\mathcal{K}(\nu)|| d\nu \Big) + \Big(\int_r^t ||\mathcal{L}(\nu)|| d\nu \Big) \\
&\qquad + \Big(\int_\mu^r ||\mathcal{K}(\nu)|| d\nu \Big) + \Big(\int_s^r ||\mathcal{K}(\nu) + \mathcal{L}(\nu)|| d\nu \Big) \Big] \Bigg) && (4.86) \\
&\leq \int_s^t dr \int_s^r d\mu \Bigg(||\big[\mathcal{L}(r), \mathcal{K}(\mu)\big]|| \exp\Big[\int_s^t \big(3||\mathcal{K}(\nu)|| + 2||\mathcal{L}(\nu)|| \big) d\nu \Big] \Bigg) && (4.87) \\
&\leq \Bigg(\int_s^t dr \int_s^r d\mu ||\big[\mathcal{L}(r), \mathcal{K}(\mu)\big]|| \Bigg) \exp\Big[\int_s^t \big(3||\mathcal{K}(\nu)|| + 2||\mathcal{L}(\nu)|| \big) d\nu \Big] && (4.88) \\
&\leq \frac{1}{2}(t-s)^2 \Big[\sup_{s \leq \mu \leq r \leq t} ||\big[\mathcal{K}(u), \mathcal{L}(r)\big]|| \Big] \\
&\qquad \times \Big[e^{\left[(t-s) \left(3 \sup_{s \leq \nu \leq t} ||\mathcal{K}(\nu)|| + 2 \sup_{s \leq \nu \leq t} ||\mathcal{L}(\nu)|| \right) \right]} \Big]. && (4.89)
\end{aligned}$$

□

Applying Lemma 4.4 to the special case of the norm

$$\Gamma \equiv ||T^j_{\sum_{z=1}^{\phi} \mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1} \mathcal{L}_z}||, \quad (4.90)$$

then yields the corollary,

Corollary 4.3. *Using the notation and setting of Sections 4.2 and 4.3, we have that, for all $2 \leq \phi \leq K$, the following inequality holds*

$$||T^j_{\sum_{z=1}^{\phi} \mathcal{L}_z} - T^j_\phi T^j_{\sum_{z=1}^{\phi-1} \mathcal{L}_z}|| \leq (K\beta^2)(\Delta t)^2 e^{(3+2K)\beta \Delta t}.$$

Theorem 4.1 now follows straightforwardly as a consequence of Corollary 4.2, Lemma 4.3 and Corollary 4.3. Finally, we provide a proof of Corollary 4.1.

Proof (Corollary 4.1). Assume that

$$0 \leq \epsilon \leq \frac{(2K^2\beta t \ln(2) e^{(K+K^2)t^{\mathrm{ID}}\beta})}{(3 + [3 + \tilde{C}K + \tilde{C}K^2])}, \tag{4.91}$$

and

$$m \geq 2K\beta^2 t^2 e^{(K+K^2)t^{\mathrm{ID}}\beta}/\epsilon. \tag{4.92}$$

It follows from Theorem 4.1 and assumptions (4.91) and (4.92) that

$$\xi \leq \frac{K^2\beta^2 t^2}{m} e^{(3+[3+\tilde{C}]K+\tilde{C}K^2)\beta(t/m)} e^{(K+K^2)t^{\mathrm{ID}}\beta} \tag{4.93}$$

$$\leq \frac{\epsilon}{2} \exp\Big[\frac{\big(3 + [3 + \tilde{C}]K + \tilde{C}K^2\big)\epsilon}{2K^2\beta t e^{(K+K^2)t^{\mathrm{ID}}\beta}}\Big] \tag{4.94}$$

$$\leq \frac{\epsilon}{2} e^{\ln(2)} \tag{4.95}$$

$$\leq \epsilon. \tag{4.96}$$

□

Bibliography

[1] R. Sweke, M. Sanz, I. Sinayskiy, F. Petruccione, and E. Solano. Digital quantum simulation of many-body non-Markovian dynamics. *Phys. Rev. A*, 94:022317, 2014.

