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QUANTUM OPTIMAL CONTROL – QUANTUM STOCHASTIC MASTER EQUATION AS MODEL BACKGROUND INTRODUCTION AND PEDAGOGICAL BENCHMARKS

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The second (quantum computing algorithms and HW-computers) and third quantum (quantum programming and SW-engineering and quantum "powerful" computing AI) revolutions have led to the necessity in developing of intelligent SW/HW platform (strong quantum computational AI) of industrial quantum technologies for mega - science projects "Industry 5.0 / 6.0". This fact, in turn, has raised the big challenge of training a new generation of quantum engineering staff in the fields of quantum end-to-end IT, quantum software engineering and quantum intelligent control. The creation of an appropriate software-algorithmic platform and hardware support in view of a quantum computer for industrial development required a radical revision of the foundations of educational processes for quantum engineering, the creation of a new technological structure and mathematical / physical / technical background in dynamically developing areas of application of quantum end-to-end IT. The lack of teaching staff and objective assessments of the necessity of industry and science for quantum engineering personnel only increased the difficulties in the development of quantum engineering. There is a certain mathematical maturity required to understand the quantum mechanics of finite dimensional systems. We review only the basics here and this is mostly to familiarize the reader with the notation used for the remainder of this Introduction.

Keywords: quantum computing, quantum end-to-end information technologies, quantum engineering.

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ОСНОВЫ ОПИСАНИЯ МОДЕЛЕЙ КВАНТОВОГО ОПТИМАЛЬНОГО УПРАВЛЕНИЯ – КВАНТОВЫЕ СТОХАСТИЧЕСКИЕ КИНЕТИЧЕСКИЕ УРАВНЕНИЯ: ВВЕДЕНИЕ И ПЕДАГОГИЧЕСКИЕ ПРИМЕРЫ

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Вторая (квантовые вычислительные алгоритмы и HW-компьютеры) и третья квантовые (квантовое программирование и SW- инженерия и квантовый «мощный» вычислительный ИИ) революции привели к необходимости разработки интеллектуальной SW/HW платформы (сильный квантовый вычислительный ИИ) промышленных квантовых технологий для мега-научных проектов «Индустрия 5.0 / 6.0». Это, в свою очередь, поставило большую задачу подготовки нового поколения кадров квантовой инженерии в области квантовых сквозных ИТ, квантовой программной инженерии и квантового интеллектуального управления. Создание соответствующей программно-алгоритмической платформы и аппаратного обеспечения с учетом квантового компьютера для промышленного развития потребовало радикального пересмотра основ образовательных процессов по квантовой инженерии, создания новой технологической структуры и математической/физической/технической базы в динамично развивающихся областях применения квантовых сквозных ИТ. Нехватка преподавательского состава и объективных оценок потребности промышленности и науки в кадрах квантовой инженерии только увеличили трудности в развитии квантовой инженерии. Для понимания квантовой механики конечномерных систем требуется определенная математическая зрелость. Здесь мы рассмотрим только основы, и это сделано главным образом для того, чтобы познакомить начинающего читателя с обозначениями и результатами, используемыми в оставшейся части этого введения.

Ключевые слова: квантовые вычисления, квантовые сквозные информационные технологии, квантовая инженерия.

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Introduction

The results obtained in the field of quantum technologies and quantum information technologies clearly demonstrate the high technological potential of quantum technologies for solving a number of problems, much more efficiently than any modern "traditional" computer.

Despite the fact that the era of noisy intermediate-scale quantum (NISQ) devices is currently on going, quantum information science as a whole is already a new, rapidly developing branch of science associated with the use of quantum systems to implement fundamentally new methods of transmitting messages, computing and technologies (quantum communication channels, quantum cryptography, quantum computer) [1].

Periodically, there are reports of achieving "quantum supremacy"4, that is, the creation of a quan tum computer capable of solving problems significantly more efficiently than any modern "traditional" computer (modern von Neumann supercomputers are also considered "traditional" tools in this ap proach) or even impossible to solve using "traditional" computing tools [1, 2].

The second (quantum computing algorithms and HW-computers) and third quantum (quantum programming and SW-engineering and quantum "powerful" computing AI) revolutions have led to the necessity in developing of intelligent SW/HW platform (strong quantum computational AI) of industrial quantum technologies for mega - science projects "Industry 5.0 / 6.0".

This fact, in turn, has raised the big challenge of training a new generation of quantum engineering staff in the fields of quantum end-to-end IT, quantum software engineering and quantum intelligent control.

The creation of an appropriate software-algorithmic platform and hardware support in view of a quantum computer for industrial development required a radical revision of the foundations of educational processes for quantum engineering, the creation of a new technological structure and mathematical / physical / technical background in dynamically developing areas of application of quantum end-to-end IT.

The lack of teaching staff and objective assessments of the necessity of industry and science for quantum engineering personnel only increased the difficulties in the development of quantum engineering. There is a certain mathematical maturity required to understand the quantum mechanics of finite dimensional systems. Here we will look at only the basics, and this is mainly to familiarize the reader with the notation used in the field of quantum computing and quantum information technology.

1. Mathematical objects of quantum mechanical control (simplified introduction)

Vector in Hilbert space. A Hilbert space is a vector space over with a complete inner product structure. By complete, we mean that all Cauchy sequences in the Hilbert space will converge to a point in the Hilbert space. For the purpose of this Introduction, all Hilbert spaces will be finite dimensional and we need not worry about the many complications which arise in infinite dimensional systems. Vectors in Hilbert space will be denoted using Dirac notation $|\psi\rangle$ and will denote an element in Hilbert space. The inner product between $|\psi\rangle$ and $|\phi\rangle$ will be $\langle\psi|\phi\rangle$ and adjoints will be denoted by Dirac bras $\langle\psi| = |\psi\rangle^{\dagger}$. Linear maps will either be denoted as matrices or as products of states and adjoints $A|\psi\rangle = \sum_{j,k} \alpha_{jk} |j\rangle\langle k|\psi\rangle$.

Pure State Quantum Mechanics. To describe a physical system as an information processor, we must discuss three components. First, we must specify the quantities *observable* via some measurement process called observables. We also must determine how these observables change with time. We finally must discuss how we can interact with these systems to bias the outcomes of observations. In order to fully describe the observation model in quantum mechanics, we first introduce a higher level of abstraction. We model the internal states of the system as vectors in a Hilbert space. This inner product structure induces a norm on the Hilbert space as $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$. We take the set of all accessible states to be the set of vectors with norm one.

The *state* of a quantum system evolves in time according to the Schrödinger equation

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle,$$

where H is a Hermitian operator called the Hamiltonian of the system and $\hbar = 1$.

We can now describe the observation model. We want to describe an interaction such that when the system is in the state $|n\rangle$, the measurement apparatus is in a state $|m(n)\rangle$. We set up a large Hilbert space, $\mathrm{H_S} \otimes \mathrm{H_A}$, where $\mathrm{H_S}$ is the Hilbert space of the system we wish to observe and $\mathrm{H_A}$ is the Hilbert space of the measurement apparatus we are using to observe the system. The interaction of the system with the apparatus is given by a Hamiltonian $\mathrm{H_{SA}}$.

The dynamics are governed by the Schrödinger equation

$$\frac{d|\psi\rangle}{dt} = -iH_{\mathrm{SA}}|\psi\rangle.$$

Let us suppose the system and the apparatus begin their interaction in the state $|\psi_{\mathrm{S}}\rangle|0_{\mathrm{A}}\rangle$ where the state $|0_{\mathrm{A}}\rangle$ represents the initialized state of the apparatus. We postulate that the measurement corresponds to a set of projection operators P_k, that sum to the identity, and a projection on the apparatus Hilbert space M_k corresponding to measuring the quantity "k." In this model, we have by the Schrödinger equation that the system will be in the state $|n_{\mathrm{S}}\rangle|m(n)\rangle_{\mathrm{A}}$.

That is, the apparatus reads "the system is in state n" and a quantum system must also be in the state $|n_{\mathrm{S}}\rangle$. In turn, we assign $|\alpha_k|^2$ to be the probability of measuring the state $|k\rangle$. Note that this measurement corresponds to a discontinuity in the dynamics of evolution.

The density matrix. While the pure state theory is fully consistent, it does not really help us to fully describe the quantum world. For example, we are unable to describe how a quantum system can interact with a macroscopic system such as a measurement apparatus. We can resolve all of these issues by remembering that our formulation only tells us how to *predict measurement* outcomes. The state of a quantum system is a convenient mathematical model only insofar as it predicts the results of experiments. It makes sense that the state should represent "*what we know*" about a quantum system at any particular time.

In this section, we will introduce a new object called *the density matrix* to describe our knowledge of a quantum system. We will also see how the density matrix gives us a powerful tool for describing how a quantum system interacts with much larger thermal systems.

Take a state $|\psi\rangle \in \mathrm{H}$ and write the matrix $|\rho\rangle = |\psi\rangle\langle\psi|$. This object is called the *density matrix* of the state $|\psi\rangle$. The density matrix is an element of $\mathrm{H} \otimes \mathrm{H}^*$. It has trace one, is positive semidefinite and is Hermitian. The Schrödinger equation now becomes

$$\frac{d\rho}{dt} = \frac{d}{dt}|\psi\rangle\langle\psi| = \frac{d|\psi\rangle}{dt}\langle\psi| + |\psi\rangle\frac{d\langle\psi|}{dt} = (-iH)|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|(-iH)^{\dagger}$$
$$= -(iH|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|iH) = -i[H,\rho].$$

Similarly, we can calculate the expectation values of observables with respect to the density matrix

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \mathrm{Tr}(A|\psi\rangle\langle\psi|) = \mathrm{Tr}(A\rho).$$

Unit vectors like $|\psi\rangle$ are called *pure states*. A pure state contains all the available physical information about the system, such as the expectation value of an observable A associated with hermitian operator A,

So, we can formulate quantum mechanics in terms of the density matrix instead of in terms of the state vector. This seems like too much work, as carrying matrices around for computation is more cumbersome than just using vectors, but the utility becomes clear when we allow any positive semidefinite Hermitian matrix with trace one to be a density matrix. Now, not only are there are more states available than we had before, but we can start to discuss the concepts of quantum ensembles and irreversible quantum processes.

Mixed states. Let H be a quantum system of dimension *N* with basis $\{|\psi_k\rangle\}$. Let $\{p_k\}$ be a probability distribution over these *N* basis vectors. Define the density matrix $\rho = \sum_{k=1}^{N} p_k |\psi_k\rangle\langle\psi_k|$ then this is a classical mixture of the states $|\psi_k\rangle$. Any measurement of this state is now biased by a classical probability distribution. Note that if all of the p_k are equal to zero except for one, the density matrix of the system is $|\psi\rangle\langle\psi|$ and this corresponds to a state in Hilbert space. We will call such a state a pure state, and note that a state is pure if and only if $\mathrm{Tr}\rho^2 = 1$. Otherwise, we say that the state is mixed. Let's explore these two cases. Given any density matrix ρ we can always diagonalize it into the form of equation $\rho = \sum_{k=1}^{N} p_k |\psi_k\rangle\langle\psi_k|$. The p_k are the eigenvalues of ρ. Since ρ is Hermitian, the $|\psi_k\rangle$ are all orthogonal, and hence we conclude that a state is pure if and only if it has 1 as an eigenvalue. Clearly, this also means that $\rho = |\psi\rangle\langle\psi|$ for a unique $|\psi\rangle$

Density operator can represent both pure and mixed states, and can be expressed in any basis $\mathrm{B} = \{|\phi_i\rangle\}_{i=1}^{d}$ of the Hilbert space H as

$$\rho = \sum_{i,j}^{d} \rho_{ij} |\phi_i\rangle\langle\phi_j| = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1d} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{d1} & \rho_{d2} & \cdots & \rho_{dd} \end{pmatrix},$$

where ρ_{ij} is the associated matrix element with row *i* and column *j*. The diagonal elements ρ_{ii} of the density matrix are known as populations and they denote the probabilities of finding the system in the respective basis states $|\phi_i\rangle$. The off-diagonal elements ρ_{ij} are known as *coherences*, and provide information about the coherent superposition of the basis states $|\phi_i\rangle$ and $|\phi_j\rangle$.

What is a mixed state then? Its eigenvalues, $\{p_k\}$, are not all ones and zeros. In this case, ρ is a probabilistic mixture of pure states. In this way, the density matrix quantifies our knowledge of a quantum state.

The density matrix allows us to consider component parts of quantum systems. If we have a state ρ in large quantum system with Hilbert space $\mathrm{H}_1 \otimes \mathrm{H}_2$ and we are only interested in the component in H_1, then if we let $|e_k\rangle$ be a basis for H_2, we can define the partial trace over H_2 as $\rho_1 = \sum_k \left(1 \otimes \langle e_k|\right) \rho \left(1 \otimes \langle e_k|\right) \equiv \mathrm{Tr}_2(\rho)$. One can readily check that this definition of partial trace is invariant under choice of the $|e_k\rangle$ and that for any $|\psi\rangle$, $|\phi\rangle$ in H_1

$$\langle\phi|\mathrm{Tr}_2(\rho)|\psi\rangle = \sum_k \langle\phi \otimes e_k|\rho|\psi \otimes e_k\rangle.$$

Returning to the discussion of measurement, consider a system-apparatus Hilbert space $\mathrm{H}_\mathrm{S} \otimes \mathrm{H}_\mathrm{A}$. The operators, $\{A_{jk}\}$, which perform measurement on an ensemble in H_S form a projection operator valued

measurement (POVM). The set of operators must satisfy $\sum_{j,k} A_{j,k}^{\dagger} A_{j,k} = 1$ and measurement corresponding to this POVM gives the result *j* with probability $p_j = \sum_{j,k} A_{jk} \rho_S A_{jk}^{\dagger}$.

In this case the system density matrix is in the state $\rho_j = \frac{1}{p_j} \sum_{j,k} A_{jk} \rho_S A_{jk}^{\dagger}$.

Again, we break down measurement into a set of probabilities and projection operators, but this is only a formal pair. A measurement still corresponds to the evolution of a Schrödinger equation corresponds to the state of the system after tracing out the measurement apparatus; ρ_j represents our knowledge of the system after a measurement.

Example. Let us consider the following bipartite pure state $|\psi(\theta)\rangle = \cos(\theta)|00\rangle + \sin(\theta)|11\rangle$, where $|00\rangle = |0\rangle_1 \otimes |0\rangle_2$, $|11\rangle = |1\rangle_1 \otimes |1\rangle_2$, and its associated density operator is given by $\rho(\theta) = |\psi(\theta)\rangle\langle\psi(\theta)|$. The state $\rho(\theta)$ is separable for $\theta = 0,\ \pi/2$, and entangled otherwise, being maximally entangled for $\theta = \pi/4$. As a result, for $\theta \neq k\pi/2$ the partial state of each subsystem $\rho_i(\theta) = \mathrm{Tr}_j[\rho(\theta)]$ is not pure, and is therefore an improper mixture.

To measure the degree of mixedness of a density operator we can use the purity P ,

$$\mathrm{P}[\rho] = \mathrm{Tr}[\rho^2] = \sum_{j=1}^{d} p_j^2 ,$$

which is bounded between 1, for pure states $\rho(\theta) = |\psi(\theta)\rangle\langle\psi(\theta)|$, and 1/*d*, for maximally mixed states $\rho = \mathbf{1}/d$.

The PYTHON script calculates the marginal state of the first subsystem, $\rho_1(\theta) = \mathrm{Tr}_2 \rho(\theta)$ showing that its purity $\mathrm{P}[\rho_1(\theta)] < 1$ for $\theta \neq k\pi/2$. Notice that $\rho_1(\theta)$ is maximally mixed when $\rho(\theta)$ is maximally entangled, i.e., $\mathrm{Tr}[\rho_1(\pi/4)] = 1/2$, as shown in Fig.1.

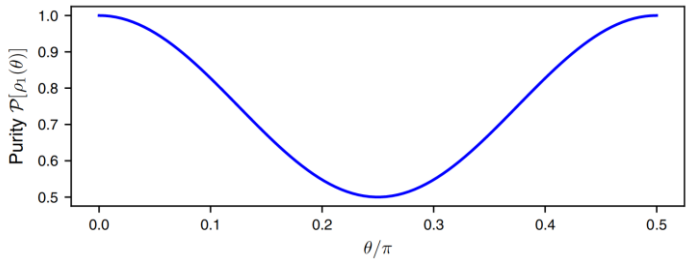


Fig. 1. Purity of the marginal state $\rho_1(\theta)$

It is easy to prove that the Hamiltonian dynamics does not change the purity of a system,

$$\frac{d}{dt}\mathrm{Tr}[\rho^2] = \mathrm{Tr}\left[\frac{d\rho^2}{dt}\right] = \mathrm{Tr}[2\rho\dot{\rho}] = -2i\mathrm{Tr}[\rho(H\rho - \rho H)] = 0 ,$$

where we have used the cyclic property of the trace. This result illustrates that the mixing rate of a state does not change due to the quantum evolution.

Remark. The evolution of an open quantum system is more complex. Suppose a system interacts with some other external system that has infinitely many degrees of freedom, which is essentially a classical system. This system is known as a bath or environment. In this case the system no longer evolves according to a Schrödinger equation. Instead, we now use a density matrix ρ to describe the system and its evolution is given

by a master equation. Assuming Markovianity, the master equation is Lindbladian. The ensemble representation allows us to further model measurement without projection at all. By a weak measurement, we mean a measurement of a quantum ensemble that only perturbs the density matrix by a small amount. If this perturbation is small enough, we can approximate the density matrix after the measurement to be identical to the density matrix before the measurement. An important feature of open quantum systems is the ability to alter these decay channels with feedback. This will be used extensively in this work. Typical quantum optical systems, such as optical cavities and two-level atoms can be modelled with relative ease due to their simple Markovian dynamics and hence their dynamics are well known.

A way of making these systems more complex is to introduce *quantum feedback*. This process has been used for a variety of tasks. Most notably in the literature, feedback is used for the stabilisation and control of quantum systems, usually for quantum information purposes. In this work, we shall see feedback used for a different purpose. In effect, the feedback used in the work acts to destabilise the system, inducing far more complex behavior in previously simple quantum optical systems. We also consider *the unravelling* of these master equations, allowing for the study of *individual quantum trajectories*.

We first consider a general quantum system that interacts with a surrounding bath. This bath is assumed to also interact with an external environment, which causes it to thermalise continuously. More concretely, the environment constantly resets the bath into its environmentally preferred state - its so-called *pointer* state. Hence, the resulting effective time evolution of the open quantum system is approximately Markovian and its density matrix ρ_{S} obeys a master equation in Lindblad form. This master equation can be unravelled into an infinite set of physically-meaningful quantum trajectories. An unravelling involves splitting the overall average evolution into its individual components and looking at a possible evolution along such a path. Considering such an unravelling and assuming that any instantaneous quantum feedback is triggered by sudden changes of the state of the quantum system, it becomes clear how to incorporate instantaneous feedback into the master equation.

2. The Lindblad equation – density operator master equations

Master equations are differential equations used to model the dynamics of systems that can be described as a probabilistic combination of some states. We can interpret p_i as the probability of being in state i and can generalize this idea to formulate master equations as first-order differential equations to the vector of probabilities $p = (p_1, \ldots, p_n)$ of being in one of the n states of some system of interest. As a result, the dynamics of the state's probabilities are prescribed by the master equation $\dot{p} = F(p,t)$ with F often being a linear function of p represented by some generating matrix A, as in $\dot{p} = Ap$. However, when dealing with quantum systems we must take into account that coherent superpositions of states participate in the evolution, as prescribed by Schrödinger's equation $\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar} H |\psi(t)\rangle$, where H is the Hamiltonian of the system, and $|\psi(t)\rangle = \sum_{j=1}^{n} c_j(t)|\phi_j\rangle$ is its state at time t, expressed as a coherent superposition of the eigenstates $\mathrm{B}_H = \{|\phi_1\rangle, \ldots, |\phi_n\rangle\}$ of the Hamiltonian, via the normalised complex coefficients $c_j(t)$ satisfying $\sum_i |c_i(t)|^2 = 1$. In this case, a vector of probabilities p, with $p_i = |c_i|^2$, is no longer sufficient to completely describe the dynamics of the system, since different phases of c_i will lead to different solutions. Master equations for the dynamics of quantum systems can then be expressed by employing another representation of the state of the system, known as the density operator ρ. As discussed in details below, the density operator contains all the information regarding the probabilities (known as *populations*) of being in each state i, given by $p_i = \langle\phi_i|\rho|\phi_i\rangle$, as well as the phases (known as *coherences*) $\varphi_{ij} = \langle\phi_i|\rho|\phi_j\rangle$ associated with the coherent superpositions between basis states $|\phi_i\rangle$ and $|\phi_j\rangle$.