[2] H. P. Breuer and F. Petruccione. *The Theory of Open Quantum Systems.* Oxford University Press, 2002.

[3] A. J. Daley. Quantum trajectories and open many-body quantum systems. *Adv. Phys.*, 63:77, 2014.

[4] A. Rivas and S. F. Huelga. *Open Quantum Systems, An Introduction.* Springer Briefs in Physics, 2012.

[5] H. P. Breuer, E. M. Laine, J. Piilo, and B. Vacchini. *Colloquium* : Non-Markovian dynamics in open quantum systems. *Rev. Mod. Phys.*, 88:021002, 2016.

[6] A. Rivas, S. F. Huelga, and M. B. Plenio. Quantum non-Markovianity: characterization, quantification and detection. *Rep. Prog. Phys.*, 77:094001, 2014.

[7] I. de Vega and D. Alonso. Dynamics of non-Markovian open quantum systems. arXiv:1511.06994 [quant-ph], 2015.

[8] L. Aolita, F. de Melo, and L. Davidovich. Open-system dynamics of entanglement:A key issues review. *Rep. Prog. Phys.*, 78:042001, 2015.

[9] B. Leggio, R. Lo Franco, D. O. Soares-Pinto, P. Horodecki, and G. Compagno. Distributed correlations and information flows within a hybrid multipartite quantum-classical system. *Phys. Rev. A*, 92:032311, 2015.

[10] Z. Man, Y. Xia, and R. Lo Franco. Harnessing non-Markovian quantum memory by environmental coupling. *Phys. Rev. A*, 92:012315, 2015.

[11] A. Chiuri, C. Greganti, L. Mazzola, M. Paternostro, and P. Mataloni. Linear optics simulation of quantum non-Markovian dynamics. *Sci. Rep.*, 2:968, 2012.

[12] A. Orieux, A. D'Arrigo, G. Ferranti, R. Lo Franco, G. Benenti, E. Paladino, G. Falci, F. Sciarrino, and P. Mataloni. Experimental on-demand recovery of entanglement by local operations within non-Markovian dynamics. *Sci. Rep.*, 5:8575, 2015.

[13] M. Žnidarič, T. Prosen, G. Benenti, G. Casati, and D. Rossini. Thermalization and ergodicity in one-dimensional many-body open quantum systems. *Phys. Rev. E*, 81:051135, 2010.

[14] M. J. Kastoryano and F. G. S. L Brandao. Quantum Gibbs Samplers: the commuting case. *Comm. Math. Phys.*, 344:915–957, 2016.

[15] I. Pizorn. One-dimensional Bose-Hubbard model far from equilibrium. *Phys. Rev. A*, 88:043635, 2013.

[16] T. Prosen and M. Žnidarič. Matrix product simulations of non-equilibrium steady states of quantum spin chains. *J. Stat. Mech.*, 02:02035, 2009.

[17] T. Prosen. Open XXZ spin chain: Nonequilibrium steady state and a strict bound on ballistic transport. *Phys. Rev. Lett.*, 106:217206, 2011.

[18] G. Benenti, G. Casati, T. Prosen, D. Rossini, and M. Žnidarič. Charge and spin transport in strongly correlated one-dimensional quantum systems driven far from equilibrium. *Phys. Rev. B*, 80:035110, 2009.

[19] T. Prosen and M. Žnidarič. Diffusive high-temperature transport in the one-dimensional Hubbard model. *Phys. Rev. B*, 86:125118, 2012.

[20] M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik. Environment-assisted quantum walks in photosynthetic energy transfer. *J. Chem. Phys.*, 129:174106, 2008.

[21] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, and A. Aspuru-Guzik. Environment-assisted quantum transport. *New J. Phys.*, 11:033003, 2009.

[22] M. B. Plenio and S. F. Huelga. Dephasing-assisted transport: quantum networks and biomolecules. *New J. Phys.*, 10:113019, 2008.

[23] A. Marais, I. Sinayskiy, A. Kay, F. Petruccione, and A. Ekert. Decoherence-assisted transport in quantum networks. *New J. Phys.*, 15:013038, 2013.

[24] I. Sinayskiy, A. Marais, F. Petruccione, and A. Ekert. Decoherence-assisted transport in a dimer system. *Phys. Rev. Lett.*, 108:020602, 2012.

[25] R. Dorner, J. Goold, and V. Vedral. Towards quantum simulations of biological information flow. *Interface Focus*, 2:522, 2012.

[26] S. F. Huelga and M. B. Plenio. Vibrations, quanta and biology. *Contemp. Phys.*, 54:181, 2013.

[27] F. Verstraete, M. M. Wolf, and J. I. Cirac. Quantum computation and quantum-state engineering driven by dissipation. *Nature Physics*, 5:633, 2009.

[28] I. Sinayskiy and F. Petruccione. Efficiency of open quantum walk implementation of dissipative quantum computing algorithms. *Quant. Inf. Proc.*, 11:1301, 2012.

[29] P. Pfeiffer, I. L. Egusquiza, M. Di Ventra, M. Sanz, and E. Solano. Quantum Memristors. *Sci. Rep.*, 6:29507, 2016.

[30] J. C. Budich, P. Zoller, and S. Diehl. Dissipative preparation of Chern insulators. *Phys. Rev. A*, 91:042117, 2015.

[31] S. Diehl, E. Rico, M. A. Baranov, and P. Zoller. Topology by dissipation in atomic quantum wires. *Nature Physics*, 7:971, 2011.

[32] C. E. Bardyn, M. A. Baranov, C. V. Kraus, E. Rico, A. Imamoğlu, P. Zoller, and S. Diehl. Topology by dissipation. *New J. Phys.*, 15:085001, 2013.

[33] B. Kraus, H. P. Büchler, S. Diehl, A. Kantian, A. Micheli, and P. Zoller. Preparation of entangled states by quantum Markov processes. *Phys. Rev. A*, 78:042307, 2008.

[34] S. Diehl, A. Micheli, A. Kantian, B. Kraus, H.P. Büchler, and P. Zoller. Quantum states and phases in driven open quantum systems with cold atoms. *Nature Physics*, 4:878, 2008.

[35] M. Kliesch, T. Barthel, C. Gogolin, M. J. Kastoryano, and J. Eisert. Dissipative Quantum Church-Turing Theorem. *Phys. Rev. Lett.*, 107:120501, 2011.

[36] T. Barthel and M. Kliesch. Quasilocality and efficient simulation of Markovian quantum dynamics. *Phys. Rev. Lett.*, 108:230504, 2012.

[37] D. G. Tempel and A. Aspuru-Guzik. The KitaevFeynman clock for open quantum systems. *New J. Phys.*, 16:113066, 2014.

[38] R. Di Candia, J. S. Pedernales, A. del Campo, E. Solano, and J. Casanova. Quantum simulation of dissipative processes without reservoir engineering. *Sci. Rep.*, 5:9981, 2015.

[39] D. S. Wang, D. W. Berry, M. C. de Oliveira, and B. C. Sanders. Solovay-kitaev decomposition strategy for single-qubit channels. *Phys. Rev. Lett.*, 111:130504, 2013.

[40] D. S. Wang and B.C. Sanders. Quantum circuit design for accurate simulation of qudit channels. *New J. Phys.*, 17:043004, 2015.

[41] H. Wang, S. Ashhab, and F. Nori. Quantum algorithm for simulating the dynamics of an open quantum system. *Phys. Rev. A*, 83:062317, 2011.

[42] R. Sweke, I. Sinayskiy, and F. Petruccione. Simulation of single qubit open quantum systems. *Phys. Rev. A*, 90:022331, 2014.

[43] R. Sweke, I. Sinayskiy, D. Bernard, and F. Petruccione. Universal simulation of Markovian open quantum systems. *Phys. Rev. A*, 91:062308, 2015.

[44] B. Dive, F. Mintert, and D. Burgarth. Quantum simulations of dissipative dynamics: Time dependence instead of size. *Phys. Rev. A*, 92:032111, 2015.