Quantum master equations (QMEs) are then formulated by generalisation of Eq. $\dot{p} = F(p,t)$, as first-order differential equations to the density operator, $\dot{\rho} = \mathrm{F}(\rho,t)$. One of the key aspects of QMEs is that they provide a coarse-grained stochastic description of the effect of unknown and

uncontrollable agents on a system of interest, leading to a computationally inexpensive ensemble-averaged picture of the dynamics of quantum systems. QMEs can be phenomenological or derived, using first principles, from a microscopic model of the system-environment interactions. They can be used to derive qualitative trends or make quantitatively accurate predictions. They are just as suitable for the derivation of analytical results as they are for the numerical simulation of complex systems with a large number of degrees of freedom.

For these reasons, QMEs, illustrated in Fig. 2, have become a standard approach to model the dynamics of quantum systems, and they have become a starting point for the formulation of more sophisticated descriptions.

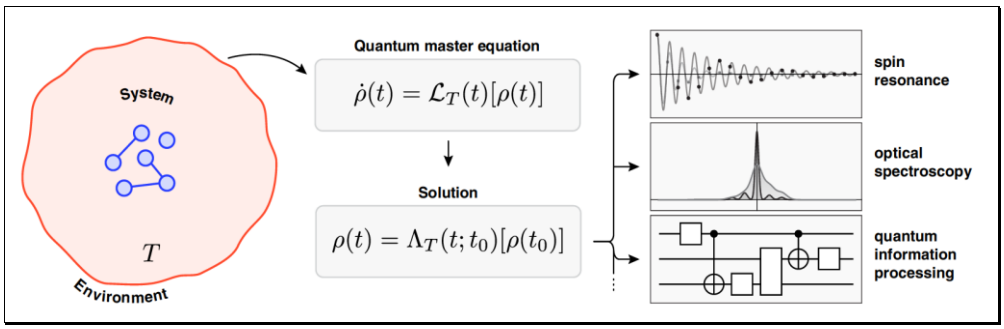


Fig. 2. QMEs provide a coarse-grained prescription for the dynamics of a quantum system (blue) that interacts weakly with its environment (red) [3]

The state ρ of the quantum system, represented by the density operator, evolves according to some master equation $\dot{\rho}(t) = \mathrm{L}_T\left[\rho(t)\right]$, where the Liouville superoperator $\mathrm{L}_T(t)$ generating the evolution may depend on time t and on the temperature T of the environment. The solution $\rho(t) = \Lambda_T(t,t_0)\left[\rho(0)\right]$ (and the master equation itself) can be used to study the steady-state and nonequilibrium properties of the system. QMEs are a staple tool for modeling spin resonance, optical spectra, and quantum information processing, and their use is certainly not limited to these fields and applications.

The power of master equations resides in the choice of ignoring the environment's dynamics, often uncontrollable and inaccessible. By neglecting the environment's degrees of freedom, we can limit the scaling of the computational requirements to a polynomial of $d = \dim \mathrm{H_S}$, where $\mathrm{H_S}$ is the system's Hilbert space.

In this section we introduce quantum master equations and focus on their numerical implementation and solution, providing direction for further readings. We briefly review the mathematical description of the state of a quantum system, focusing on the numerical implementation of state vectors and density operators.

3. Quantum Information

Let us consider examples of quantum information that in context of textbook are used.

3.1 Quantum entropy and information amount

Defining the entropy of a density matrix as $S(\rho) = -\mathrm{Tr}(\rho \ln \rho)$ it is straightforward to show that

$$S(\rho) = -\mathrm{Tr}(\rho \log \rho) = -\mathrm{Tr}\left(\sum_k p_k |\psi_k\rangle\langle\psi_k|\right)\log\left(\sum_k p_k |\psi_k\rangle\langle\psi_k|\right) = -\mathrm{Tr}\left(\sum_k p_k \log p_k |\psi_k\rangle\langle\psi_k|\right)$$
$$= -\sum_k p_k \log p_k$$

The meaning of this derivation is that quantum entropy measures the classical entropy of the probability distribution $\{p_k\}$. It should be clear from this definition that a state is pure if and only if its entropy is zero.

Remark. The usual definition of entropy in quantum mechanics is von Neumann entropy (von Neumann, 1932), which is the natural analog to Shannon entropy. One can likewise define a quantum analog to Renyi

entropy. These definitions are for the standard representation of quantum mechanics. The question in this section is what are the natural definitions of Shannon and Renyi entropy in phase-space representations of quantum mechanics (Wigner, 1932; Feynman, 1987; Wootters, 1987; Gibbons, Hoffman, and Wootters, 2004). The issue is the negativity of phase-space probabilities – what are often called quasi-probabilities. Since both Shannon and Renyi entropies involve log terms, they can both become complex-valued in this case, which does not admit an obvious interpretation in terms of the amount of uncertainty about a system. and modify the axioms so that entropy retains its natural meaning in the presence of negative probabilities. In fact, it is possible axiomatize what was called signed Shannon and signed Renyi entropies for all signed measures, not just those normalized to sum to 1, to increase the scope of application of developed theory. Interestingly, the usual relationship between Shannon entropy and Renyi entropy – namely, that Shannon entropy is the limit of Renyi entropy as the free parameter α in Renyi entropy tends to 1 – no longer holds in this case. Renyi entropy and Shannon entropy are no longer nested (in the sense of a limit) once signed measures are admitted.

That is, we can obtain two quite distinct notions of entropy for signed measures.

Definition 1. Given a signed measure Q with $w(Q) \neq 0$ (the quantity $w(Q) = \sum_{i=1}^{n} q_i$ is called the weight of Q), the signed Shannon entropy of Q is defined by:

$$H_{Sh}(Q) = -\frac{\sum_{i=1}^{n} |q_i| \log_2 |q_i|}{\left| \sum_{i=1}^{n} |q_i| \right|}.$$

Definition 2. Given a signed measure Q with $w(Q) \neq 0$, the signed Renyi entropy of Q is defined, for $\alpha > 0$ with $\alpha \neq 1$, by:

$$H_{\alpha}(Q) = -\frac{1}{1-\alpha} \log_2 \left[\frac{\sum_{i=1}^{n} |q_i|^{\alpha}}{\left| \sum_{i=1}^{n} |q_i| \right|} \right].$$

Remark. In their extension of Renyi entropy to signed probabilities, Koukouledikis and Jennings (2022) assume that $\alpha = 2a/(2b - 1)$, where a, b are positive integers with $a \geq b$, so that q_i^{α} is non-negative real-valued and the usual Renyi formula remains real-valued. Of course, in this same case, we can drop the absolute-value operations. Moreover, if Q is a signed probability measure, then, again in this case, further reduces to the usual definition of Renyi entropy, and the definition coincides with the Koukouledikis-Jennings one.

Example. While signed Renyi entropy is non-decreasing, signed Shannon entropy may not be. Let the matrix of transition rates be given by:

$$\Lambda = \begin{pmatrix} -1 & 1/2 & 1/2 \\ 1/2 & -1 & 1/2 \\ 1/2 & 1/2 & -1 \end{pmatrix},$$

and choose the initial signed probability measure: $Q(0) = (-1/7, 3/7, 5/7)$.

Figure 3 (generated by ChatGPT 4o) shows the evolution of signed Renyi 2-entropy $H_2(t)$ and signed Shannon entropy $H_{Sh}(t)$. While signed Shannon entropy converges to the same limit $\log 2\ 3 \approx 1.585$ as does signed Renyi 2-entropy, we see that it is transiently non-monotonic.

We can also use arguments about entropy to characterize the state of a quantum system based only on the information that we have about it. For example, suppose we have a quantum system with Hamiltonian H and we know that the total energy of the system is E. Let $|\psi_k\rangle$ be the eigenstates of H with the eigenvalues E_k. Given no other information, we can assign a state to this system by imposing the maximum entropy principle. This principles states that we should assign the state with the largest entropy satisfying the constraint equations for the system.

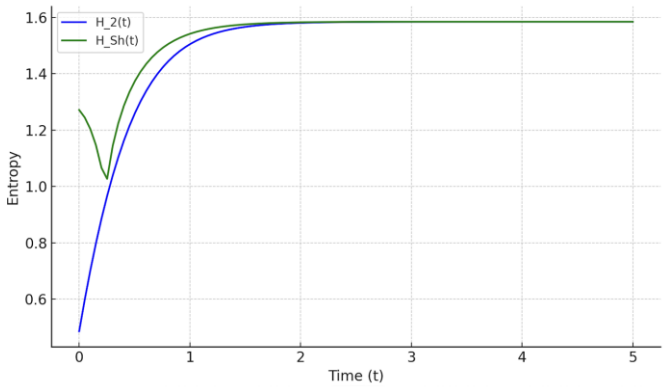


Fig. 3. Evolution of signed Renyi and signed Shannon entropies [4].

That is, the quantum state we assign only represents the information that we have about the system. Such a state can be found using variational methods $\rho_B = \frac{\sum_k \exp(-\beta E_k)|\psi_k\rangle\langle\psi_k|}{\sum_k \exp(-\beta E_k)}$ and is called the Boltzmann distribution. The quantity $\beta = k_B T$ is the familiar function of temperature from thermodynamics and $\mathrm{Z} = \sum_k \exp(-\beta E_k)$ is called the partition function of the system. Extending these definitions of quantum information, we can introduce a measure of quantum correlations called entanglement, which definitively distinguishes between quantum and classical distributions.

3.2. Entanglement

Entanglement is what makes quantum mechanics quantum. The odd behaviors and correlations that we don't typically see in the macroscopic world arise from parts of the density matrix that are not classical. Indeed, to show that unitary correction schemes can preserve inherently quantum in-formation, it suffices to show that entangled states can be preserved for an arbitrarily long time.

First, we can quantify the entanglement of a pure quantum system. Given two coupled quantum systems with Hilbert Space $\mathrm{H}_A \otimes \mathrm{H}_B$, we say that a state $|\psi\rangle$ is entangled if it cannot be expressed as a product $|\psi_1\rangle_A |\psi_2\rangle_B$. We can measure the entanglement of identical systems as follows. First, we note that any pure quantum state can be written as $|\psi\rangle = \sum_k \alpha_k |k\rangle_A |k\rangle_B$ where the $|k\rangle_A$ and $|k\rangle_B$ are an orthonormal set of states for *A* and *B* respectively and the α_k, called the Schmidt coefficients of $|\psi\rangle$, are positive real numbers. The Schmidt coefficients are unique for a given $|\psi\rangle$ and hence the measure $E(\psi) = S(\alpha_k) = -\sum \alpha_k \log \alpha_k$ is well defined. It is called the *entanglement* of $|\psi\rangle$ and ranges between 0 and 1.

Now what about for mixed states? We can define the entanglement of formation as

$$E(\rho) = \min \sum_k p_k E(\psi_k),$$

where the minimum is taken over all ensembles of pure states satisfying $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$.

It is called the *entanglement of formation* as it is the minimum entanglement required to produce a particular mixed state from pure states. Whenever $E(\rho) > 0$, we can say that the density matrix describes a state which is allowed by the laws of quantum mechanics but not by the classical laws of probability.

4. Open Quantum Systems

We will generalize the notion of unitary evolution to a new concept of quantum dynamical semigroups and show that these dynamics are generated by a differential equation called the *Lindblad equation*. This equation describes the dynamics of all decoherence processes.

4.1 Kraus Operators

Let's return to the evolution of a quantum system coupled to an environment that we initially discussed in the pure state case. Let the system of interest have Hilbert space $\mathrm{H_S}$ and the environment have Hilbert space H_E. Their joint Hilbert space is $\mathrm{H_S} \otimes \mathrm{H}_E$. We'll use the word "environment" as an umbrella term to describe any quantum system which interacts with $\mathrm{H_S}$, but whose dynamics are not of interest themselves. The environment could be a measurement apparatus, a thermal heat bath, or even another microscopic quantum system. The goal will be to find the state of the quantum system after it interacts with an environment. Assume that we begin initially uncorrelated in the state $\rho_S \otimes \rho_A$. The system and environment will then evolve according to unitary dynamics $U_t \rho_S \otimes \rho_A U_t^\dagger$. The resulting state of our system can be found by tracing out the environment $\rho(t) = \mathrm{Tr}_A\left(U_t \rho_S \otimes \rho_A U_t^\dagger\right)$. What if we want to ignore the environment altogether? If we are only interested in a particular mode of interaction and not the environment itself, can we find a class of dynamics which describes all possible interactions with all possible environments? These questions are intentionally leading.

We can, in fact, describe all physically allow-able transformations on density matrices in a compact form. The key insight is to introduce a basis $\left\{\left|e_l\right\rangle\right\}$ for the Hilbert space H_E such that $\rho_A = \sum_l \lambda_l \left|e_l\right\rangle\left\langle e_l\right|$ and a basis $\left\{\left|\psi_j\right\rangle\right\}$ for $\mathrm{H_S}$ such that $\rho_S = \sum_j p_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$. The unitary evolution can be written in this basis as $U\left|\psi_j\right\rangle\left|e_l\right\rangle = \sum_{m,n} U_{jl,mn}\left|\psi_m\right\rangle\left|e_n\right\rangle$ and acting on the state $\rho_S \otimes \rho_A$, we find

$$U_t \rho_S \otimes \rho_A U_t^\dagger = \sum_{j,l,m,n,r,s} p_j \lambda_l U_{jl,mn}\left|\psi_m\right\rangle\left|e_n\right\rangle\left\langle\psi_r\right|\left\langle e_s\right|\bar{U}_{rs,jl}.$$

The partial trace can now be written by setting $r = s$ and removing the $\left|e_l\right\rangle$'s

$$\mathrm{Tr}_E\left(U_t \rho_S \otimes \rho_A U_t^\dagger\right) = \sum_{j,l,m,n,r} p_k \lambda_l U_{jl,mn}\left|\psi_m\right\rangle\left|\psi_r\right\rangle\bar{U}_{rn,jl}$$

$$= \sum_{l,n}\sum_j p_j \left(\sum_m \sqrt{\lambda_l} U_{jl,mn}\left|\psi_m\right\rangle\right)\left(\sum_r \left\langle\psi_r\right|\sqrt{\lambda_l} U_{jl,mn}\left|\psi_m\right\rangle\right) \equiv \sum_k E_k \sum_j p_j \left|\psi_j\right\rangle\left\langle\psi_j\right| E_k^\dagger = \sum_k E_k \rho_S E_k^\dagger$$

where the E_k are operators on $\mathrm{H_S}$ and are defined by summing over l and n. It is straightforward to check that $\left(\sum_k E_k^\dagger E_k\right)_{rs} = \sum_{l,n,a} \lambda_l \bar{U}_{rl,an} U_{sl,an} = \sum_l \lambda_l \delta_{rs} = \delta_{rs}$.

That is $\sum_k E_k^\dagger E_k = 1$. The operators E_k are called *Kraus operators*, named for their discoverer Karl Kraus. The map in last equation is called a quantum operation.

The reduced map is given by the Kraus operators we started with. Indeed, when the environment begins in the state $\rho_E = \left|e_1\right\rangle\left\langle e_1\right|$ we have

$$\mathrm{Tr}_E\left(U \rho_S \otimes \rho_E U^\dagger\right) = \mathrm{Tr}_E\left(\sum_{j,k} E_j \rho_S E_k^\dagger \left|e_j\right\rangle\left\langle e_k\right|\right) = \sum_{j,k,l} E_j \rho_S E_k^\dagger \left\langle e_l\right|e_j\rangle\left\langle e_k\right|e_l\rangle = \sum_k E_k \rho_S E_k^\dagger.$$

So, we have found that the most general form of quantum dynamics is the set of all maps of the form $\rho \mapsto \sum_k E_k \rho_S E_k^\dagger$ where $\sum_k E_k^\dagger E_k = 1$. Many different unitary processes can give rise to the same Kraus operators. Similarly, there is a large freedom in the representation of the E_k.

4.2. The Lindblad equation

Let E be a quantum process which satisfies $\mathrm{E}_t \mathrm{E}_s = \mathrm{E}_{t+s}$. That is, if the operation acts for time *s* and then for time *t* then this is equivalent to the operation acting for time *t* + *s*. The dynamics of such a system would be Markovian, and a map satisfying $\mathrm{E}_t \mathrm{E}_s = \mathrm{E}_{t+s}$ is called a *quantum dynamical semigroup*. It is only "semi" as the inverses of the maps E_t are not necessarily defined. Indeed, only in the case where E_t is unitary is a quantum process reversible (i.e., invertible). Just as in the case of unitary dynamics, a quantum dynamical semigroup is completely characterized by its generator, or its derivative at *t* = 0. This is because the maps E are linear, and hence there exists a linear map *L* satisfying E_t = exp (*Lt*).

The generator must satisfy $\frac{d\mathrm{E}_t(\rho)}{dt} = L\mathrm{E}_t^\dagger(\rho)$ and is the *Lindblad Equation*. We can derive the form of the Lindblad equation as follows. Let F_k be a basis for M_N with $F_0 = 1$. Then

$$\mathrm{E}_t(\rho) = \sum_k E_k \rho E_k = \sum_{k,l,m} \left(r_{kl}(t) F_l\right) \rho \left(\bar{r}_{km}(t) F_m^\dagger\right) = \sum_{k,l,m} r_{kl}(t) \bar{r}_{km}(t) F_l \rho F_m^\dagger = \sum_{l,m} c_{lm}(t) F_l \rho F_m^\dagger ,$$

where $c_{lm} = \sum_k r_{kl}(t) \bar{r}_{km}(t)$. Note that $c_{lm} = \bar{c}_{ml}$ and $c_{00}(0) = 1$ and $c_{lm}(0) = 0$ for all *l*, *m*.

The time derivative is easily evaluated:

$$\begin{aligned} L(\rho) &= \lim_{\varepsilon \to 0} \frac{\mathrm{E}_t - 1}{\varepsilon}(\rho) = \lim_{\varepsilon \to 0} \frac{c_{00}(\varepsilon) - 1}{\varepsilon} \rho + \sum_l \frac{c_{l0}}{\varepsilon} F_l \rho + \sum_m \frac{\bar{c}_{m0}}{\varepsilon} \rho F_m^\dagger + \sum_{l,m} \frac{c_{lm}}{\varepsilon} F_l \rho F_m^\dagger \\ &= A\rho + \rho A^\dagger + \sum_{l,m} \alpha_{lm} F_l \rho F_m^\dagger \end{aligned} .$$

Bear with us for a second, we will simplify these calculations into a much more compact form.

First note that the dynamics must preserve the trace of ρ and, subsequently, Tr($L(\rho)$) = 0.

This means that for all

$$\rho : \mathrm{Tr}\left(A\rho + \rho A^\dagger + \sum_{l,m} \alpha_{lm} F_l \rho F_m^\dagger \right) = \mathrm{Tr}\left(\left[A + A^\dagger + \sum_{l,m} \alpha_{lm} F_l F_m^\dagger \right] \rho \right) = 0$$

using the cyclic property of the trace. But this in turn means that $A + A^\dagger = -\sum_{l,m} \alpha_{lm} F_l F_m^\dagger$.