[45] P. Zanardi, J. Marshall, and L. Campos Venuti. Dissipative universal Lindbladian simulation. *Phys. Rev. A*, 93:022312, 2016.

[46] M. Müller, K. Hammerer, Y. L. Zhou, C. F. Roos, and P. Zoller. Simulating open quantum systems: From many-body interactions to stabilizer pumping. *New J. Phys.*, 13:085007, 2011.

[47] P. Schindler, M. Müller, D. Nigg, J. T. Barreiro, E. A. Martinez, M. Hennrich, T. Monz, S. Diehl, P. Zoller, and R. Blatt. Quantum simulation of dynamical maps with trapped ions. *Nature Physics*, 9:361, 2013.

[48] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C.F. Roos, P. Zoller, and R. Blatt. An open-system quantum simulator with trapped ions. *Nature*, 470:486, 2011.

[49] H. Weimer, M. Müller, H. P. Büchler, and I. Lesanovsky. Digital quantum simulation with Rydberg atoms. *Quant. Inf. Proc.*, 10:885, 2011.

[50] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H. P. Büchler. A Rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[51] J. Prior, A. W. Chin, S. F. Huelga, and M. B. Plenio. Efficient simulation of strong system-environment interactions. *Phys. Rev. Lett.*, 105:050404, 2010.

[52] J. Cerrillo and J. Cao. Non-Markovian dynamical maps: Numerical processing of open quantum trajectories. *Phys. Rev. Lett.*, 112:110401, 2014.

[53] R. Rosenbach, J. Cerrillo, S. F. Huelga, J. Cao, and M. B. Plenio. Efficient simulation of non-Markovian system-environment interaction. *New. J. Phys.*, 18:023035, 2016.

[54] M. P. Woods, M. Cramer, and M. B. Plenio. Simulating bosonic baths with error bars. *Phys. Rev. Lett.*, 115:130401, 2015.

[55] P. C. Cárdenas, M. Paternostro, and F. L. Semião. Non-Markovian qubit dynamics in a circuit-QED setup. *Phys. Rev. A*, 91:022122, 2015.

[56] F. Brito and T. Werlang. A knob for Markovianity. *New. J. Phys.*, 17:072001, 2015.

[57] U. Alvarez-Rodriguez, R. Di Candia, J. Casanova, M. Sanz, and E. Solano. Algorithmic quantum simulation of memory effects. arXiv:1604.02992 [quant-ph], 2015.

[58] H. P. Breuer, B. Kappler, and F. Petruccione. Stochastic wave-function method for non-Markovian quantum master equations. *Phys. Rev. A*, 59:1633, 1999.

[59] H. P. Breuer. Genuine quantum trajectories for non-Markovian processes. *Phys. Rev. A*, 70:012106, 2004.

[60] A. A. Budini. Non-Markovian quantum jumps from measurements in bipartite Markovian dynamics. *Phys. Rev. A*, 88:012124, 2013.

[61] R. Barends, L. Lamata, J. Kelly, L. García-Álvarez, A. G. Fowler, A. Migrant, E. Jeffrey, T. C. White, D. Sank, J. Y. Mutus, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, I. C. Hoi, C. Neill, P. J. J. O Malley, C. Quintana, P. Roushan, A. Vainsencher, J. Wenner, E. Solano, and J. M. Martinis. Digital quantum simulation of fermionic models with a superconducting circuit. *Nature Comm.*, 6:7654, 2015.

[62] R. Barends, A. Shabani, L. Lamata, J. Kelly, A. Mezzacapo, U. Las Heras, R. Babbush, A. G. Fowler, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, E. Jeffrey, E. Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, P. J. J. OMalley, C. Quintana, P. Roushan, D. Sank, A. Vainsencher, J. Wenner, T. C. White, E. Solano, H. Neven, and J. M. Martinis. Digitized adiabatic quantum computing with a superconducting circuit. *Nature*, 534:222, 2016.

[63] Y. Salathé, M. Mondal, M. Oppliger, J. Heinsoo, P. Kurpiers, A. Potočnik, A. Mezzacapo, U. Las Heras, L. Lamata, E. Solano, S. Filipp, and A. Wallraff. Digital quantum simulation of spin models with circuit quantum electrodynamics. *Phys. Rev. X*, 5:021027, 2015.