Performing some rearranging yields

$$\begin{aligned} A\rho + \rho A^\dagger &= \frac{1}{2}\left(A\rho + A\rho + \rho A - \rho A + \rho A^\dagger + \rho A^\dagger + A^\dagger \rho - A^\dagger \rho \right) \\ &= \frac{1}{2}\left(A\rho - A^\dagger \rho - \rho A + \rho A^\dagger \right) + \frac{1}{2}\left(A\rho + A^\dagger \rho + \rho A + \rho A^\dagger \right) \\ &= \left[\frac{1}{2}\left(A - A^\dagger \right), \rho \right] + \frac{1}{2}\left(A + A^\dagger \right)\rho + \frac{1}{2}\rho\left(A + A^\dagger \right) \end{aligned}$$

and for any *A*, $A-A^{\dagger}$ is skew symmetric. This means that $H=\frac{i}{2}\left(A-A^{\dagger}\right)$ is Hermitian. Plugging these results into $L(\rho)$ gives $L\rho=-i[H,\rho]-\frac{1}{2}\sum_{l,m}\alpha_{lm}\left(F_m^{\dagger}F_l\rho+\rho F_m^{\dagger}F_l-2F_l\rho F_m^{\dagger}\right)$ or, breaking the second term into commutators

$$L\rho=-i[H,\rho]+\frac{1}{2}\sum_{l,m}\alpha_{lm}\left(\left[F_l\rho,F_m^{\dagger}\right]+\left[F_l,\rho F_m^{\dagger}\right]\right).$$

This fully describes all possible quantum dynamical semigroups.

Once we have chosen a basis F_k, we need only specify a Hermitian matrix *H* and a positive semidefinite operator $A = (a_{jk})$. Of course, this structure is dependent on the basis F_k, and the form of equation $L\rho$ is not unique.

Note that in the case $A = 0$, the Lindblad equation reduces to the Schrödinger equation and the dynamics are unitary. The term $-i[H,\rho]$ is the Hermitian part of the Lindblad equation. On the other hand, all of the dissipative non-unitary dynamics can be found in the double commutator terms. These are called the *dissipative part* of the Lindblad equation.

Note that if we diagonalize the matrix *A*, we are left with the Lindblad equation

$$L\rho=-i[H,\rho]+\frac{1}{2}\sum_{k}\left(\left[L_k\rho,L_k^{\dagger}\right]+\left[L_k,\rho L_k^{\dagger}\right]\right)$$

in the form originally discovered by Lindblad (see, Preface).

Finally, by definition of the coefficients, α_{ij} can be arranged to form a Hermitian, and therefore diagonalizable, matrix. By diagonalizing it, we obtain the diagonal form of the Lindblad master equation. We can also derive the Lindblad equation from the old unitary picture as following:

$$\dot{\rho}=-\frac{i}{\hbar}[H,\rho]+\sum_{k}\Gamma_k\left(L_k\rho(t)L_k^{\dagger}-\frac{1}{2}\left\{L_kL_k^{\dagger},\rho(t)\right\}\right), \qquad (1)$$

where ρ is the system's density operator, *H* is the Hamiltonian of the system, and $\{L_k\}$ are the Lindblad operators representing some nonunitary processes such as relaxation or decoherence that occur at some rates $\{\Gamma_k\}$. The operators [.,.] and {.,.} denote the commutator and anticommutator of the operands. From now on, *H* represents the Hamiltonian of the system, unless specified otherwise.

Example: *Solving the dynamics of the system*. Let us discuss how to solve Eq. (1) in order to obtain the state of the system $\rho(t)$ at any time *t* from a given initial condition $\rho_0 = \rho(t_0)$. We can represent the solution with the dynamical map $\rho(t)=\Lambda(t,t_0)\rho_0$. For linear, time-independent generators L, the solution to $\dot{\rho}=\mathrm{L}\rho$ can be obtained by calculating the following matrix exponential: $\rho(t)=\exp\left[\mathrm{L}(t-t_0)\right]\rho(t_0)$; the operator $P(t,t_0)=\exp\left[\mathrm{L}(t-t_0)\right]$ is called the "*propagator*" of the evolution.

We have implicitly represented the propagator $P(t,t_0)$ as a matrix, i.e., by applying the same reshaping function that we used to vectorize $\rho \rightarrow \boldsymbol{\rho}$ to both of its index pairs. Then one can represent the solution as a density operator $\rho(t)$ just by applying the inverse reshaping on $\rho(t)$.

Example. Let us study the eff ect of temperature on a physical implementation of a quantum logic gate. We consider the Hadamard–controlled NOT (CNOT) gate, given by the sequential composition of the Hadamard gate *H* on the first qubit

$$U_1 = H \otimes 1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes 1,$$

and the CNOT gate

$$U_2 = \text{CNOT} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

In practice, the gate is implemented by means of two time-independent Hamiltonians H_1 and H_2,

$$H_1 = \frac{1}{2}\left(1 - \frac{\sigma_z + \sigma_x}{\sqrt{2}}\right) \otimes 1, \quad H_2 = \frac{1-\sigma_z}{2} \otimes \frac{1-\sigma_x}{2}$$

that act on some initial state for some time $\tau = \pi$.

The *resulting* gate, shown in Fig. 4, can be used to obtain the (maximally entangled) Bell state

$$\left|\Phi_+\right\rangle = \frac{\left|00\right\rangle + \left|11\right\rangle}{\sqrt{2}} = U_2 U_1 \left|00\right\rangle,$$

starting from the fiducial input state $\left|00\right\rangle$.

The purity of the output state $\mathrm{P}\left[\rho_{\text{out}}\right] = \mathrm{Tr}\left[\rho_{\text{out}}^2\right]$ shows that as the temperature increases, the implemented gate is no longer unitary, and instead maps an initially pure state to a mixed state.

A temperature-dependent decoherence process affects the performance of the gate implementation via dephasing and relaxation rates $\{\gamma_k(T)\}$, which are greater as the thermal energy $k_B T$ increases with respect to the energy gap $\hbar\omega_0$ between ground $\left|0\right\rangle$ and excited $\left|1\right\rangle$ states, with k_B being. As a result, the output state $\rho_{\text{out}} = \Lambda_2(\tau)\left[\Lambda_1(\tau)\left[\rho_{\text{in}}\right]\right]$ differs from the target state $\left|\Phi_+\right\rangle = U_2 U_1 \left|00\right\rangle$.

In practice, decoherence processes, such as dephasing and relaxation, prevent us from implementing ideal unitary gates as U_1 and U_2. As a result, the output state is, in general, a mixed state, $\rho_{\text{out}} = \Lambda_2(\tau)\left[\Lambda_1(\tau)\left[\rho_0\right]\right]$. In this example, the effect of temperature is modeled via some temperature-dependent transition rates $\gamma_k(T)$, which are greater as the temperature increases, as prescribed by Bloch-Redfield theory.

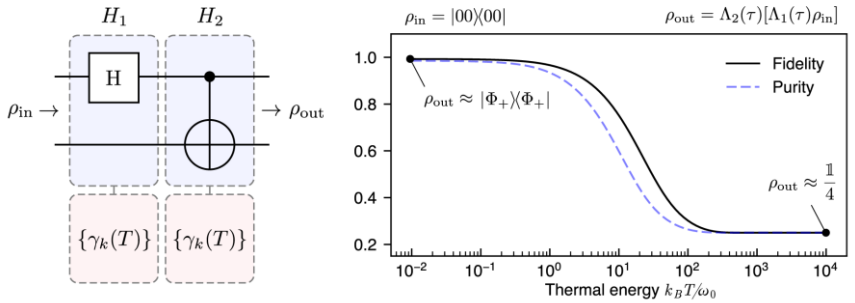


Fig. 4. Left: A Hadamard-CNOT gate is implemented with two time-independent Hamiltonians H_1 and H_2. Right: The difference is measured here with use of the fidelity [3]; $\mathrm{F}\left(\rho,\sigma\right) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]\right)^2$ which is equal to 1 when $\rho = \sigma$ i.e., when $\rho_{\text{out}} = \left|\Phi_+\right\rangle\left\langle\Phi_+\right|$

Remark. Like the Hamiltonian generates coherent dynamics, the Lindblad operators generate incoherent transitions in the space of states. Unlike the Hamiltonian, they do not need to be Hermitian. For example, a decay transition from some excited state $|e\rangle$ to some ground state $|g\rangle$ is mediated by the Lindblad operator $L_{\downarrow} = |g\rangle\langle e|$. Indeed, when we apply $L_{\downarrow}$ to $|e\rangle$, we obtain $|g\rangle = L_{\downarrow}|e\rangle$. Note that $L_{\downarrow}^{*} = |e\rangle\langle g| \neq L_{\downarrow}$. Eq. (1) is used to approximate the evolution of the density operator of a system S with Hamiltonian *H* that is weakly coupled to a *Markovian* (memoryless stochastic process) environment. The GKSL master equation is the general form for a completely positive and trace-preserving Markovian and time-homogeneous map for the evolution of the system's density operator *ρ*.

Example: *Time dependency of the two-level system with decay*. Continuing example of a two-level atom, we can make it more realistic by including the possibility of atom decay by the emission of a photon. This emission happens due to the interaction of the atom with the surrounding vacuum state. (This is why atoms decay.) The complete quantum system would be in this case the "atom + vacuum" system, and its time evolution should be given by the von Neumann equation, where *H* represents the total "atom + vacuum" Hamiltonian. This system belongs to an infinite-dimension Hilbert space, as the radiation field has infinite modes. If we are interested only in the time dependence of the state of the atom, we can derive a Markovian master equation for the reduced density matrix of the atom. The master equation we will study is

$$\frac{d}{dt}\rho(t) = -i[H,\rho] + \Gamma\left(\sigma^{-}\rho\sigma^{=} - \frac{1}{2}\{\sigma^{-}\sigma^{=},\rho\}\right), \qquad (2)$$

where Γ is the coupling between the atom and the vacuum.

We show some results of solving Eq. (2) and calculating the density matrix as a function of time. A Mathematica notebook solving this problem. To illustrate the time behavior of this system, we calculate the evolution for different state parameters. In all cases, we start with an initial state that represents the state being excited $\rho_{11} = 1$, with no coherence between different states, meaning $\rho_{01} = \rho_{10} = 0$. If the decay parameter Γ is equal to zero, the problem reduces to solve the von Neumann equation, and the result is displayed in Fig. 5.

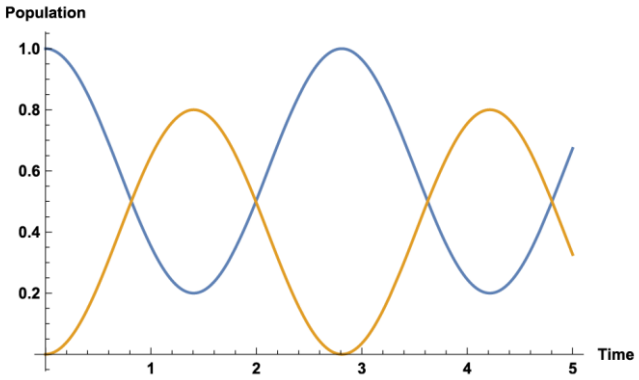


Fig. 5. Population dynamics under a quantum dynamic (parameters are Ω = 1 and E = 1) [5]. [The blue line represents ρ_{11} and the orange one ρ_{00}.]

In this case the evolution of our isolated two-level system is described by its Hamiltonian, $H_{\text{Free}} = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$. As the system was already in an eigenvector of the Hamiltonian, its time-evolution consists only in adding a phase to the state, without changing its physical properties. (If an excited state does not change, why do atoms decay?)

Without losing any generality, we can fix the energy of the ground state as zero, obtaining $H_{\text{Free}} = E_1|1\rangle\langle 1|$ with $E \equiv E_1$. To make the model more interesting, we can include a driving that coherently switches between both states. The total Hamiltonian would be then $H = E|1\rangle\langle 1| + \Omega\,(|0\rangle\langle 1| + |1\rangle\langle 0|)$, where Ω is the frequency of driving. The system is then driven between the states, and the populations present Rabi oscillations, as it is shown in Fig. 6.

The other extreme case would be a system with no coherent dynamics ($\Omega = 0$) but with decay. In this case, as shown in Fig. 6, we observe an exponential decay of the population of the excited state. Finally, we can calculate the dynamics of a system with both coherent driving and decay. This is displayed in Fig. 7.

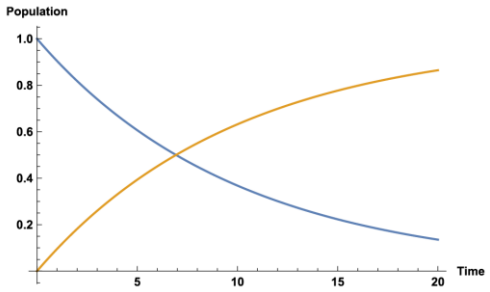


Fig. 6. Population dynamics under a pure incoherent dynamic ($\Gamma = 0.1$, $n = 1$, $\Omega = 0$, and $E = 1$). [The blue line represents ρ_{11} and the orange one ρ_{00}.]

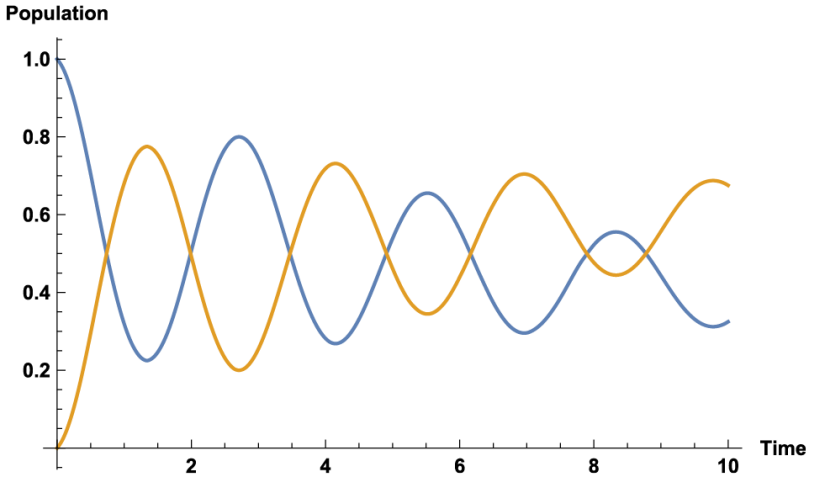


Fig. 7. Population dynamics under a pure incoherent dynamic ($\Gamma = 0.2$, $n = 1$, $\Omega = 0$, and $E = 1$). [The blue line represents ρ_{11} and the orange one ρ_{00}.]

In this case, both behaviors coexist and there are oscillations and decay.

4.3. Reduced Hamiltonian control

Open Markovian quantum systems with fast and full Hamiltonian control can be reduced to an equivalent control system on the standard simplex modelling the dynamics of the eigenvalues of the density matrix describing the quantum state. In practice of quantum control it explore this reduced control system for answering questions on reachability and stabilizability with immediate applications to the cooling of Markovian quantum systems. For certain tasks of interest, the control Hamiltonian can be chosen time-independent. The reduction picture is an example of dissipative interconversion between equivalence classes of states, where the classes are induced by fast controls. Often a major obstacle towards realizing quantum technologies roots in uncontrolled or unmitigated noise. Hence systematic effort is being put into achieving significant progress in reducing noise in current hardware (see, e.g., the [6-8] and refs. therein) on one hand. On the other hand, quantum optimal control [9-14] lends itself to complement these efforts to further mitigate noise on the ‘software’ side, or in other cases to modulate noise in order to even exploit it as additional control resource beyond coherent controls (see, e.g., the quantum control roadmap [7] and refs. therein). A practical instance is quantum error correction with noise-assisted quantum feedback. In any case, every quantum system that can be externally controlled must interact with its environment and hence is also subject to decoherence. Thus, we accept noise as natural ‘part of the game’ when studying what can be achieved in spite of (or even thanks to) such noise.

The main tool used here is a reduction of a full bilinear control system $\dot{X}(t)=\left(A+\sum_j u_j B_j\right)X(t)$ evolving on the space of Hermitian matrices X(t), to a reduced one $\dot{\lambda}=-L_U\lambda(t)$ describing the dynamics of the eigenvalues of X(t). The reduced system is obtained by factoring out the unitary action, which is possible as soon as one has fast unitary controllability. In the finite-dimensional quantum dynamical systems treated here, henceforth X(t) ≡ ρ(t) is a density matrix representing the state of the system, and so its eigenvalues sum up to 1. Thus λ(t) lives in the standard simplex, which then forms the reduced state space. Obviously, such a reduced system is easier to analyze (and visualize) than the full set of density matrices. See Fig. 8 for an illustration of this approach.

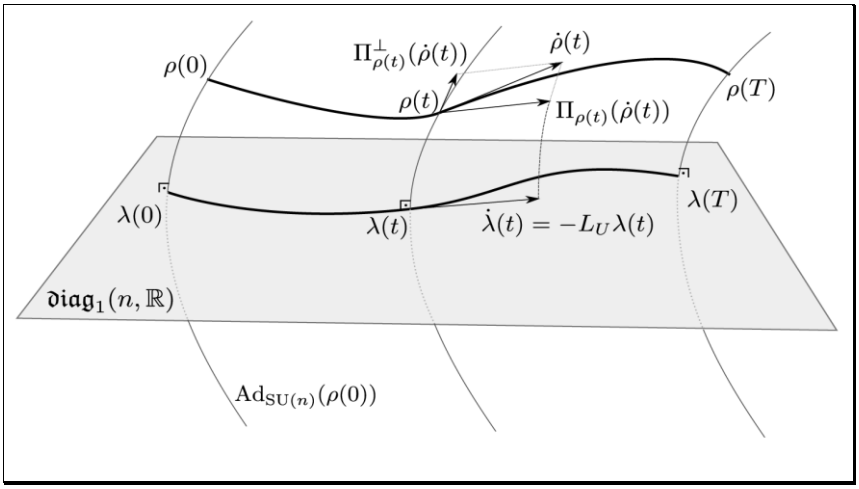


***Fig. 8**. Relationship between the time evolutions of a bilinear control system (B) on density matrices ρ(t) and the reduced control system (R) governing the dynamics of the eigenvalues of ρ(t), where "the" vector λ(t) of eigenvalues is depicted by the respective diagonal matrix diag(λ(t)). The derivative $\dot{\rho}(t)$ can always be split into a part orthogonal to the orbit (using the orthogonal projection $\Pi_{\rho(t)}$ onto the commutant of ρ(t)), and a part tangent to the orbit (using the complementary projection $\prod^{\perp}_{\rho(t)}$) [15]*

The general idea of reducing control systems admitting fast control on a Lie group action has been addressed. However, under two simplifying assumptions: (i) commuting controls and (ii) that the reduced state space has no singularities. (In this work, the singularities are exactly the collisions of eigenvalues of the density matrix).

4.4. Properties of the Lindblad master equation

Some interesting properties of the Lindblad equation are the following [3, 5, 16-20]:

- Under a Lindblad dynamics, if all the jump operators are Hermitian, the purity of a system fulfills

$$\frac{d}{dt}\left(\mathrm{Tr}\left[\rho^2\right]\right)\le 0\,.$$

- The Lindblad master equation is invariant under unitary transformations of the jump operators, $\sqrt{\Gamma_i}L_i\to\sqrt{\Gamma_i'}L'=\sum_j \upsilon_{ij}\sqrt{\Gamma_i}L_i$, with υ representing a unitary matrix. It is also invariant under inhomogeneous transformations in the form

$$L_i\to L_i+a_i;\quad U\to H'=H+\frac{1}{2i}\sum_j\Gamma_i\left(a_j^*A_j-a_jA_j^*\right)+b\,,$$

where $a_i\in\square$, $b\in\square$;

- Thanks to the previous properties, it is possible to find traceless jump operators without loss of generality.

Remark. We are looking for maps that transform density matrices into density matrices. We define $\rho(\mathrm{H})$ as the space of all density matrices in the Hilbert space H. Therefore, we are looking for a map of this space onto itself, $\mathrm{V}:\rho(\mathrm{H})\to\rho(\mathrm{H})$. To ensure that the out-put of the map is a density matrix, this should fulfill the following properties:

- Trace preserving. Tr[$\mathrm{V}A$] = Tr[A], $\forall A \in O(\mathrm{H})$;
- Completely positive (see below).

Any map that fulfills these two properties is called a *completely positive* and *trace-preserving* map (CPT-*maps*). The first property is quite apparent, and it does not require more thinking. The second one is a little more complicated, and it requires an intermediate definition.

Definition 1. A map V is positive iff $\forall A \in \mathrm{B}(\mathrm{H})$ s.t. $A \geq 0 \Rightarrow \mathrm{V}A \geq 0$.

This definition is based on the idea that, as density matrices are positive, any physical map should transform positive matrices into positive matrices. One could naively think that this condition must be sufficient to guarantee the physical validity of a map; it is not.

As we know, there exist composite systems, and the density matrix could be the partial trace of a more complicated state. Because of that, we need to impose a more general condition.

Definition 2. A map V is completely positive iff $\forall n \in \mathbb{N}$, $\mathrm{V} \otimes \mathbf{1}_n$ is positive.

To prove that not all positive maps are completely positive, we need a counterexample.

Example: *A canonical example of an operation that is positive but fails to be completely positive is the matrix transposition*. If we have a Bell state in the form $|\psi_B\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$, its density matrix can be expressed as $\rho_B = \left(|0\rangle\langle 0|\otimes|1\rangle\langle 1| + |1\rangle\langle 1|\otimes|0\rangle\langle 0| + |0\rangle\langle 1|\otimes|1\rangle\langle 0| + |1\rangle\langle 0|\otimes|0\rangle\langle 1|\right)$, with a matrix representation

$$\rho_B = \frac{1}{2}\left\{\begin{pmatrix}1&0\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&0\\0&1\end{pmatrix} + \begin{pmatrix}0&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&0\end{pmatrix} + \begin{pmatrix}0&0\\1&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix} + \begin{pmatrix}0&1\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix}\right\}.$$

A little algebra shows that the full form of this matrix is $\rho_B = \begin{pmatrix}0&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&0\end{pmatrix}$ and it is *positive.*

It is easy to check that the transformation $\mathbf{1} \otimes T_2$, meaning that we transpose the matrix of the second subsystem leads to a *nonpositive* matrix

$$(1\otimes T_2)\rho_B = \frac{1}{2}\left\{\begin{pmatrix}1&0\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix} + \begin{pmatrix}0&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix} + \begin{pmatrix}0&0\\1&0\end{pmatrix}\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix} + \begin{pmatrix}0&0\\0&1\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix}\right\}.$$

The total matrix is

$$(1\otimes T_2)\rho_B = \begin{pmatrix}0&0&0&1\\0&1&0&0\\0&0&1&0\\1&0&0&0\end{pmatrix}$$

with (−1) as an eigenvalue.

This example illustrates how the non-separability of quantum mechanics restricts the operations we can perform in a subsystem. By imposing these two conditions, we can derive a unique master equation as the generator of any possible Markovian CPT-map.

Example. Given a system environment interaction Hamiltonian H_{int}, we can expand the unitary dynamics to second order

$$\begin{aligned} U_t\left(\rho_S \otimes \rho_E\right)U_t^\dagger &= \exp\left(-iH_{\text{int}}t\right)\left(\rho_S \otimes \rho_E\right)\exp\left(iH_{\text{int}}t\right) \\ &= \left(1-iH_{\text{int}}t+\frac{1}{2}H_{\text{int}}^2t^2\right)\left(\rho_S \otimes \rho_E\right)\left(1+iH_{\text{int}}t+\frac{1}{2}H_{\text{int}}^2t^2\right) \\ &= \left(\rho_S \otimes \rho_E\right)-i\left[H_{\text{int}},\rho_S \otimes \rho_E\right]t+\left(-\frac{1}{2}H_{\text{int}}^2\left(\rho_S \otimes \rho_E\right)-\frac{1}{2}\left(\rho_S \otimes \rho_E\right)H_{\text{int}}^2+H_{\text{int}}\rho_S H_{\text{int}}\right)t^2 \end{aligned}.$$

We can write H_{int} as a sum of tensored operators $\sum_k H_k^S \otimes H_k^A$. When we trace over the environment, the first order terms become

$$\begin{aligned} \text{Tr}_2\left[H_k^S \otimes H_k^E,\rho_S \otimes \rho_E\right] &= \text{Tr}_2\left[H_k^S\rho_S \otimes H_k^E\rho_E-\rho_S H_k^S \otimes \rho_E H_k^E\right] \\ &= H_k^S\rho_S\text{Tr}\left(H_k^E\rho_E\right)-\rho_S H_k^S\text{Tr}\left(\rho_E H_k^E\right)=\left[H_k^S,\rho_S\right]\text{Tr}\left(\rho_E H_k^E\right) \end{aligned}.$$

The last term follows from the cyclic property of the trace.

These first order terms, called *Lamb Shifts*, are perturbations on the system Hamiltonian due to an environmental coupling. We can also trace out the environment on the second order terms to recover the full Lindblad equation.

This derivation from a unitary process is a more physically intuitive version of the Lindblad equation. If we know the specific mode of interaction between the environment and the system, then this form of the Lindblad equation is probably the better to work with.

On the other hand, if we want to concoct an arbitrary quantum dynamical semigroup without mention of the coupling to an external environment, equation

$$L\rho=-i\left[H,\rho\right]+\frac{1}{2}\sum_{l,m}\alpha_{lm}\left(\left[F_l\rho,F_m^\dagger\right]+\left[F_l,\rho F_m^\dagger\right]\right)$$

is more appropriate.

Example: Coherence vectors presentation of Lindblad equation. Now let F_k be a basis for *su*(*N*) with $\text{Tr}\left(F_iF_j\right)=\delta_{ij}$. Note that any density matrix can be written in the form

$$\rho=\frac{1+\sum_{k=1}^{N^2-1}r_kF_k}{N},$$

$\vec{r}=\left(r_k\right)$ is the coherence vector. $\vec{r}$ is a real vector and is the analog of the Bloch vector for single spins (see, Chapter 2). Consider the trace norm of ρ given by

$$\left\|\rho\right\|^2=\text{Tr}\left(\rho\rho^\dagger\right)=\text{Tr}\left(\frac{1+\sum_k r_kF_k+\sum_{k,j}r_kr_jF_kF_j}{N^2}\right)=\frac{1}{N^2}\left(N+\sum_k r_k^2\right).$$

Since the density matrix is positive semidefinite and has trace one, all of the eigenvalues of ρ lie between zero and one. It follows that $\frac{1}{\sqrt{N}} \le \|\rho\| \le 1$ which means that $0 \le \|\vec{r}\| \le \sqrt{N^2 - N}$.

Hence any map on a quantum system cannot increase the lengths of coherence vectors. In other words, the dynamics of the coherence vector have eigenvalues with real parts strictly less than one. Note that it is only a necessary, not a sufficient, condition for the length of a coherence vector.

In particular it does not imply that the density matrices form a sphere. Indeed, we can define three operators on a 4-level Hilbert space as

$$M_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad M_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

These matrices are trace orthogonal and can be extended to a basis for the coherence vectors.

The state $\rho = (1+M_1+M_2+M_3)/4$ is a pure state and has coherence vector length $\sqrt{3}$. But the matrix $\rho_{bad} = (1 + 3M_1)/4$ has eigenvalues 1/2, − 1/4 and is not positive semidefinite. So, we must be careful. We can bound the length of the coherence vector, but the intrinsic geometry of density matrices does not necessarily form a nice sphere except in the special case of *su*(2).

Let's reformulate some of the last sections results in terms of this coherence vector. First, consider commutation with $H = \sum_k h_k F_k$ as:

$$-i[H, \rho] = \frac{1 + \sum_{k=1}^{N^2-1} r_k [H, F_k]}{N} = \frac{1 + \sum_{k,l=1}^{N^2-1} r_k h_l [F_l, F_k]}{N} = \frac{1 + \sum_{k,l,m=1}^{N^2-1} r_k h_l g_{lkm} F_m}{N},$$

where g_{lkm} are the structure constants of *su*(*N*). Evidently, we can define the matrix $C_{nm} = \sum_k g_{kml} h_k$ and then in this representation $\vec{r} \mapsto \vec{C}\vec{r}$ under *H*. We have $\vec{r} = A\vec{r} + \vec{b}$ with $A_{mn} = -\frac{1}{4} \sum_{j,k,l} a_{jk} \left(z_{jln} f_{klm} + \overline{z}_{kln} f_{jlm} \right) b_m = \frac{1}{N} \sum_{j,k} a_{jk} f_{jmk}$. Here $z_{mnl} = f_{mnl} + i d_{mnl}$ where f_{mnl} and d_{mnl} are the symmetric and antisymmetric structure constants of *su*(*N*).

The computations involving structure constants are often difficult in practice, but the form of equation A_{mn} describes all of the possible transformations on density matrices in an intuitive way. We see that the only admissible maps are a subset of the linear affine transformations of the coherence vectors. Hence the general Lindblad equation is rewritten in a much more familiar form

$$\frac{d\vec{r}}{dt} = A\vec{r} + \vec{b} + C\vec{r}.$$

Unfortunately, we cannot impose any symmetry conditions on the matrix *A* except when *N* = 2. But we can still analyze the properties of this ODE to determine what it tells us about open system evolution. Using this notation to analyze the structure of the Lindblad equation, first consider when *A* = 0 and $\vec{b}$ = 0. Then we are left with an ODE $\frac{d\vec{r}}{dt} = C\vec{r}$, where *C* is skew-symmetric. Then exp (*Ct*) is an orthogonal matrix for all t and hence the dynamics are orthogonal. It is not surprising that the coherence vector doesn't change length under these dynamics as we know the dynamics under a Schrödinger equation are unitary.

When *C* = 0 and $\vec{b}$ = 0, science the dynamics of the Lindblad equation must not increase the length of coherence vectors, the real parts of the eigenvalues of *A* must be less than or equal to zero. Unfortunately,

again we have to reiterate that this is all we can say about the structure of *A*. Remember, that *A* is not usually diagonalizable when $N > 2$.

We will close this section with two definitions. A quantum operation is called relaxing or a relaxation process if $\vec{b} \neq 0$. In this case, all density matrices damp exponentially to a unique fixed point. If $\vec{b} = 0$ and *A* has negative eigenvalues, we say that the process is dephasing. The distinction between these two types of decoherence is essential for what follows as the main result of this section is that relaxation processes can be corrected by unitary operations while dephasing processes cannot.

Example: *the Bloch sphere*. Defining the array of matrices $\vec{\sigma} = (X, Y, Z)$ allows any density matrix over *su*(*N*) to be written as $\rho = \frac{1 + \vec{r} \cdot \vec{\sigma}}{2}$ where $\vec{r}$ s the coherence vector. In this case we call it the Bloch vector in honor of Felix Bloch and $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$, $Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Under the relabeling $\sigma_1 = X$, $\sigma_2 = Y$, $\sigma_3 = Z$, we get the algebraic relations

$$\left[\sigma_i, \sigma_j\right] = i2\varepsilon_{ijk}\sigma_k; \quad \sigma_i\sigma_j = \delta_{ij}1 + 2\varepsilon_{ijk}\sigma_k .$$

The Bloch vectors are now the set of all vectors in $\mathbb{R}^3$ with norms less than or equal to one. Hence, the set of all Bloch vectors hence forms a 3-dimensional sphere with radius one. We call this sphere the Bloch Sphere. It is useful to link the thermodynamics of a density matrix to the geometry of the Bloch vector. Given a density matrix $\rho = \begin{pmatrix} 1 + r_z & r_x + ir_y \\ r_x - ir_y & 1 - r_z \end{pmatrix}$. It is easy to compute the characteristic polynomial

$$c_\rho(\lambda) = \lambda^2 - \mathrm{Tr}(\rho)\lambda + \det(\rho) = \lambda^2 - \lambda + \frac{1 - r_x^2 - r_y^2 - r_z^2}{4} = \lambda^2 - \lambda + \frac{1 - \|\vec{r}\|^2}{4} .$$

The eigenvalues of the density matrix are then given by $\lambda_i = \frac{1 \pm \|\vec{r}\|}{2}$. We recall that for any two Hermitian matrices *M* and *N*, there exists a unitary matrix *U* satisfying $M = UNU^\dagger$ if and only if *M* and *N* have the same eigenvalues. We see from equation for λ_i that any two Bloch vectors with the same norm have corresponding density matrices with the same eigenvalues.

Furthermore, we can compute the entropy of a density matrix

$$S(\rho) = -\lambda_1 \log \lambda_1 - \lambda_2 \log \lambda_2 = -\frac{1 + \|\vec{r}\|}{2} \log \frac{1 + \|\vec{r}\|}{2} - \frac{1 - \|\vec{r}\|}{2} \log \frac{1 - \|\vec{r}\|}{2}$$

showing that the entropy only depends on the length of the Bloch vector.

The geometry of the Bloch vector is simple and aesthetically pleasing because the Lie Algebras *su*(2) and *so*(3) are isomorphic. Thus, there is a perfect correspondence between the transformations of 2×2 density matrices and the geometry of $\mathbb{R}^3$.

For any initial density matrix described by a nonzero Bloch vector $\vec{r}$, the norm of the density matrix is strictly decreasing and $S(\rho) < S(\mathrm{E}(\rho))$. In the Bloch Sphere picture, the *x* and *y* components of the Bloch vector are dissipated leaving the projection of the Bloch vector on the *z*-axis. If quantum process acts for time *t*, then we can try, for example, to push the spin system back to where it started. If our pushes are unitary then we cannot change the length of the Bloch vector. Though in general quantum processes are free to change the Bloch vector length, but there is no reason why they must do so. We can correct the quantum process with a unitary operation only when the Bloch vector hasn't changed length under its evolution. We formulate this as following:

a quantum state is stabilizable under a quantum process E_t if there is a unitary operation U such that $\mathrm{E}_t(\rho) = U\rho U^\dagger$ and it follows immediately that a quantum state is stabilizable under E_t if and only if the corresponding Bloch vector at time t has the same norm as at time 0. A quantum operation E_t can be corrected by unitary operations if the manifold of stabilizable states has dimension 2.

A large class of open quantum systems can be described by Lindblad equations for the dynamics of density operators. In many atomic physics and quantum optics applications, this is an accurate description of physical phenomena. Lindblad dynamics can be viewed as an ensemble average over stochastic pure-state trajectories. The stochastic trajectories may be interpreted as the state of an individual experimental quantum system conditioned on a measurement record. The nature of the measurement record determines the types of trajectories in the ensemble, and intriguingly can lead to strikingly different microscopic dynamics and behaviors, while averaging to the same Lindblad dynamics.

This section presents a novel approach to simulating the Lindblad equation. The method leverages the intimate relationship between Lindblad dynamics, stochastic diff erential equations (SDEs), and Hamiltonian simulations. By adding extra ancilla qubits, the Lindblad dynamics can be incorporated into a unitary dynamic in a larger Hilbert space. Moreover, the unitary dynamics can be simulated using a quantum circuit that only involves Hamiltonian simulation and tracing out the ancilla qubits (see Fig. 9).

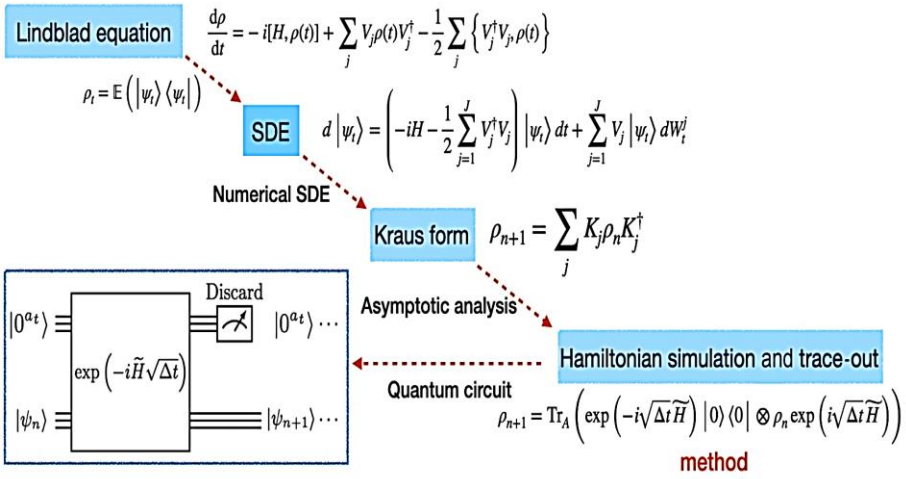


Fig. 9. A flowchart illustrating the derivation of the numerical scheme and the quantum circuit (one step) for simulating the time-independent Lindbladian dynamics [21]

Algorithm using the following steps: (1) unraveling of the Lindblad equation into stochastic diff erential equations (SDEs); (2) expressing classical numerical SDE schemes as the Kraus-representation form for the density operator; (3) mapping the Kraus form to the dilated Hamiltonian in the Stinespring form.

A sequence of unitary dynamics in an enlarged Hilbert space that can approximate the Lindblad dynamics up to an arbitrarily high order. This unitary representation can then be simulated using a quantum circuit that involves only Hamiltonian simulation and tracing out the ancilla qubits. There is no need for additional postselection in measurement outcomes, ensuring a success probability of one at each stage. The method can be directly generalized to the time-dependent setting. Numerical examples provide that simulate both time-independent and time-dependent Lindbladian dynamics with accuracy up to the third order. The simulation on the circuit advances a Hamiltonian simulation for a time duration of $\sqrt{\Delta t}$, after which the ancilla qubits are measured. The outcomes of these measurements on the ancilla qubit are disregarded and the ancilla qubits are subsequently reset to the state $\left|0^{a_k}\right\rangle$ in preparation for the next iteration. The inherent unitary and trace-out design ensures that the algorithm achieves a success probability of one, eliminating the need for any additional amplitude-amplification steps.

5. Lindblad open quantum systems with quantum feedback

As abovementioned two of the most important unravellings [3, 5, 16, 17, 19] are given by *stochastic Schrödinger equations* (SSEs) and *quantum-jump* trajectories, respectively. The SSE dynamics is a good description, for example, of certain homodyne and heterodyne detection schemes in quantum optics arising from constant weak continuous measurements. Quantum-jump dynamics, on the other hand, may arise in photodetection experiments and is theoretically described by periods of deterministic evolution under an effective non-Hermitian Hamiltonian, stochastically interrupted by discrete measurements. In both SSE and quantum-jump scenarios, if the measurement channel is not recorded, then the best estimate for the state is obtained by averaging over all possibilities, resulting in Lindblad dynamics. There are other interpretations of the unravellings of the Lindblad equation, viewing them as candidate laws of nature in an effort to explain the wavefunction collapse in quantum measurement [19].

Stochastic Schrödinger equation. In this section an introduction to the theory of stochastic quantum molecular dynamics (SQMD) is given. For completeness, this includes general aspects of open quantum systems as well as the basic theorem of SQMD. For simplicity, we will consider only a single bath (an electron-ion many-body system coupled to a bosonic bath), but the formulation is trivially extended to the case of several environments. The total Hamiltonian of the entire system is then $\hat{H} = \hat{H}_{\mathrm{S}} \otimes \hat{I}_B + \hat{I}_{\mathrm{S}} \otimes \hat{H}_B + \lambda \hat{H}_{\mathrm{SB}}$. The system of interest is described by the many-body Hamiltonian $\hat{H}_{\mathrm{S}}$ and the environment degrees of freedom are given in terms of $\hat{H}_B$. The interaction of the system with the environment is given by the Hamiltonian $\hat{H}_{\mathrm{SB}}$ and is assumed to be weak in the sense that a perturbation expansion in terms of this coupling can be performed. With λ we denote the corresponding coupling parameter for the system-bath interaction. The total system described by the Hamiltonian $\hat{H}$ follows a unitary time-evolution, which can be formulated for pure states either in terms of the time-dependent Schrödinger equation (TDSE), with $\hbar$ = 1: $i\partial_t \psi(t) = \hat{H}(t)\psi(t)$, or, alternatively for mixed states, in terms of the Liouville-von Neumann equation $\frac{d}{dt}\hat{\rho}(t) = -i\left[\hat{H}(t), \hat{\rho}(t)\right]$, where $\hat{\rho}(t)$ is the statistical operator. We are only interested in the dynamics of the system degrees of freedom. It is therefore desirable to find an effective description for the system only.