[64] H. F. Trotter. On the product of semi-groups of operators. *Proc. Amer. Math. Soc.*, 10:545, 1959.

[65] M. Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. *Phys. Lett. A*, 146:319, 1990.

[66] M. Suzuki. General theory of fractal path integrals with applications to manybody theories and statistical physics. *J. Math. Phys.*, 32:400, 1991.

[67] U. Las Heras, U. Alvarez-Rodriguez, E. Solano, and M. Sanz. Genetic algorithms for digital quantum simulations. *Phys. Rev. Lett.*, 116:230504, 2016.

[68] J. Watrous. Theory of quantum information (book draft). https://cs.uwaterloo.ca/ watrous/TQI/, 2016.

[69] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 2000.

[70] L. D. Brown, T. T. Cai, and A. DasGupta. Interval estimation for a binomial proportion. *Statistical Science*, 16:101, 2001.

[71] S. Wallis. Binomial confidence intervals and contingency tests: Mathematical fundamentals and the evaluation of alternative methods. *J. Quant. Ling.*, 20:178, 2013.

[72] E. B. Wilson. Probable inference, the law of succession, and statistical inference. *J. Am. Stat. Ass.*, 22:209, 1927.

[73] I. Arrazola, J. S. Pedernales, L. Lamata, and E. Solano. Digital-analog quantum simulation of spin models in trapped ions. *Sci. Rep.*, 6:30534, 2016.

[74] A. Mezzacapo, U. Las Heras, J. S. Pedernales, L. DiCarlo, E. Solano, and L. Lamata. Digital quantum Rabi and Dicke models in superconducting circuits. *Sci. Rep.*, 4:7482, 2014.

[75] L. García-Álvarez, U. Las Heras, A. Mezzacapo, M. Sanz, E. Solano, and L. Lamata. Quantum chemistry and charge transport in biomolecules with superconducting circuits. *Sci. Rep.*, 6:27836, 2016.

[76] J. Salmilehto, F. Deppe, M. Di Ventra, M. Sanz, and E. Solano. Quantum memristors with superconducting circuits. arXiv:1603.04487 [quant-ph], 2016.

[77] M. Schuld, I. Sinayskiy, and F. Petruccione. An introduction to quantum machine learning. *Cont. Phys.*, 56:172, 2015.

[78] J. D. Dollard and C. N. Friedman. Product integrals and the Schrödinger equation. *J. Math. Phys.*, 18:1598–1607, 1977.

Chapter 5

Conclusion

At this point we have introduced and analysed a variety of algorithms for the quantum simulation of the time evolution of various classes of intrinsically specified open quantum systems. As the main contributions and results of this work have already been summarised in Section 1.5 of Chapter 1, we will not repeat that summary here. However, as has been previously mentioned in the conclusion of each chapter, the results obtained in this thesis naturally suggest a variety of new research directions, and allow one to formulate a number of important open questions. Mindful of the rapid pace with which the study of many-body physics and the development of quantum algorithms is proceeding, we will attempt in this concluding chapter to briefly synthesise some of the perspectives emerging from this thesis, within the context of current research.

In particular, as discussed at length in the introduction, it is becoming increasingly clear that *hybrid* simulation methodologies offer the most promising path towards the experimental implementation of quantum simulations which exhibit *quantum supremacy* over the best possible classical simulation methods. As such, it is of interest to interrogate how such methodologies, centred around the notion of "dissipation as a resource", might be utilised to both augment and ensure the implementation of the methods presented in this thesis on a scale which allows for the study of the plethora of phenomena discussed in Chapter 1. Firstly, within the context of Markovian open quantum systems, it is clear that the results presented in Chapters 2 and 3 allow one to focus ones effort on developing methods for the simulation of processes from a well specified universal set, with the knowledge that efficient simulation of these processes can be efficiently recombined to allow for the simulation of arbitrary Markovian open quantum systems. As such, the development of practical and experimentally feasible methods for the simulation of these universal processes is clearly of the utmost importance if one wants to utilise the meth-