To accomplish this, we may trace out the bath degrees of freedom at the level of the statistical operator, namely we perform the operation $\hat{\rho}_{\mathrm{S}} = \mathrm{Tr}_B(\hat{\rho})$, where $\hat{\rho}_{\mathrm{S}}$ is called the reduced statistical operator of system S. It is worth pointing out here that this procedure does not generally lead to a closed equation of motion for the reduced statistical operator and one needs further approximations. Depending on the approximations involved, one may arrive at an effective quantum master equation for the reduced density operator $\hat{\rho}_{\mathrm{S}}$. This approach has some drawbacks when used within a density-functional formulation, both fundamental - in view of the theorems of DFT - and practical, since solving for the density matrix is computationally more demanding than solving directly for state vectors. We therefore take here a different route. Instead of working with a derived/composite quantity like the statistical operator, we summarize briefly how the bath degrees of freedom can be traced out directly at the level of the wavefunction. The derivation that follows has been reported elsewhere in the literature. We repeat some steps here for completeness and to clarify starting point. To this end let us consider the set of eigenfunctions $\{\chi_n(x_B)\}$ of the bath Hamiltonian $\hat{H}_B \chi_n(x_B) = \varepsilon_n \chi_n(x_B)$, with x_B the bath's coordinates (including possibly spin), and expand the total wavefunction of TDSE in the complete set of orthonormal states formed by $\{\chi_n(x_B)\}$, namely $\psi(x_{\mathrm{S}}, x_B, t) = \sum_n \phi_n(x_{\mathrm{S}}, t)\chi_n(x_B)$. with $\phi_n(x_{\mathrm{S}}, t)$ some functions (not necessarily normalized) in the Hilbert space of the system S.

Let us define the following projection operators: $\hat{P}_n = \hat{I}_{\mathrm{S}} \otimes |\chi_n\rangle\langle\chi_n|$, $\hat{Q}_n = \hat{I}_{\mathrm{S}} \otimes \sum_{k\neq n} |\chi_k\rangle\langle\chi_k|$. The rationale behind the choice of the above operators is to obtain the equation of motion of a representative coefficient $\phi_n(x_{\mathrm{S}}, t)$. By acting with these projection operators on the many-body TDSE for the combined system and bath in $i\partial_t \psi(t) = \hat{H}(t)\psi(t)$ we arrive at

$$i\partial_t \hat{P}\psi(t) = \hat{P}\hat{H}\hat{P}\hat{P}\psi(t) + \hat{P}\hat{H}\hat{Q}e^{-i\hat{Q}\hat{H}\hat{Q}t}\hat{Q}\psi(0) - i\int_0^t \hat{P}\hat{H}\hat{Q}e^{-i\hat{Q}\hat{H}\hat{Q}(t-\tau)}\hat{Q}\hat{H}\hat{P}\hat{P}\psi(\tau)d\tau\,, \qquad (3)$$

where we have omitted the index *n* for brevity. The first term on the right-hand side of Eq. (3) contains only projections on the system manifold, and describes the coherent evolution of the system degrees of freedom. The second term is a source term that carries a dependence on initial conditions ($\hat{Q}\psi(0)$ are the initial conditions of all system's states except the one we are considering), and the third term on the right-hand side is a memory term that is recording the history of the time evolution. The time evolution given by Eq. (3) is still fully coherent.

Remark. The solution of Eq. (3) is very involved [22, 23] and, apart from model systems, not feasible in practice. Furthermore, a solution would require the initial conditions for all the microscopic degrees of freedom of the bath. These cannot all be determined simultaneously by a measurement. In practice, one rather has only knowledge about macroscopic thermodynamic properties of the bath, like temperature and pressure. It is therefore common to perform the following additional approximations which are motivated by the form of the system - bath interaction and the thermodynamic properties of the bath: (i) due to the assumed weak coupling between system and bath the source and memory terms are expanded up to second order in the system-bath coupling parameter λ, (ii) the bath and subsystem S are assumed to be uncorrelated at the initial time, (iii) a random phase approximation is performed for the phases in the source and memory terms, and (iv) it is assumed that the bath degrees of freedom form a dense energy spectrum and are in local thermal equilibrium characterized by $\hat{\rho}_B = \frac{1}{\mathrm{Tr}\left(e^{-\beta\hat{H}_B}\right)}e^{-\beta\hat{H}_B}$, where $\beta = 1/k_B T$. The random phase approximation invoked in the derivation of the Markovian stochastic Schrödinger equation might seem at first sight surprising. The derivation of the Lindblad equation from the Markovian stochastic Schrödinger equation on the other hand shows, that both describe the exact same dynamics if the Hamiltonian does not depend on internal degrees of freedom or any time-dependent or stochastic field.

Let us then write the interaction Hamiltonian as $\hat{H}_{\mathrm{SB}} = \sum_\alpha \hat{S}_\alpha \hat{B}_\alpha$, where $\hat{S}_\alpha$ and $\hat{B}_\alpha$ are - in the most general case - many-body operators that act on the Hilbert spaces of the system and bath, respectively. In the following we will also assume that the average of the operators $\hat{B}_\alpha$ vanishes on the *n*-th eigenstate of the bath, namely $\sum_\alpha \hat{S}_\alpha \langle \chi_n | \hat{B}_\alpha | \chi_n \rangle = 0$. The term $\langle \chi_n | \hat{B}_\alpha | \chi_n \rangle$ contributes to the unitary evolution of the system by renormalizing its eigenvalues (a typical example of this is the Lamb shift). With these approximations in place, the source term can be regarded as a stochastic driving term.

This is because, the system's state we have singled out now interacts with a (practically infinite) large set of bath states densely distributed in energy. The previously coherent Eq. (3) then has to be regarded as a non-Markovian stochastic Schrödinger equation for the general state vector $\psi(t) \equiv \phi_n(x_{\mathrm{S}}, t) / \langle \phi_n(x_{\mathrm{S}}, t) | \phi_n(x_{\mathrm{S}}, t) \rangle$ as

$$i\partial_t \psi(t) = \hat{H}_{\mathrm{S}}\psi(t) + \lambda\sum_\alpha l_\alpha \hat{S}_\alpha \psi(t) - i\lambda^2 \sum_{\alpha\beta}\int_0^t C_{\alpha\beta}(t-\tau)\hat{S}_\alpha^\dagger e^{-i\hat{H}_{\mathrm{S}}(t-\tau)}\hat{S}_\beta \psi(\tau)\,d\tau + \mathrm{O}\left(\lambda^3\right), \qquad (4)$$

where $l_\alpha(t)$ are stochastic processes with zero ensemble average, $\langle l_\alpha(t) \rangle = 0$, and correlation functions $\langle l_\alpha(t) l_\beta(t') \rangle = 0$, $\langle l_\alpha^*(t) l_\beta(t') \rangle = C_{\alpha\beta}(t-t')$.

Eq. (4) is a general *non-Markovian stochastic* Schrödinger equation.

Indeed, it still contains a time-integral over the past dynamics which is originating from the memory term of Eq. (3). Even though the theorem of SQMD could be formulated with non-Markovian baths we will focus in the following only on the Markovian limit $C_{\alpha\beta}(t-t') = \delta_{\alpha\beta}\delta(t-t')$, namely, we consider baths that are δ-correlated.

Remark. Physically, this means that the bath does not retain memory of the interaction with the system which is valid when the typical thermalization time-scales inside the bath are much faster than the thermalization time-scales of the system. This approximation is well justified for a large number of bath degrees of freedom. If this assumption does not hold, one has to resort to the solution of the more involved Eq. (4).

By inserting the Markov approximation, $C_{\alpha\beta}\left(t-t'\right)=\delta_{\alpha\beta}\delta\left(t-t'\right)$, into Eq. (4) we then arrive at the *stochastic Schrödinger* equation in the *Born-Markov* limit

$$i\partial_t\psi\left(t\right)=\hat{H}_{\mathrm{S}}\left(t\right)\psi\left(t\right)-\frac{i}{2}\sum_{\alpha}\hat{S}_{\alpha}^{\dagger}\hat{S}_{\alpha}\psi\left(t\right)+\sum_{\alpha}l_{\alpha}\left(t\right)\hat{S}_{\alpha}\psi\left(t\right) \tag{5}$$

where the parameter λ has been absorbed in the operators $\hat{S}_{\alpha}$. The first term on the right-hand side of Eq. (5) is the usual unitary evolution of the system under the action of the system Hamiltonian $\hat{H}_{\mathrm{S}}$, the second term describes the dissipation effects introduced by the bath and would indeed make the probability density generated by $\psi\left(t\right)$ decay in time. The last term, however, introduces fluctuations so that the norm of the state vector $\psi\left(t\right)$ averaged over the ensemble is conserved, namely $\left\langle\left\langle\psi\left(t\right)\middle|\psi\left(t\right)\right\rangle\right\rangle=1+\mathrm{O}\left(\lambda^4\right)$. Due to the stochastic nature of this equation, the stochastic process described by Eq. (5) has to be simulated in terms of an ensemble of state vectors $\psi\left(t\right)$. Each member $\psi\left(t\right)$ of the ensemble evolves differently in time due to the random variables $l_{\alpha}\left(t\right)$ in the third term on the rhs of Eq. (5).

It is possible to derive the Lindblad equation from the stochastic Schrödinger Eq. (5).

Derivation of the Lindblad equation and stochastic Hamiltonians. Let us denote in the following discussion with $\psi\left(t\right)$ a single member of the stochastic ensemble $\left\{\left|\psi_k^j\right\rangle\right\}$. If we consider for simplicity the case of a single bath operator in Eq. (3), and observe that in the Markovian limit $W\left(t\right)=\int_0^t l\left(t'\right)dt'$ is a Wiener process with properties $\left\langle W\left(t\right)\right\rangle=0$ and $\left\langle dW^{\dagger}dW\right\rangle=dt$, we can formulate the stochastic Schrödinger Eq. (5) for a single bath in differential form according to

$$d\left|\psi\right\rangle=\left[-iH_{\mathrm{S}}\left|\psi\right\rangle-\frac{1}{2}\hat{S}^{\dagger}\hat{S}\left|\psi\right\rangle\right]dt-i\hat{S}\left|\psi\right\rangle dW\,. \tag{6}$$

Next, we employ Ito stochastic calculus in order to compute the following differential

$$d\left|\psi\right\rangle\left\langle\psi\right|=\left(d\left|\psi\right\rangle\right)\left\langle\psi\right|+\left|\psi\right\rangle\left(d\left\langle\psi\right|\right)+\left(d\left|\psi\right\rangle\right)\left(d\left\langle\psi\right|\right). \tag{7}$$

Unlike in normal calculus, we also have to keep the third term in the product rule above. This becomes necessary, since a statistical average over the Wiener increment $dW^{\dagger}dW$ is proportional to *dt*, which will cause terms quadratic in *dW* to contribute to first order in *dt*. Inserting Eq. (6) and its Hermitian conjugate into Eq. (7) we arrive after elementary algebra at

$$\begin{aligned}d\left|\psi\right\rangle\left\langle\psi\right|=&-i\hat{S}\left|\psi\right\rangle\left\langle\psi\right|dW+h.c.-i\left[\hat{H}_{\mathrm{S}},\left|\psi\right\rangle\left\langle\psi\right|\right]dt-\frac{1}{2}\left\{\hat{S}^{\dagger}\hat{S},\left|\psi\right\rangle\left\langle\psi\right|\right\}dt\\&+\hat{S}\left|\psi\right\rangle\left\langle\psi\right|\hat{S}^{\dagger}dW^{\dagger}dW+\hat{S}\left|\psi\right\rangle\left\langle\psi\right|\hat{H}_{\mathrm{S}}dWdt+h.c.+\frac{i}{2}\hat{S}\left|\psi\right\rangle\left\langle\psi\right|\hat{S}^{\dagger}\hat{S}dWdt+h.c.\\&+\hat{H}_{\mathrm{S}}\left|\psi\right\rangle\left\langle\psi\right|\hat{H}_{\mathrm{S}}dt^2+\frac{1}{4}\hat{S}^{\dagger}\hat{S}\left|\psi\right\rangle\left\langle\psi\right|\hat{S}^{\dagger}\hat{S}dt^2+\frac{i}{2}\left\{\hat{H}_{\mathrm{S}},\left|\psi\right\rangle\left\langle\psi\right|\hat{S}^{\dagger}\hat{S}\right\}dt^2\end{aligned} \tag{8}$$

In order to construct the statistical operator from the state vectors of the statistical ensemble $\left\{\left|\psi_k^j\right\rangle\right\}$, we perform in the next step the statistical average over all members in the ensemble, i.e. $d\hat{\rho}=d\left\langle\left|\psi\right\rangle\left\langle\psi\right|\right\rangle$. Taking

the properties $\langle dW \rangle = \langle dWdt \rangle = 0$ and $\langle dW^{\dagger} dW \rangle = dt$ of the stochastic process $l(t)$ into account, we see that only

$$(-i\left[\hat{H}_{\mathrm{S}}, |\psi\rangle\langle\psi|\right]dt - \frac{1}{2}\left\{\hat{S}^{\dagger}\hat{S}, |\psi\rangle\langle\psi|\right\}dt) \text{ and } (\hat{S}|\psi\rangle\langle\psi|\hat{H}_{\mathrm{S}}dWdt + \frac{i}{2}\hat{S}|\psi\rangle\langle\psi|\hat{S}^{\dagger}dWdt)$$

terms in Eq. (8) contribute to first order in *dt* and we arrive at

$$d\hat{\rho} = -i\left\langle\left[\hat{H}_{\mathrm{S}}|\psi\rangle\langle\psi|\right]\right\rangle dt - \frac{1}{2}\left\{\hat{S}^{\dagger}\hat{S}, \langle|\psi\rangle\langle\psi|\rangle\right\}dt + \hat{S}\langle|\psi\rangle\langle\psi|\rangle\hat{S}^{\dagger}dt + O\left(dt^2\right). \qquad (9)$$

At this point, note that this equation of motion is not necessarily closed for $\hat{\rho} = \langle|\psi\rangle\langle\psi|\rangle$ because the first term on the right-hand side of Eq. (9) is not equal to the commutator $-i\left[\hat{H}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}\right]$ unless $\hat{H}_{\mathrm{S}} \neq \hat{H}_{\mathrm{S}}\left[\left\{|\psi_k^j\rangle\right\}\right]$, or $\hat{H}_{\mathrm{S}}$ does not depend on any stochastic field, or the system is in a pure state at all times - which would amount to the case $\hat{S} = 0$.

However, if the Hamiltonian is stochastic, one has to deal with an ensemble of Hamiltonians, and the statistical average of the first term on the right-hand side of Eq. (9) involves also a statistical average over these Hamiltonians.

For the moment being, let us assume that $\hat{H}_{\mathrm{S}} \neq \hat{H}_{\mathrm{S}}\left[\left\{|\psi_k^j\rangle\right\}\right]$ and furthermore that the Hamiltonian $\hat{H}_{\mathrm{S}}$ does not depend on some external stochastic field. In this case we find

$$d\hat{\rho} = -i\left[\hat{H}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}\right] - \frac{1}{2}\left\{\hat{S}^{\dagger}\hat{S}, \hat{\rho}_{\mathrm{S}}\right\} + \hat{S}\hat{\rho}_{\mathrm{S}}\hat{S}^{\dagger} \qquad (I0)$$

which is the well-known quantum master equation in Born-Markov limit (or Lindblad equation if the bath operators and the Hamiltonian, do not depend on time) [24].

We have thus shown that the stochastic Schrödinger equation of Eq. (5) and the master equation (10) lead to the same statistical operator, if and only if the Hamiltonian is not stochastic. However, in order to prove any DFT theorem one is led to consider the dynamics of the actual many-body system and that of any auxiliary one (including the Kohn-Sham system) with different interaction potentials, but reproducing the exact many-body density or current density. It is then at this stage that a choice has to be made - in the case of a many-body system open to one or more environments - regarding the basic equation of motion to work with. If we choose to work with a quantum master equation of the type (10), then we are assuming from the outset that the Kohn-Sham Hamiltonian is not stochastic. But this is a hypothesis that constitutes part of the final description, namely we have to prove that this statement is correct, not assume it a priori. This issue does not arise with the stochastic Schrödinger equation (5), because in that case we can consider all possible Hamiltonians, including those that are stochastic.

The construction of the statistical operator from stochastic trajectories effectively selects only the physical solutions of the associated quantum master equation while the latter also permits non-physical solutions. Therefore, the above issues make the equation of motion of the statistical operator a less solid starting point for a DFT theory of open quantum systems.

The dynamics of Gaussian states for open quantum systems described by Lindblad equations can be solved analytically for systems with quadratic Hamiltonians and linear Lindbladians, showing the familiar phenomena of dissipation and decoherence. It is well known that the Lindblad dynamics can be expressed as an ensemble average over stochastic pure-state dynamics, which can be interpreted as individual experimental implementations, where the form of the stochastic dynamics depends on the measurement setup. Here we consider quantum-jump and stochastic Schrödinger dynamics for initially Gaussian states. While both unravellings converge to the same Lindblad dynamics when averaged, the individual dynamics can differ qualitatively.

For the stochastic Schrödinger equation, Gaussian states remain Gaussian during the evolution, with stochastic differential equations governing the evolution of the phase-space centre and a deterministic evolution of the covariance matrix. In contrast to this, individual pure-state dynamics arising from the

quantum-jump evolution do not remain Gaussian in general. Applying results developed in the non-Hermitian context for Hagedorn wavepackets, we formulate a method to generate quantum-jump trajectories that is described entirely in terms of the evolution of an underlying Gaussian state. To illustrate the behaviours of the different unravellings in comparison to the Lindblad dynamics, we consider two examples in detail, which can be largely treated analytically, a harmonic oscillator subject to position measurement and a damped harmonic oscillator. In both cases, we highlight the differences as well as the similarities of the stochastic Schrödinger and the quantum-jump dynamics.

C. *Posssible unravellings of the Lindblad equation*. The Lindblad equation was initially derived as the most general Markovian dynamical equation that preserves the trace, Hermiticity and positivity of the density matrix. Physically, it can be used to describe certain quantum systems that are weakly coupled to a memoryless environment. In this spirit, dynamics of Lindblad form can be obtained for the reduced density matrix by averaging over the effect of a bath of quantum harmonic oscillators [24]. Any linear and Markovian (local in time) master equation that preserves the Hermiticity and trace of the density matrix may be expressed in Lindblad form (1),

$$i\hbar\frac{d}{dt}\hat{\rho}(t)=\left[\hat{H},\hat{\rho}\right]+i\sum_k\left(\hat{L}_k\hat{\rho}(t)\hat{L}_k^\dagger-\frac{1}{2}\left\{\hat{L}_k\hat{L}_k^\dagger,\hat{\rho}(t)\right\}\right),\quad \left\{\hat{L}_k\hat{L}_k^\dagger,\hat{\rho}(t)\right\}=\hat{L}_k\hat{L}_k^\dagger\hat{\rho}(t)+\hat{\rho}(t)\hat{L}_k\hat{L}_k^\dagger .$$

Here $\hat{H}$ is a Hamiltonian and $\hat{L}_k$ are general Lindblad operators, the properties of which are system-specific. For simplicity in what follows we shall confine the discussion to a single Lindblad operator.

Much like the deterministic Fokker–Planck equation for the dynamics of probability distributions in classical physics admits *unravellings* in terms of single trajectories of the stochastic Langevin equation, the deterministic Lindblad equation for the dynamics of the density operator may be unravelled in terms of stochastic pure-state trajectories. There are infinitely many such unravellings that differ from each other in the stochastic driving processes. The two types of unravellings most commonly considered in the literature are SSE trajectories driven with continuous Gaussian distributed noise, and quantum-jump trajectories driven by discrete Poissonian distributed noise [25].

Example. The *SSE* we consider here is given by

$$|d\psi\rangle=\frac{i}{\hbar}\left(-i\hat{H}-\frac{1}{2}\hat{L}^\dagger\hat{L}+\langle\hat{L}^\dagger\rangle\hat{L}-\frac{1}{2}\langle\hat{L}^\dagger\rangle\langle\hat{L}\rangle\right)|\psi\rangle dt+\frac{1}{\sqrt{2\hbar}}\left(\hat{L}-\langle\hat{L}\rangle\right)|\psi\rangle\left(d\xi_R+id\xi_I\right),$$

where $d\xi_R$ and $d\xi_I$ are independent ($\mathrm{E}[d\xi_R d\xi_I] = 0$) Ito stochastic processes with mean zero ($\mathrm{E}[d\xi_R] = \mathrm{E}[d\xi_I] = 0$) and normalisation $d\xi_R^2 = d\xi_I^2 = 0$. The SSE trajectories are driven with a continuous stochastic process and are often used to model systems undergoing weak continuous measurement such as heterodyne detection in quantum optics or quantum Brownian motion.

In the *quantum-jump* description, on the other hand, the pure-state trajectories deterministically evolve under an effective non-Hermitian Hamiltonian $\hat{H}-i\hat{\Gamma}$ with $\hat{\Gamma}=\frac{1}{2}\hat{L}^\dagger\hat{L}$, periodically interrupted by stochastic quantum jumps. These jumps may be used to represent random discrete measurements of quantum systems such as photodetection from a microwave cavity. The cumulative effect of these jumps when averaged over many trajectories induces the "jump term" contribution $\hat{L}_k\hat{\rho}(t)\hat{L}_k^\dagger$ in the density operator dynamics. Concretely, quantum-jump pure-state dynamics can be described by the dynamical equation

$$|d\psi\rangle=\frac{i}{\hbar}\left(-i\hat{H}-\frac{1}{2}\hat{L}^\dagger\hat{L}\right)|\psi\rangle(1-dN)dt+\left(\frac{\hat{L}}{\sqrt{\langle\hat{L}^\dagger\hat{L}\rangle}}-1\right)|\psi\rangle dN .$$

Here dN is a Poisson process, taking the values 0 (no jump) or 1 (jump) with expectation value $\mathrm{E}[dN]=\langle\hat{L}^\dagger\hat{L}\rangle dt$. Considering quantum-jump trajectories of a Markovian open system described by the

Lindblad master equation and post-selecting only trajectories in which no jumps have occurred, thus leads to effective non-Hermitian Hamiltonian dynamics.

Quantum dynamics generated by non-Hermitian Hamiltonians is an active area of research on its own, and we will make use of some techniques developed in this context. It should be noted that $\hat{L}^\dagger \hat{L}$ is a positive operator and thus non-Hermitian Hamiltonians, $\hat{H} - \frac{i}{2}\hat{L}^\dagger \hat{L}$, arising in the context of post-selection of Lindblad/quantum-jump dynamics may only describe loss (but not gain).

Remark. Despite converging to the same ensemble dynamics, the SSE and quantum-jump trajectories can differ not just quantitatively but qualitatively. We will analyse these differences in detail for quadratic Hamiltonians and linear Lindbladians with initially Gaussian states. While for Lindblad and SSE dynamics the state remains Gaussian for all times for quadratic Hamiltonians and linear Lindbladians, this is in general not the case for quantum-jump dynamics, even though averaging over quantum-jump trajectories recovers the Gaussian Lindblad results. For Hermitian Lindbladians, the Lindblad term in the central dynamics vanishes, leaving only Hamiltonian dynamics, as expected for these *purely decohering* systems. In general, non-Hermitian Lindbladians lead to both decoherence (that may be characterised by the evolution and dissipation that leads to non-Hamiltonian dynamics of the centre of the Gaussian.

Example: *Non-Hermitian evolution.* The propagation of a coherent state under a time evolution generated by a non-Hermitian operator and the special case of quadratic Hamiltonians in the context of Hagedorn wave packets has been studied in [3]. In order to apply these results we need first to rewrite the Hamiltonian $\hat{H} - \frac{i}{2}\hat{L}^\dagger \hat{L}$ slightly; since we assume that *L* is linear, we have $\left(\bar{L} \circ L\right)(z) = \bar{L}(z)L(z) + \frac{i\hbar}{2}\left\{\bar{L}, L\right\}$ and the term $\left\{\bar{L}, L\right\} = \nabla\bar{L} \cdot \Omega \nabla L$ is constant. This gives us $\hat{L}^\dagger L = \bar{L}L + \frac{i\hbar}{2}\left\{\bar{L}, L\right\}$, and we obtain

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\left(\hat{H} - \frac{i}{2}\hat{L}^\dagger \hat{L}\right)t} = e^{-\frac{i}{4}\nabla\bar{L}\cdot\Omega\nabla L t} e^{-\frac{i}{\hbar}\hat{K}t} \sqrt{a^2 + b^2} \text{ where } K(z) = H(z) - \frac{i}{2}\left|L(z)\right|^2.$$

The dynamics of a Gaussian wavepacket under a non-Hermitian Hamiltonian can be derived following a similar procedure to the one we have outlined for the Lindblad and SSE cases. Substituting the effective non-Hermitian Hamiltonian *K*(*z*) yields the parameter dynamics

$$\frac{d\tilde{z}}{dt} = \Omega\nabla H - G^{-1}\,\mathrm{Re}\left(\bar{L}\nabla L\right),\ \frac{dG}{dt} = -G\Omega H'' + H''\Omega G + \mathrm{Re}\left(\nabla\bar{L}\nabla L^{\mathrm{T}}\right) + G\Omega\,\mathrm{Re}\left(\nabla\bar{L}\nabla L^{\mathrm{T}}\right)\Omega G,$$

where the evolution equation for *G* is the same as the one for the SSE case. As expected, this fulfils $\frac{d}{dt}\det G = 0$ for $\det G = 1$, and an initially pure state remains pure.

The dissipative part of the central motion of the non-Hermitian dynamics can appear either quite different or very similar to that of the Lindblad case, depending on the structure of the Lindblad operator. For a Lindblad operator that is an analytic function of $\hat{a}$ or $\hat{a}^\dagger$, for example, the dissipative term in the central dynamics, given by $\Omega\,\mathrm{Im}\left(L\nabla\bar{L}\right)$ can be rewritten as $-\mathrm{Re}\left(\bar{L}\nabla L\right)$, which is very similar to the non-Hermitian dissipation, with the difference that the latter is modulated by the changing covariance metric *G*.

An example for which Lindblad and non-Hermitian central dynamics are very different, are Hermitian Lindbladians, for which the dissipative term in the Lindblad dynamics vanishes entirely. The quantum-jump evolution turns the non-Hermitian behaviour into the Lindblad one, by averaging over different quantum jumps that in general do not leave an initially Gaussian state Gaussian.

We will return to this issue after considering the Gaussian Lindblad and SSE dynamics.

6. Gaussian dynamics

Gaussian states are well suited for the analysis of quantum dynamics, since they are localised in phase space on order $\hbar$ (in appropriate coordinates they are minimum uncertainty states), and are the only states with a completely positive Wigner function. In this regard, they may be thought of as the most 'classical' of quantum states, and Gaussian approximations of the full quantum dynamics lead to simple phase-space dynamics. As has been observed by Schrödinger already in the early days of quantum mechanics, Gaussian wavepackets remain Gaussian in the dynamics of quantum harmonic oscillators and follow classical trajectories.

For open systems described by Lindblad equations or Schrödinger dynamics generated by non-Hermitian Hamiltonians, a similar statement holds, which allows one to reduce the full quantum Hilbert space dynamics to a simple phase-space dynamics described by a handful of parameters for Gaussian states for quadratic Hamiltonians and linear Lindbladians. Gaussian evolution for stochastic Schrödinger equations with quadratic Hamiltonian and linear Lindbladians in position representation has been considered and here too, an initially Gaussian state remains Gaussian.

In what follows we shall provide a brief review of the derivation and result for Lindblad dynamics, and then extend the idea to stochastic Schrödinger dynamics in quantum phase space, where we use the Wigner–Weyl formalism that illuminates the underlying phase-space geometry and allows for a better direct comparison with the Lindblad dynamics. At the heart of the Wigner–Weyl scheme is the Weyl transformation, a bijective map that maps observables on Hilbert spaces to their corresponding Weyl symbols. The Weyl symbol corresponding to an observable $\hat{O}\left(\hat{X},\hat{P}\right)$ is a distribution on classical phase space and is given by

$$O(x,p)=\int ds\left\langle x-\frac{s}{2}\middle|\hat{O}\left(\hat{X},\hat{P}\right)\middle|x+\frac{s}{2}\right\rangle e^{\frac{ips}{\hbar}}.$$

The Weyl symbol corresponding to the density operator is known as the Wigner function. We will consider Gaussian states with Wigner functions of the form

$$W(z)=\frac{\sqrt{\det G}}{\pi\hbar}e^{-\frac{i}{\hbar}\delta z G\delta z} \text{ with } \delta z=\begin{pmatrix} x-\langle x\rangle \\ p-\langle p\rangle \end{pmatrix}, \tag{11}$$

with a real symmetric matrix *G*, that encodes the phase-space covariance matrix of the system as

$$\sum_{ij}=\Delta\left(z_i z_j\right)^2=\frac{\hbar}{2}G_{ij}^{-1}. \tag{12}$$

This describes a pure state if and only if det *(G)* = 1. Inserting an ansatz of the form $W(z)$ with time-dependent (and in the SSE case stochastic) parameters *G* and $\tilde{z}$ into the evolution equation for the Wigner function yields dynamical equations for the parameters.

6.1. Gaussian dynamics of the Lindblad equation

The Lindblad equation in Weyl representation takes the form

$$\frac{dW}{dt}=\frac{i}{\hbar}\left(-\left(H\,\mathrm{e}\,W-W\,\mathrm{e}\,H\right)+L\,\mathrm{e}\,W\,\mathrm{e}\,\bar{L}-\frac{1}{2}\bar{L}\,\mathrm{e}\,L\,\mathrm{e}\,W-\frac{1}{2}W\,\mathrm{e}\,\bar{L}\,\mathrm{e}\,L\right)$$

with the Moyal (star) product of Weyl symbols given by

$$(A\,\mathrm{e}\,B)(q,p)=A(q,p)e^{\frac{i\hbar}{2}\overleftarrow{\nabla}\cdot\Omega\cdot\vec{\nabla}}B(q,p).$$

Since we are considering only quadratic Hamiltonians and linear Lindbladians, the Moyal products in this equation can be fully expanded to yield

$$\frac{dW}{dt}=-i\nabla\bar{L}\cdot\Omega\nabla LW+\nabla H\cdot\Omega\nabla W+\mathrm{Im}\left(L\nabla\bar{L}\right)\cdot\Omega\nabla W-\frac{\hbar}{2}\mathrm{Re}\left(\nabla L\cdot\Omega\nabla W''\Omega\nabla\bar{L}\right), \tag{13}$$

where $\Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ is the symplectic matrix. It is useful to rewrite H and L as polynomials in δz

$$H(z) = H(\tilde{z}) + \nabla H\big|_{z=\tilde{z}} \cdot \delta z + \frac{1}{2}\delta z \cdot H''\big|_{z=\tilde{z}}\, \delta z, \qquad L(z) = L(\tilde{z}) + \nabla L\big|_{z=\tilde{z}} \cdot \delta z \tag{14}$$

An initial Gaussian state remains Gaussian for all times. We can obtain the dynamical equations for parameters in the Wigner function (13) as

$$\frac{d\tilde{z}}{dt} = \Omega\nabla H + \Omega\,\mathrm{Im}\left(L\nabla L\right),$$
$$\frac{dG}{dt} = \left(H'' + \mathrm{Im}\left(\nabla L\nabla \bar{L}^{\mathrm{T}}\right)\right)\Omega G - G\Omega\left(H'' - \mathrm{Im}\left(\nabla L\nabla \bar{L}^{\mathrm{T}}\right)\right) + 2G\Omega\,\mathrm{Re}\left(\nabla L\nabla \bar{L}^{\mathrm{T}}\right)\Omega G$$

for the dynamics of the Gaussian parameters. The first order differential equation describing the central motion is linear and can be trivially integrated. The dynamical equation for the covariance matrix G decouples from the central motion as the Hamiltonian and Lindbladian dependent terms become constant.

For Hermitian Lindbladians, the Lindblad term in the central dynamics vanishes, leaving only Hamiltonian dynamics, as expected for these *purely decohering* systems. In general, non-Hermitian Lindbladians lead to both decoherence (that may be characterised by the evolution of G in this case) and dissipation that leads to non-Hamiltonian dynamics of the center of the Gaussian.

6.2. Gaussian Stochastic Schrödinger dynamics

Let us now use the same approach to derive parameter dynamics for the SSE. We begin by writing the SSE in projector form as

$$d\left(|\psi\rangle\langle\psi|\right) = |d\psi\rangle\langle\psi| + |\psi\rangle\langle d\psi| + |d\psi\rangle\langle d\psi| = \frac{i}{\hbar}\left(-i\hat{H} - \frac{1}{2}\hat{L}^{\dagger}\hat{L} + \langle\hat{L}^{\dagger}\rangle\hat{L} - \frac{1}{2}\langle\hat{L}^{\dagger}\rangle\langle\hat{L}\rangle\right)|\psi\rangle\langle\psi|\,dt$$
$$+ \frac{1}{\sqrt{2\hbar}}\left(\hat{L}\hat{\rho} + \hat{\rho}\hat{L}^{\dagger} - \langle\hat{L} + \hat{L}^{\dagger}\rangle\rho\right)d\xi_R + \frac{1}{\sqrt{2\hbar}}\left(\hat{L}\hat{\rho} - \hat{\rho}\hat{L}^{\dagger} - \langle\hat{L} - \hat{L}^{\dagger}\rangle\rho\right)d\xi_I \tag{15}$$

The deterministic (dt) part of Eq. (I.15) is the same as that of the Lindblad, which can evolve pure states into mixed states. In the SSE case, however, the state remains pure for all times, since the stochastic terms conspire to conserve the purity of the state.

We can translate Eq. (15) into the Wigner-Weyl representation to obtain

$$dW = -\frac{i}{\hbar}\left(H \,\mathrm{e}\, W - W \,\mathrm{e}\, H + i\left(L \,\mathrm{e}\, W \,\mathrm{e}\, \bar{L} - \frac{1}{2}\bar{L} \,\mathrm{e}\, L \,\mathrm{e}\, W - \frac{1}{2}W \,\mathrm{e}\, \bar{L} \,\mathrm{e}\, L\right)\right)dt$$
$$+ \frac{1}{\sqrt{2\hbar}}\left[L \,\mathrm{e}\, W + W \,\mathrm{e}\, \bar{L} - i\hat{H} - \langle\hat{L} + \hat{L}^{\dagger}\rangle W\right]d\xi_R + \frac{i}{\sqrt{2\hbar}}\left(L \,\mathrm{e}\, W - W \,\mathrm{e}\, \bar{L} - i\hat{H} - \langle\hat{L} - \hat{L}^{\dagger}\rangle W\right)d\xi_I$$

.

Since the deterministic part is the same as that of the Lindblad system Eq. (13), we need only calculate the stochastic terms. As result we have

$$dW = \left[\{H, W\} + \mathrm{Im}\left(L\{\bar{L}, W\}\right) - i\{\bar{L}, L\}W + \frac{\hbar}{2}\mathrm{Re}\{L, \{\bar{L}, W\}\}\right]dt$$
$$+ \left(\sqrt{\frac{2}{\hbar}}\left(L^R - \langle L^R\rangle\right)W + \sqrt{\frac{\hbar}{2}}\{W, L^I\}\right)d\xi_R - \left(\sqrt{\frac{2}{\hbar}}\left(L^I - \langle L^I\rangle\right)W - \sqrt{\frac{\hbar}{2}}\{W, L^R\}\right)d\xi_I$$

After algebraic transformations we can obtain the (stochastic) dynamical equations

$$d\tilde{z} = \left(\Omega\nabla H + \Omega\,\mathrm{Im}\left(L\nabla\bar{L}\right)\right)dt + \sqrt{\frac{\hbar}{2}}\left(G^{-1}\nabla L^{R} - \Omega\nabla L^{I}\right)d\xi_{R},$$

$$\frac{dG}{dt} = -G\Omega H'' + H''\Omega G + \mathrm{Re}\left(\nabla\bar{L}\nabla L^{\mathrm{T}}\right) + G\Omega\,\mathrm{Re}\left(\nabla\bar{L}\nabla L^{\mathrm{T}}\right)\Omega G$$

for the Gaussian parameters.

We notice that the deterministic part of the dynamics of the centre $\tilde{z}$ is the same as that of the Lindblad equation; however, the SSE dynamics have an additional stochastic component as expected. This stochastic component contains covariance dependent terms and unlike in the Lindblad case, we can no longer simulate the centre trajectories without calculating the covariance dynamics. For quadratic systems the evolution of the covariance matrix *G* is deterministic and independent of the motion of the centre but different from that of the Lindblad evolution. This difference is not surprising considering that the *G* matrix in the SSE describes the covariances of the individual pure-state trajectories, while the *G* matrix of the Lindblad evolution describes that of the total density matrix arising from the ensemble average. In fact, the dynamics of *G* for the SSE are the same as those arising from deterministic non-Hermitian Hamiltonian dynamics, which we shall briefly review in the next section as the first phase of quantum-jump dynamics.

6.3. Quantum-jump dynamics

Quantum-jump dynamics do not preserve Gaussian states for arbitrary linear Lindbladians. As an example, consider the Lindblad operator $\hat{L} = \hat{a}^{\dagger}$. The first jump maps a state $|\psi_g\rangle$ to $\hat{a}^{\dagger}|\psi_g\rangle$ and thus transforms a Gaussian state into a non-Gaussian one. We will show in what follows, that it is still possible to calculate the quantum-jump dynamics building on the propagation of Gaussian states, leading again to just a handful of time-dependent parameters. In the quantum jump unravelling of the Lindblad dynamics, we propagate the initial state $|\psi_0\rangle$ with the time evolution generated by the non-Hermitian Hamiltonian $H - \frac{i}{2}\hat{L}^{\dagger}\hat{L}$, and intersperse it with jumps at discrete times t_j,

$$|\psi\rangle \mapsto \frac{\hat{L}|\psi\rangle}{\sqrt{\langle\psi|\hat{L}^{\dagger}\hat{L}|\psi\rangle}}.$$

The non-Hermitian nature of time evolution $\hat{U}(t) = e^{-\frac{i}{\hbar}\left(\hat{H} - \frac{1}{2}\hat{L}^{\dagger}\hat{L}\right)t}$ will lead to a decreasing norm of the propagated state, and the quantum jumps reset the norm to one due to the inclusion of the denominator. After *k* quantum jumps at times $t_1, t_2, \ldots, t_k$, i.e, $t \in [t_k, t_{k+1})$, the state will be of the form

$$|\psi(t)\rangle = \frac{1}{\left\||\psi(t_k)\rangle\right\|}\hat{U}(t_k - t_{k-1})\hat{L}\hat{U}(t_k - t_{k-1})\hat{L}\hat{U}(t_{k-1} - t_{k-2})\hat{L}\cdots\hat{U}(t_2 - t_1)\hat{L}\hat{U}(t_1)|\psi_0\rangle.$$

To compute this expression, we will introduce a basis which is moving with the state $\hat{U}(t)|\psi_0\rangle$, the so-called Hagedorn basis. An example for which Lindblad and non-Hermitian central dynamics are very different, are Hermitian Lindbladians, for which the dissipative term in the Lindblad dynamics vanishes entirely. The quantum-jump evolution turns the non-Hermitian behaviour into the Lindblad one, by averaging over different quantum jumps that in general do not leave an initially Gaussian state Gaussian.