ods presented here. As previously mentioned, and explicitly demonstrated in Chapter 2, while *any* alternative method for the simulation of Markovian open quantum systems could be used for the implementation of the universal building blocks, it will be interesting to investigate the extent to which naturally occurring dissipation and decoherence can be exploited for this task. In particular, inspired by experimental developments in the simulation of open quantum systems in superconducting circuits [1], as well as the small scale open quantum simulators in trapped ion and Rydberg atom systems [2–8], it would be of interest to catalogue the platform specific dissipative resources *currently available*, and investigate the extent to which both the universality results of this thesis, as well as the various "dissipative gadget" constructions [9–11], might be rephrased in terms of these currently available experimental resources. In some sense one might think of this as a "bottom up approach", in contrast with the "top-down" approach adopted in this thesis for the construction of the universal sets themselves. In line with the philosophy of hybrid simulation methodologies, the hope is that these approaches might converge to provide pragmatically motivated and practically feasible methods with the minimum number of prohibitive experimental constraints.

In a similar vein, but within the context of non-Markovian open quantum systems, the rigorous SLT results proven in Chapter 4 provide the foundation required to simulate complex many-body models through the simulation of simpler building blocks. Although we have provided an explicit proposal for how one might algorithmically simulate the required non-completely-postive propagators using feedback with a universal quantum computer, it is clear that there are fundamental obstacles involved in achieving *efficient* simulation algorithms in this way. As such, it is once again clearly of interest to both investigate methods for engineering simple non-Markovian open quantum systems [12–15], and to catalogue experimentally accessible natural non-Markovian systems, which might be utilised as building blocks within a hybrid digital/analog simulation strategy.

Although from a pragmatic point of view the investigation of hybrid simulation methodologies capable of exploiting naturally occurring and simple to engineer dissipation is of the utmost importance, from a foundational complexity-theoretic perspective it would also be extremely interesting if one was able to construct *provably optimal* digital simulation strategies for arbitrary open quantum systems from specific classes. Furthermore, we note that Hamiltonian simulation has become a crucial subroutine in various quantum machine learning algorithms [16, 17], and as such the development of optimal algorithms for Hamiltonian simulation has become important outside of the physically motivated context. This motivation has led to a plethora of new techniques for Hamiltonian simulation, resulting in algorithms which are close to provable complexity lower

bounds in almost all relevant parameters [18–20]. With this in mind, it is interesting to ask whether any of the innovative new tools or techniques from Hamiltonian simulation could be generalised into the open quantum systems context, and whether the simulation of specific open quantum systems might be of any computational use as a subroutine for algorithms outside of the physically motivated context. In particular, it would be worthwhile investigating the extent to which non-trivial memory effects present in certain open quantum systems might be used as an algorithmic tool.

Finally, directly in line with this last point, given the rapid development of methods for the simulation of open quantum systems, and the development of quantum technologies to implement these methods, it is important to ask how one might exploit the dynamics of open quantum systems. As discussed in Chapter 1, there are by now a large number of proposals for dissipative state preparation, but one might argue that there is as of yet no "killer application" of dissipation as a resource. Considering our rapidly improving ability to implement the dynamics of open quantum systems there is therefore potentially a lot to be gained from creatively re-examining the potential applications of dissipation and decoherence. One particularly interesting direction in this regard is the recent suggestion of fault-tolerant dynamical decoders for topological quantum memories which can be implemented through the evolution of Markovian open quantum systems [21, 22], and it would be worthwhile to examine both how these suggestions like this can be extended, and how these proposals can be realised through existing simulation methodologies such as the ones presented in this thesis.

In conclusion, one can certainly say that we are living in an extremely exciting period in the history of physics. The birth of quantum information science from a merger of mathematics, physics and theoretical computer science has given us a new lens through which to view the world, and a rapidly developing toolbox to approach difficult and foundational questions throughout the natural sciences. Quantum simulations are definitely at the forefront of this development and innovation, and despite the rapid progress we have made, there remain endless rich directions to explore, which promise a continued stream of fresh insights and new knowledge.