7. Examples

Let us consider the Lindblad dynamics and the two unravellings for a harmonic oscillator Hamiltonian $\hat{H} = \frac{\omega}{2}\left(\hat{p}^2 + \hat{x}^2\right)$ with two different Lindblad operators, one Hermitian and one non-Hermitian. Let us first

consider a quantum harmonic oscillator with a Hermitian Lindblad operator $\hat{L} = \sqrt{\gamma}\hat{x}$ which can be thought of as modelling a position measurement.

7.1. Position measurement

Since the Lindbladian is Hermitian (purely decohering), in the Lindblad dynamics $\hat{L}$ yields no contribution to the dynamics of the expectation values z_t, which simply follow the familiar harmonic oscillator trajectories. Conversely for individual SSE and quantum-jump trajectories $\hat{L}$ will affect the central dynamics. The dynamical equations for the Gaussian parameters in the Lindblad dynamics equation simplify to

$$\frac{d\tilde{z}}{dt} = \omega\Omega\tilde{z}, \qquad \frac{dG}{dt} = \omega\left(\Omega G - G\Omega\right) + 2G\Omega\Gamma\Omega G, \tag{16}$$

where we have defined $\Gamma = \mathrm{Re}\left(\nabla L \nabla \bar{L}^{\mathrm{T}}\right) = \begin{pmatrix} \gamma & 0 \\ 0 & 0 \end{pmatrix}$. While the central dynamics is that of the unitary harmonic oscillator, the dynamics of the covariances encoded by $G(t)$, are influenced by the position measurement. Let us consider the simple example of an initially squeezed state with,

$$G(0) = \begin{pmatrix} \zeta & 0 \\ 0 & \dfrac{1}{\zeta} \end{pmatrix}.$$

Solving equation (I.16) we find the physical variances as

$$\Delta x^2(t) = \frac{\hbar}{4}\left(\frac{\zeta^2 + 2\gamma\zeta t + 1}{\zeta} - \frac{\gamma}{\omega}\sin(2\omega t) - \frac{\zeta^2 - 1}{\zeta}\cos(2\omega t)\right)$$
$$\Delta p^2(t) = \frac{\hbar}{4}\left(\frac{\zeta^2 + 2\gamma\zeta t + 1}{\zeta} + \frac{\gamma}{\omega}\sin(2\omega t) + \frac{\zeta^2 - 1}{\zeta}\cos(2\omega t)\right).$$
$$\Delta xp(t) = \frac{\hbar}{4}\left(\frac{\gamma}{\omega^2\zeta} + \frac{\zeta^2\omega - \omega - \gamma\zeta}{\zeta^2\omega^2}\cos(2\omega t)\right)$$

This behaviour is illustrated in Fig. 10.

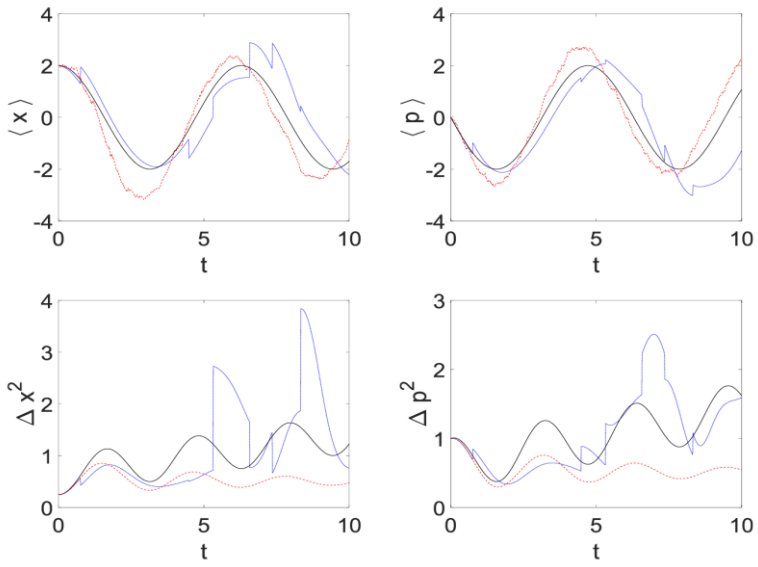


Fig. 10. Lindblad dynamics (solid black line) compared with single trajectories of the SSE (dashed red line) and quantum-jump method (dotted blue line) for the position measurement, with ω = 1 and γ = 0.2.

[The initial Gaussian is a squeezed state (i.e. $G=\begin{pmatrix}2 & 0\\ 0 & \frac{1}{2}\end{pmatrix}$*), centered at* $\tilde{z}_t=(2,0)^{\mathrm{T}}$*. We show the time dependence of the position expectation* $\langle\hat{x}\rangle$ *(top left), the momentum expectation* $\langle\hat{p}\rangle$ *(top right), the positional variance* Δx^2 *(bottom left) and the momentum variance* Δp^2 *(bottom right).The Lindblad dynamics are depicted as solid black lines]*

Figure 10 depicts the expectation values of position and momentum and their uncertainties as a function of time for an example with $\omega = 1$ and $\gamma = 0.2$ for an initially squeeze state centred at $\tilde{z}_t=(2,0)^{\mathrm{T}}$. That is, we observe the typical harmonic oscillations with frequency 2ω in the covariances as they appear in the unitary harmonic oscillator, accompanied by a linear growth of the position and momentum uncertainties Δx^2 and Δp^2, associated with the effect of the position measurement.

The SSE dynamical equations become

$$d\tilde{z}=\omega\Omega\tilde{z}dt+\sqrt{\frac{\hbar\gamma}{2}}G^{-1}\begin{pmatrix}1\\0\end{pmatrix}d\xi_R+\sqrt{\frac{\hbar\gamma}{2}}\begin{pmatrix}1\\0\end{pmatrix}d\xi_I,\quad \frac{dG}{dt}=\omega(\Omega G-G\Omega)+\Gamma+G\Omega\Gamma\Omega G\,.$$

That is, for the central motion we again have the familiar unitary Hamiltonian flow term, and no damping term, but now there is an additional width-dependent stochastic noise. The equation for the covariances differs from that in the Lindbladian case, as expected.

As a result, independent of the initial value $G(0)$, $\Sigma(t)$ tends to a fixed point as $t\to\infty$ given by

$$\Sigma(t)\to\frac{\hbar}{2\gamma}\begin{pmatrix}\sqrt{2\omega(\lambda-\omega)} & \lambda-\omega\\ \lambda-\omega & \lambda\sqrt{\frac{2(\lambda-\omega)}{\omega}}\end{pmatrix}.$$

This is in stark contrast to the behaviour of the Lindblad covariances, with their linear growth in Δx^2 and Δp^2. We can see this in Fig. 10 which shows the SSE dynamics as red dashed lines. For the parameter choices corresponding to the example in Fig. 1 ($\omega = 1$, $\gamma = 0.2$) we have $\lambda=\frac{\sqrt{26}}{5}$, and the covariances approach

$$\Delta x^2(t)\to\frac{5\sqrt{2(\lambda-1)}}{2}\approx 0.497,\quad \Delta p^2(t)\to\frac{5\lambda\sqrt{2(\lambda-1)}}{2}\approx 0.507,\quad \Delta xp(t)\to\frac{5(\lambda-1)}{2}\approx 0.049\,,$$

that is, the final state is very close to a coherent state, due to the relatively small value of γ. For the central dynamics we observe *stochastic fluctuations* around the average Lindblad dynamics.

The *quantum-jump trajectories*, on the other hand, depicted for an example run as blue dotted lines in Fig.10, show *very different* behaviour. Here up to the first jump, the centre of the Gaussian state follows the non-Hermitian dynamics, which in the present case reduce to

$$\begin{pmatrix}\dot{x}_t\\ \dot{p}_t\end{pmatrix}=\omega\begin{pmatrix}p_t\\ -x_t\end{pmatrix}-\frac{2\gamma x_t}{\hbar}\begin{pmatrix}\Delta x^2(t)\\ \Delta xp(t)\end{pmatrix},$$

where $G(t)$ evolves dynamically as in the SSE case. That is, there is an additional position dependent damping term in the evolution, modulated by the covariances of the state. This damping in comparison to the Lindblad evolution is visible in the example depicted in Fig. 10.

We also observe in Fig. 10 that, as expected, the dynamics of position and momentum variances agree between the quantum jump and the SSE dynamics up to the first jump. What is not shown here, but has been numerically verified, is that averaging over many (quantum) jump trajectories simulated in the Hagedorn basis does indeed recover the Lindblad dynamics, the same is true of the SSE parameter dynamics as expected.

We observe clear differences between the Lindblad, SSE and quantum-jump dynamics for the harmonic oscillator with position measurement, which can be understood to a large degree using the analytical treatment developed in the previous sections.

Figure 11 shows the Wigner functions of the state at $t = 10$ for the three different realisations together with the central trajectory up until this time (see, Fig. 10).

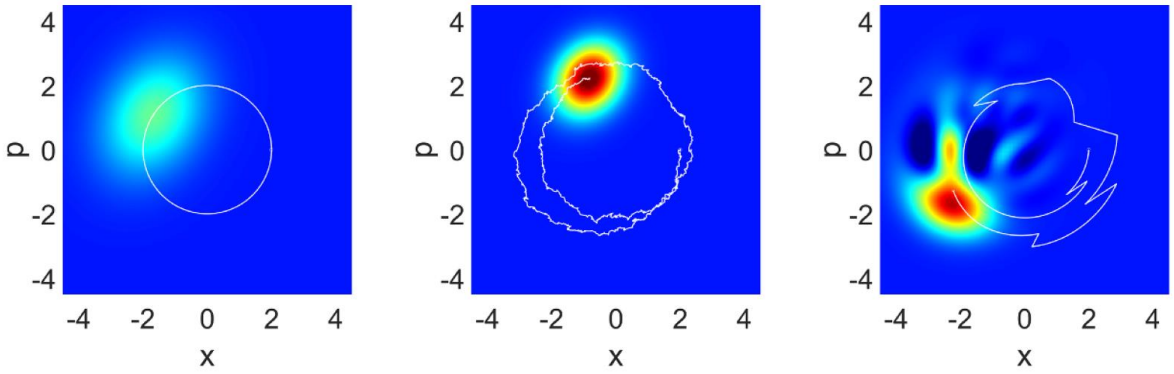


Fig. 11. Lindblad dynamics (left) compared with a single trajectory of the SSE (middle) and quantum jump (right) for the position measurement model equation with $\omega = 1$ and $\gamma = 0.2$ [25]. [In each case, a snap-shot of the Wigner function at t = 10 is plotted in phase space, with a white line displaying the precedent central motion]

In the right panel, corresponding to the Lindblad dynamics the state remains Gaussian, and its central motion follows the usual unitary harmonic oscillator trajectory. The increased uncertainties in position and momentum lead to the broadening of the Gaussian apparent here. The SSE dynamics in the central picture, on the other hand, also remains Gaussian in shape and stays well localised as predicted by the dynamical behaviour of G. The central trajectory performs a Brownian motion around the harmonic oscillator trajectory. Finally, the quantum-jump trajectory performs smooth stretches of damped harmonic oscillations interrupted by discrete jumps, and crucially, the state does not remain Gaussian.

Let us consider the generic problem of state preparation for open quantum systems.

As is well known, open quantum systems can be simulated by quantum trajectories described by a stochastic Schrödinger equation. In this context, the state preparation problem becomes a stochastic optimal control (SOC) problem. The SOC problem requires the solution of the Hamilton-Jacobi-Bellman equation, which is generally challenging to solve. A notable exception are the so-called path integral (PI) control problems for which one can estimate the optimal control solution by sampling. It is possible to derive a class of quantum state preparation problems that can be solved with PI control. Since the method only requires the propagation of state vectors ψ, it presents a quadratic advantage over density-centered approaches, such as Pontryagin Maximum Principle (PMP)-based methods. Unlike most conventional quantum control algorithms, it does not require computing gradients of the cost function to determine the optimal controls. Instead, the optimal control is computed by iterative importance sampling. The SOC setting allows in principle for a state feedback control solution, whereas Lindblad-based methods are restricted to open-loop control. Here, we illustrate the effectiveness of the approach through some examples of open loop control solutions for single- and multi-qubit systems.

7.2. Stochastic optimal control of open quantum systems

Control problems, as abovementioned, can be divided into two categories: open-loop and closed-loop/feedback control. In feedback quantum optimal control (QOC), the controls depend on the system's state, requiring full or partial information about the state at each time. In contrast, open-loop QOC involves state-independent controls that are solely functions of time. The most widely used approach considers a closed quantum system, which is a quantum system in isolation where effects from the environment can be ignored and whose dynamics is unitary. For such systems one formulates an open-loop QOC which is solved using gradient-based methods such as Gradient Ascent Pulse Engineering (GRAPE) and its variants, direct search-based methods like Chopped RAndom Basis (CRAB), variational methods such as Krotov optimization and techniques grounded in the Pontryagin Maximum Principle (PMP). These methods have been extensively

applied to address a range of tasks. In reality, quantum systems are not isolated from their environment, and the interaction with it decoheres the quantum system and destroys its unique quantum features. The theoretical framework to study how quantum systems evolve in interaction with an environment is the theory of open quantum systems. When the coupling with the environment is sufficiently weak, and the system's dynamics is much faster compared to the environment's dynamics, then the system's dynamics becomes Markovian and can be described by the so-called Lindblad equation, which contains additional non-unitary terms describing the interaction of the system with the environment.

Remark. All these methods can be computationally expensive, essentially because they require to propagate the density matrix instead of the wave function. Moreover, these methods are gradient-based, and they have several shortcomings. In some cases, the gradients can be computed analytically or numerically. But, in most cases, the gradients can only be computed approximately (such as in *k*-order Open GRAPE) and the gradient optimization is difficult due to the temporal dependencies inherent in the control problem, an issue that occurs classically as well in dynamic programming. Secondly, the optimal control solution is an open-loop controller, not a feedback controller that can correct for errors and stabilize the system. The reason a feedback controller is not possible in these frameworks is that the Lindblad equation is a deterministic equation that treats the effect of noise on average.

In order to obtain a feedback controller, the Lindblad equation needs to be replaced by a stochastic dynamics that explicitly models the effects of individual disturbances due to the environment and due to measurement. Such stochastic dynamics have been proposed under the name of quantum trajectories as stochastic generalizations of the Schrödinger equation. The Lindblad equation emerges then as the dynamics of the average $\langle \psi\psi^{\dagger} \rangle$ over quantum trajectories. Different ways of defining SSEs that lead to the same master equation constitute different unravelings of the master equation and can take the form of a Markov jump process or a diffusion process. The mathematical framework was formulated in Introduction. Stochastic unravelings for non-Markovian scenarios can be traced back to Dios and Wiseman. Quantum trajectories have been shown experimentally on different platforms, such as superconducting circuits, optomechanical systems and hybrid quantum systems.

Control of open quantum systems using unravelings naturally results in a stochastic optimal control problem, where the optimal solution is a feedback controller (see Chapter 1). The solution of the stochastic optimal control problem requires the solution of the Bellman equation or a stochastic version of PMP involving backward stochastic differential equations, which in either case is very difficult in general. A notable exception are the linear quadratic Gaussian (LQG) problems, where the dynamics is linear in the state, the cost is quadratic, and the noise is additive Gaussian. The stochastic Schrödinger equation is generally not of the LQG form: it contains a bi-linear term $u\psi$, with u the control and ψ the quantum state and it may contain more non-linearities due to a state normalization constraint. However, the bi-linearity does not necessarily preclude the formulation of an LQG control problem in the Heisenberg picture, and this has been used to control quantum systems. It was demonstrated for cooling and position localization of a quantum particle, the cooling of the vibrations of a mechanical resonator and the position of an optically trapped nano particle at room temperature etc.

Remark. The bilinearity of the control term uρ in the Lindblad equation, with u the control and ρ the density matrix, does not necessarily preclude a linear dynamics in the Heisenberg picture. A classical analogy is that a linear stochastic classical dynamical system $dx = udt + dW$ is described by a Fokker-Planck equation $\dot{p} = -\nabla(up) + \frac{1}{2}\nabla^2 p$ that describes the evolution of the instantaneous probability density $p(x,t)$. The FP equation (being the classical analog of the Lindblad equation) is bi-linear in u, while the stochastic dynamics is linear in u. As a result, quantum systems described by position and momentum operators can be treated within the LQG optimal control framework.

The feedback controller requires information about the quantum state through measurement. Since the quantum state is only partially observable through measurement, the control problem becomes what is known as a partial observable control problem. A unique quantum feature, not present in classical systems, is that measurement will disrupt the quantum state by projecting the state onto one of the measurement eigenstates (quantum back-action). A compromise between information gain and minimal disruption of the quantum state is given by the so-called weak or continuous measurement. The issue of partial observability and measurement is not so important for LQG control problems, because of a property called certainty equivalence, which essentially states that the optimal control depends on the expected latent state only.

However, partial observability and the correct treatment of measurement becomes important for stochastic optimal control problems beyond the LQG regime. Measurement can be elegantly formalized by the so-called hybrid dynamics, which describes the simultaneous time evolution of the quantum state and the classical observation(s). The theory of unravelings of the hybrid dynamics in terms of discrete time quantum jumps was first described]. Its generalization to continuous time measurements was recently proposed as a theoretical framework to unify quantum physics with gravity and generalizes earlier work on continuous measurement.

Although the theory of stochastic optimal control of quantum systems is well developed, its application has so far been mostly restricted to the LQG case. There exists another class of control algorithms that can solve a large class of non-linear stochastic optimal control problems, known as the path integral (PI) control method. This presents a quite large class of stochastic optimal control problems with non-linear dynamics, non-Gaussian noise and non-linear control cost. A strong requirement for the control problem to be of the PI form is that the noise *dW* and the control *udt* should appear in the dynamics as their sum *udt* + *dW*. The advantage of the PI control problem is that the optimal control solution can be expressed in closed form as a path integral, without the need to solve a Bellman equation or the PMP equations. The path integral can be estimated relatively efficiently through sampling.

The sampling is optimized using a procedure called adaptive importance sampling which estimates gradients based on self-generated quantum trajectories and is well suited for parallel computing with virtually no overhead. PI control has been very succesfully applied to many high dimensional non-linear stochastic optimal control problems with real-time requirements that occur in robotics where all other methods fail.

We describe the proposal to apply the PI control method to control an open quantum system whose dynamics can be written in Lindblad form. To simulate the Lindblad equation, continuous unravelings used that yield a quantum diffusion process and that is formulated as stochastic differential equations (SDE) with Brownian noise. These unravelings are not unique and in general not of the PI control form. For certain combinations of control Hamiltonian and Lindblad operators we can use this freedom to define a PI control problem. We consider the problem of quantum state preparation. This problem can be formalized as a finite-horizon stochastic optimal control problem that can be efficiently solved using the PI control method. We will focus, as a concrete example, on open loop control because closed-loop control requires the inclusion of quantum measurement in the unravelings, which is a topic that we will consider in the future as the attempt in combining state-centered quantum trajectories techniques with path integral control theory.

We describe a class of transformations on the Lindblad operators and the noise matrix that leaves the Lindblad equation invariant while changing the unraveling. This transformation proves instrumental for mapping many interesting control problems originally formulated in Lindblad form onto stochastic optimal control problems of the PI form. The optimal control that results from solving the path integral equations is a feedback controller, i.e. it depends on the system state. In practice, computing the optimal controller exactly can be challenging if not unfeasible due to the infinite dimensionality of the control. Quantum control algorithm by combining quantum unravelings with path integral control can be described.