Bibliography

[1] A. A. Houck, H. E Türeci, and J. Koch. On-chip quantum simulation with superconducting circuits. *Nature Physics*, 8:292, 2012.

[2] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H. P. Büchler. A rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[3] M. Müller, K. Hammerer, Y. L. Zhou, C. F. Roos, and P. Zoller. Simulating open quantum systems: from many-body interactions to stabilizer pumping. *New J. Phys.*, 13:085007, 2011.

[4] R. Blatt and C. F. Roos. Quantum simulations with trapped ions. *Nature Physics*, 8:277, 2012.

[5] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C.F. Roos, P. Zoller, and R. Blatt. An open-system quantum simulator with trapped ions. *Nature*, 470:486, 2011.

[6] M. Müller, G. Diehl, S.and Pupillo, and P. Zoller. Engineered open systems and quantum simulations with atoms and ions. *Adv. Atom. Mol. Opt. Phys*, 61:1, 2012.

[7] P Schindler, M Mueller, D Nigg, J. T. Barreiro, E. A. Martinez, M. Hennrich, T. Monz, S. Diehl, P. Zoller, and R. Blatt. Quantum simulation of open-system dynamical maps with trapped ions. In *APS Division of Atomic, Molecular and Optical Physics Meeting Abstracts*, volume 1, page 5005, 2013.

[8] H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, and H.-P. Büchler. A rydberg quantum simulator. *Nature Physics*, 6:382, 2010.

[9] P. Zanardi, J. Marshall, and L. C. Venuti. Dissipative universal lindbladian simulation. *Phys. Rev. A*, 93:022312, 2016.

[10] J. Marshall, L. C. Venuti, and P. Zanardi. Modular quantum information processing by dissipation. arXiv:1607.03207 [quant-ph], 2016.

[11] M. J. Kastoryano, M. M. Wolf, and J. Eisert. Precisely timing dissipative quantum information processing. *Physical review letters*, 110:110501, 2013.

[12] P. C. Cárdenas, M. Paternostro, and F. L. Semião. Non-Markovian qubit dynamics in a circuit-QED setup. *Phys. Rev. A*, 91:022122, 2015.

[13] F. Brito and T. Werlang. A knob for Markovianity. *New. J. Phys.*, 17:072001, 2015.

[14] P. Pfeiffer, I. L. Egusquiza, M. Di Ventra, M. Sanz, and E. Solano. Quantum Memristors. *Sci. Rep.*, 6:29507, 2016.

[15] J. Salmilehto, F. Deppe, M. Di Ventra, M. Sanz, and E. Solano. Quantum memristors with superconducting circuits. arXiv:1603.04487 [quant-ph], 2016.

[16] M. Schuld, I. Sinayskiy, and F. Petruccione. An introduction to quantum machine learning. *Cont. Phys.*, 56:172, 2015.

[17] A. W. Harrow, A. Hassidim, and S. Lloyd. Quantum algorithm for linear systems of equations. *Phys. Rev. Lett.*, 103:150502, 2009.

[18] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma. Simulating Hamiltonian dynamics with a truncated Taylor series. *Phys. Rev. Lett.*, 114:090502, 2015.

[19] D. W. Berry, A. M. Childs, and R. Kothari. Hamiltonian simulation with nearly optimal dependence on all parameters. *Proceedings of the 56th IEEE Symposium on Foundations of Computer Science (FOCS 2015)*, pages 792–809, 2015.

[20] D. W. Berry and L. Novo. Corrected quantum walk for optimal Hamiltonian simulation. arXiv:1606.03443 [quant-ph], 2016.

[21] M. Herold, E. T. Campbell, J. Eisert, and M. J. Kastoryano. Cellular-automaton decoders for topological quantum memories. arXiv:1406.2338 [quant-ph], 2014.

[22] M. Herold, M. J. Kastoryano, E. T. Campbell, and J. Eisert. Fault tolerant dynamical decoders for topological quantum memories. arXiv:1511.05579 [quant-ph], 2015.