Example: *Unravelling formalism for noises.* An alternative way to account for noises is to unravel the master equation and consider explicitly the noise acting on the wavefunction. Consider the following master equation, which - for the sake of simplicity - is taken as Markovian

$$\frac{d\hat{\rho}_t}{dt} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}_t\right] + \varepsilon^2 \sum\left(\hat{L}_k \hat{\rho}_t \hat{L}_k^\dagger - \frac{1}{2}\left\{\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}_t\right\}\right), \tag{17}$$

where $\hat{H}$ is the Hamiltonian, and ε quantifies the coupling of the noises, while the Lindblad operator $\hat{L}_k$ can embed also relative strengths between diff erent noise channels.

Remark. We want to construct a stochastic unravelling of the Lindblad dynamics in Eq. (17). This is a dynamical stochastic equation for the wavefunction $|\psi_t\rangle$ from which one can derive exactly Eq. (17) for the corresponding statistical operator obtained as $\hat{\rho}_t = \mathrm{E}\left[|\psi_t\rangle\langle\psi_t|\right]$, where E indicates the average over the stochastic process. There are two advantages in using the unravelling approach in place of that based on the master equation. The first one is that, for a *N* level system, the master equation approach is equivalent to solve N^2 ordinary coupled diff erential equations of the first order, while the unravelling approach has *N* stochastic ordinary coupled diff erential equation of the first order. Clearly, there is a computational advantage in the

scaling, however it is only polynomial and it has to be compared with the necessity of performing stochastic averages. The second advantage is that for every master equation there are infinite equivalent unravellings corresponding to it. Depending on the specific problem, some of these can be solved or simulated more easily than others or than the master equation. In this family of equivalent unravellings, the linear stochastic unravelling has a special place due to its simplicity.

In the so-called Ito form, it reads

$$d|\psi_t\rangle = \left[-\frac{i}{\hbar}\hat{H}dt + \sum\left(i\varepsilon\hat{L}_k dW_{k,t} - \frac{1}{2}\varepsilon^2\hat{L}_k^\dagger\hat{L}_k dt \right) \right] |\psi_t\rangle , \tag{18}$$

where $dW_{k,t}$ are diff erentials of standard independent Wiener processes, such that

$$\mathrm{E}\left[dW_{k,t} \right] = 0 \text{ and } \mathrm{E}\left[dW_{k,t} dW_{m,t} \right] = \delta_{m,t} dt . \tag{19}$$

The first term of Eq. (18) is the standard Schrödinger equation. The second term introduces the stochasticity of the noise process, while the last term is necessary to preserve the normalisation of $|\psi_t\rangle$ in time. We now proceed in showing that the dynamics in Eq. (18) is equivalent to that in Eq. (17). We start by diff erentiating the statistical operator:

$$d\hat{\rho}_t = d\mathrm{E}\left[|\psi_t\rangle\langle\psi_t| \right] = \mathrm{E}\left[d\left(|\psi_t\rangle\langle\psi_t| \right) \right],$$

where the second equality follows from the linearity of the average. Then, one has

$$d\hat{\rho}_t = \mathrm{E}\left[|d\psi_t\rangle\langle\psi_t| \right] + \mathrm{E}\left[|\psi_t\rangle\langle d\psi_t| \right] + \mathrm{E}\left[|d\psi_t\rangle\langle d\psi_t| \right],$$

where the last term is needed to account all the terms of the first order in dt, which includes that in the second order in *dW*, see Eq. (19). Now, one substitutes, up to the first order in *dt* and second order in $dW_{k,t}$, Eq. (18) in place of $|\psi_t\rangle$, and its conjugate in place of $|d\psi_t\rangle$. Then, we obtain

$$\begin{aligned} d\hat{\rho}_t = {} & \mathrm{E}\left\{ \left[-\frac{i}{\hbar}\hat{H}dt + \sum_k\left(i\varepsilon\hat{L}_k dW_{k,t} - \frac{1}{2}\varepsilon^2\hat{L}_k^\dagger\hat{L}_k dt \right) \right] |\psi_t\rangle\langle\psi_t| \right\} \\ & + \mathrm{E}\left\{ |\psi_t\rangle\langle\psi_t| \left[\frac{i}{\hbar}\hat{H}dt + \sum_k\left(-i\varepsilon\hat{L}_k dW_{k,t} - \frac{1}{2}\varepsilon^2\hat{L}_k^\dagger\hat{L}_k dt \right) \right] \right\} - \mathrm{E}\left[\sum_k i\varepsilon\hat{L}_k dW_{k,t} |\psi_t\rangle\langle\psi_t| \sum_m i\varepsilon\hat{L}_m dW_{m,t} \right] \end{aligned}$$

Under the Markovian assumption, i.e. that the noises $dW_{k,t}$ and $dW_{k,s}$ for $t \neq s$ are independent, then in the state $|\psi_t\rangle$ there are only noises up to time $s < t$ and thus independent from $dW_{k,t}$. Thus, in last Equation one can separate the average acting on $dW_{k,t}$ and that acting on the state $|\psi_t\rangle$. Namely, we find

$$\begin{aligned} & \mathrm{E}\left[dW_{k,t} |d\psi_t\rangle\langle\psi_t| \right] = \mathrm{E}\left[dW_{k,t} \right] \mathrm{E}\left[|d\psi_t\rangle\langle\psi_t| \right] = \mathrm{E}\left[dW_{k,t} \right] \hat{\rho}_t = 0, \\ & \mathrm{E}\left[dW_{k,t} |d\psi_t\rangle\langle\psi_t| dW_{m,t} \right] = \mathrm{E}\left[dW_{k,t} dW_{m,t} \right] \mathrm{E}\left[|d\psi_t\rangle\langle\psi_t| \right] = \delta_{k,m} dt \hat{\rho}_t \end{aligned} .$$

By substituting these expressions in last Equation, we obtain

$$d\hat{\rho}_t = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}_t \right] + \varepsilon^2 \sum_k \left(\hat{L}_k \hat{\rho}_t \hat{L}_k^\dagger - \frac{1}{2}\left\{ \hat{L}_k^\dagger\hat{L}_k, \hat{\rho}_t \right\} \right) dt ,$$

which can be easily recasted in the form of Eq. (17).

Consider the evolution of a quantum system *S* that is coupled to an environment *E*. The total system *S* + *E* is described by a quantum state ψ_{S+E} that evolves according to a unitary dynamic dictated by the Schrödinger equation. The density matrix of the system *S* is obtained by tracing out the degrees of freedom of the

environment and is denoted as $\rho = \mathrm{Tr}_E\left(\psi_{S+E}\psi_{S+E}^{\dagger}\right)$. The evolution law of the state ρ can be complicated or inaccessible in general but, under certain conditions such as weak coupling between system and environment and the environment being sufficiently large, one can derive an evolution law for ρ that satisfies some attractive properties such as Markovianity and trace-preservation. The most general form of this class of dynamics is given by the celebrated Lindblad equation

$$\dot{\rho} = -i\left[H,\rho\right] + \mathrm{D}\left[D,C\right]\rho \tag{20}$$

with the dissipation super operator

$$\mathrm{D}\left[D,C\right]\rho := D_{ab}\left(C_a\rho C_b^{\dagger} - \frac{1}{2}\left\{C_b^{\dagger}C_a,\rho\right\}\right).$$

The first term in (20) describes the unitary dynamics of the closed system *S* with Hamiltonian *H*. The second term describes the influence of the environment on the evolution of ρ in terms of *m* Lindblad operators C_a, $a = 1, \ldots, n_c$. The noise matrix *D* is assumed to be positive semidefinite. This is a sufficient condition, although not necessary, for ensuring positive evolution maps. Here we restrict *D* to be real symmetric.

The Lindblad operators encode decoherence and dissipation channels that arise from the interaction of the systems with the environmental degrees of freedom. The dynamical maps $\rho \to C_a\rho C_b^{\dagger} - \frac{1}{2}\left\{C_b^{\dagger}C_a,\rho\right\}$ are complete positive and trace-preserving maps. Therefore, the maximum number of these channels is $2^{2n} - 1$, with *n* the total number of qubits. Some examples of Lindblad operators are measurement operators in which case C_a is Hermitian. Usually, Hermitian operators are related to dephasing/decoherence processes. In single-qubit systems, dissipation operators such as $\sigma^{\pm}$ serves to model e.g. the emission and absorption of light quanta with the electromagnetic field. Due to the many ways of interacting with the environment, it is not surprising that any initial state that is pure will not remain so under Lindblad evolution.

Alternatively, the Lindblad equation can be interpreted as an average dynamics obtained from considering all particular time realizations of the quantum state ψ. This leads to the theory of stochastic unravelings. Stochastic quantum unravelings are usually encoded as a stochastic differential equation (SDE) of the state ψ. The SDE is designed in such a way that the density operator $P = \psi\psi^{\dagger}$, which now is a stochastic quantity, follows in average a Lindblad evolution, i.e. $\rho = \left\langle \psi\psi^{\Diamond} \right\rangle$, with ρ satisfying (20). One can define unravelings in many ways, for instance using stochastic jumps at discrete times or using continuous Wiener noise. In this section we use the latter. Assume the following SSE

$$d\psi = -iH\psi dt - \frac{1}{2}D_{ab}\left(C_b^{\dagger}C_a - 2c_aC_a + c_ac_b\right)\psi dt + \left(C_a - c_a\right)\psi dW_a \tag{21}$$

with dW_a a real-valued Wiener process with $\langle dW_a\rangle = 0$ and $\langle dW_a dW_b\rangle = D_{ab}dt$, with *D* a symmetric matrix. The C_a are the Lindblad operators appearing in (I.20) and $c_a := \psi^{\dagger}C_a^{(h)}\psi$ with $C_a^{(h)} := \frac{1}{2}\left(C_a + C_a^{\dagger}\right)$, the Hermitian part of C_a. Given these definitions, one can state the following result: Eq. (I.21) is an unraveling of the Lindblad equation (20).

The specific form of Eq. (21) is not arbitrary and its derivation satisfies very general physical constraints. If one considers that the term $C_a\psi dW_a$ in Eq. (21) implements the basic stochastic action from the environment onto the quantum state, then the remaining terms are needed to ensure that ψ remains normalized under the dynamics ($d\|\psi\|^2 = 0$). The c_a terms introduce non-linearities in the dynamics. This is a natural consequence of the stochastic non-Hermitian interaction of the system with the environment, which makes the evolution non-unitary and, therefore, violates norm preservation. A non-unitary norm preserving dynamics is necessarily non-linear.

It remains interesting to construct quantum ODE algorithms with improved efficiency by reducing the ODE to other quantumly solvable tasks. One notable candidate is the dynamics of open quantum systems with the Lindblad master equation (Lindbladian) as a typical example. Lindbladian itself is a universal quantum computing model. Recently, there have been several works proposing quantum algorithms based on

Lindbladians, where they aim to encode states of interest such as Gibbs states and ground states as the steady states of Lindbladians. Inspired by these rapid developments, our question arises:

Is it possible to solve linear ODEs via Lindbladians?

7.3. Linear ODEs solution via Lindbladians

Differential equations have long served as an essential tool for modeling and describing the dynamic of systems in natural and social science. A general linear ordinary differential equation (ODE) is typically expressed as

$$\frac{d}{dt}\vec{\mu}(t) = -V(t)\vec{\mu}(t) + \vec{b}(t), \text{ where } V(t) \in \mathbb{C}^{2^n \times 2^n},\ \vec{\mu}(t),\ \vec{b}(t) \in \mathbb{C}^{2^n}, \text{ and } \vec{\mu}(0) = \vec{\mu}_0.$$

Classical simulation algorithms often become highly inefficient for large systems due to their polynomial dependence on the system dimension. On the other hand, quantum algorithms with appropriate input access can produce a quantum state that encodes the solution of the ODE with only poly-logarithmic dependence on the system dimension, which makes solving ODE as a promising application of quantum computers. In particular, the Hamiltonian simulation, which aims to simulate the Schrödinger equation, a special case of ODEs on quantum computers, is arguably one of the most important applications and may be among the first to achieve practical quantum advantages.

Remark. Since $V(t)$ is generally not anti-Hermitian and the time evolution operator of the ODE is not necessarily unitary for many important problems in such, as example, non-Hermitian physics and fluid dynamics. The central challenge in designing quantum algorithms for linear ODEs is thus how to embed non-unitary dynamics into intrinsically unitary quantum dynamics. When $V(t)$ is a time-independent normal matrix and $\vec{b}(t) \neq \vec{0}$, the problem of solving an ODE can be efficiently addressed by the powerful quantum singular value transformation (QSVT) algorithm. However, an ODE with a time-dependent non-normal matrix $V(t)$ and a possibly inhomogeneous term $\vec{b}(t) \neq \vec{0}$ is beyond the reach of QSVT due to the mismatch between the singular value transformation and the eigenvalue transformation.

Previous works have developed two strategies for general linear ODEs. One is the linear-system-based approach, which discretizes the ODE by a numerical scheme, formulates the discretized ODE as a dilated linear system of equations, and solves the linear system by quantum linear system algorithms. The first efficient linear-system-based approach was proposed by Berry, applying multi-step methods for time discretization and HHL algorithm for solving the resulting linear system. Since then, there have been several subsequent works on linear-system-based approach by higher-order time discretization and more advanced quantum linear system algorithms. The other is the evolution-based approach, which directly embeds the time evolution operator into the subspace of an efficiently implementable unitary by time-marching, reducing to Hamiltonian simulation problems, or quantum eigenvalue processing.

Remark. The motivation comes from two remarkable features of Lindbladians. First, unlike previous evolution-based algorithms where non-unitary dynamics is embedded into the subspace of unitaries (block encoding), Lindbladians are naturally non-unitary due to the interaction with the environment. It is thus tempting to use this non-unitary dynamics to solve non-unitary ODEs. We call this a subsystem approach. Second, there exist various quantum algorithms for simulating Lindbladians, which makes it amenable to solve linear ODEs via Lindbladians on quantum computers as long as we can establish a connection between them. Solving linear ordinary differential equations (ODE) is one of the most promising applications for quantum computers to demonstrate exponential advantages. The challenge of designing a quantum ODE algorithm is how to embed non-unitary dynamics into intrinsically unitary quantum circuits.

A new quantum algorithm for solving ODEs by harnessing open quantum systems developed. Specifically, the natural non-unitary dynamics of Lindbladians utilized with the aid of a new technique called the non-diagonal density matrix encoding to encode general linear ODEs into non-diagonal blocks of density matrices. This framework enables us to design a quantum algorithm with both theoretical simplicity and good performance. Combined with the state-of-the-art quantum Lindbladian simulation algorithms, the algorithm can outperform all existing quantum ODE algorithms and achieve near-optimal dependence on all parameters under a plausible input model.

Thus, it is possible to embed general linear ODEs into Lindbladians with the aid of a new technique called non-diagonal density matrix encoding. The solution to an ODE can be encoded into a non-diagonal block of a density matrix, from which we can prepare the normalized solution state or merely measure its properties. Based on this connection between general linear ODEs and Lindbladians, we construct an efficient quantum algorithm for solving ODEs by applying the state-of-the-art Lindbladian simulation quantum algorithms, with two different input models for the coefficient matrix $V(t)$, namely the access to the original matrix $V(t)$ or to its square root information. The algorithm, especially under the second input model, can outperform all existing quantum algorithms and achieve near-optimal dependence on all parameters.

Consider putting a system in an environment that is large enough such that the Markovian approximation is valid, the dynamics of the system can be modeled by the Lindbladian

$$\frac{d\rho}{dt} = \mathrm{L}[\rho] = -i\left[H(t),\rho\right] + \sum\left(F_i(t)\rho F_i(t)^{\dagger} - \frac{1}{2}\left\{\rho, F_i(t)^{\dagger}F_i(t)\right\}\right), \qquad (22)$$

where $\rho = \sum_{ij}\rho_{ij}|i\rangle\langle j|$ is the density matrix of the system, $H(t)$ is the internal Hamiltonian, and $\{F_i(t)\}$ are *quantum jump* operators. By treating ρ as $\vec{u}(t)$ in ODE, the Lindbladian naturally corresponds to an ODE with non-normal $V(t)$. While so, the problem is that the Lindbladian has to be a completely positive trace-preserving (CPTP) map and cannot be used to program general ODE problems.

Similar to the idea of block encoding where a matrix M of interest is encoded into the upper-right block of a unitary operator, non-diagonal density matrix encoding (NDME) aims to encode the matrix M into a non-diagonal block of a density matrix to jump out of the restrictions of Hermiticity and positive semi-definiteness:

Definition 4 (NDME)). Given an (l + n)-qubit density matrix ρ_M and an n-qubit matrix M, if ρ_M satisfies $\left(\langle s_1|_l \otimes I_n\right)\rho_M\left(|s_2\rangle_l \otimes I_n\right) = \gamma M$, where $|s_1\rangle_l$ and $|s_2\rangle_l$ are two different computational basis states of the l-qubit ancilla system and $\gamma \geq 0$, then ρ_M is called an (l + n, $|s_1\rangle$, $|s_2\rangle$, γ)-NDME of M.

We will focus on (1 + n, $|0\rangle$, $|1\rangle$, γ) - NDME where ρ_M has the form

$$\rho_M = \begin{pmatrix} 0 & \gamma M \\ \gamma M^{\dagger} & 0 \end{pmatrix}.$$

Since ρ_M is Hermitian, it is also a (1 + n, $|1\rangle$, $|0\rangle$, γ) - NDME of $M^{\dagger}$.

We now show how to combine Lindbladians and NDME to encode general linear ODEs.

Starting from a (1 + n)-qubit initial state $\rho_0 = |+\rangle\langle+| \otimes |\mu_0\rangle\langle\mu_0|$ which is a (1 + n, $|0\rangle$, $|1\rangle$, $\frac{1}{2}$) - NDME of $|\mu_0\rangle\langle\mu_0|$, we consider a Lindbladian with $H(t) = \begin{pmatrix} H_1(t) & 0 \\ 0 & \alpha I_n \end{pmatrix}$ and $F_i(t) = \begin{pmatrix} G_i(t) & 0 \\ 0 & \beta_i I_n \end{pmatrix}$.

Focusing on the upper-right block of ρ_0, $\mathrm{L}[\rho_0]$ described as

$$\frac{1}{2}|\mu_0\rangle\langle\mu_0| \to \frac{1}{2}\left(-i\left(H_1(t)-\alpha\right) - \left(\frac{1}{2}\sum_i G_i(t)^{\dagger}G_i(t) - \sum_i \beta_i^{*}G_i(t) + \frac{1}{2}\sum_i|\beta_i|^2\right)\right)|\mu_0\rangle\langle\mu_0|.$$

Here, since the α term can be absorbed into $H_1(t)$ and $\frac{1}{2}\sum_i G_i(t)^{\dagger}G_i(t)$ is positive semi-definite, for semi-dissipative ODEs (the Hermitian part of $V(t)$ is positive semi-definite), we can simply set $\alpha = \beta_i = 0$ such that on the left vector of this upper-right block, we realize the homogeneous linear ODE as

$$\frac{d\vec{\mu}(t)}{dt} = -V(t)\vec{\mu}(t) = \left(-iH_1(t) - \frac{1}{2}\sum_i G_i(t)^{\dagger}G_i(t)\right)\vec{\mu}(t), \text{ with } \vec{\mu}(0) = |\mu_0\rangle.$$

This equation shows the interesting (but expected) connection between the anti-Hermitian (oscillating) part of $V(t)$ and the internal Hamiltonian of the Lindbladian, the connection between the Hermitian (dissipative) part of $V(t)$ and the environment induced jump operators of the Lindbladian. The non-Hermitian coefficient matrix appeared in this equation, sometimes, is also known as the effective non-Hermitian Hamiltonian for approximately describing the short-time dynamics of the Lindbladian. Evolving the Lindbladian for a time T, we will have

$$\rho_T = \frac{1}{2}\begin{pmatrix} 0 & \eta_T |\mu_0\rangle\langle\mu_T| \\ \eta_T |\mu_0\rangle\langle\mu_T| & 0 \end{pmatrix},$$

where $|\mu_T\rangle = \vec{\mu}(T)/\eta_T$ is the normalized solution with $\eta_T = \|\vec{\mu}(T)\|$.

A high-level picture of these procedures is shown in Fig. 12.

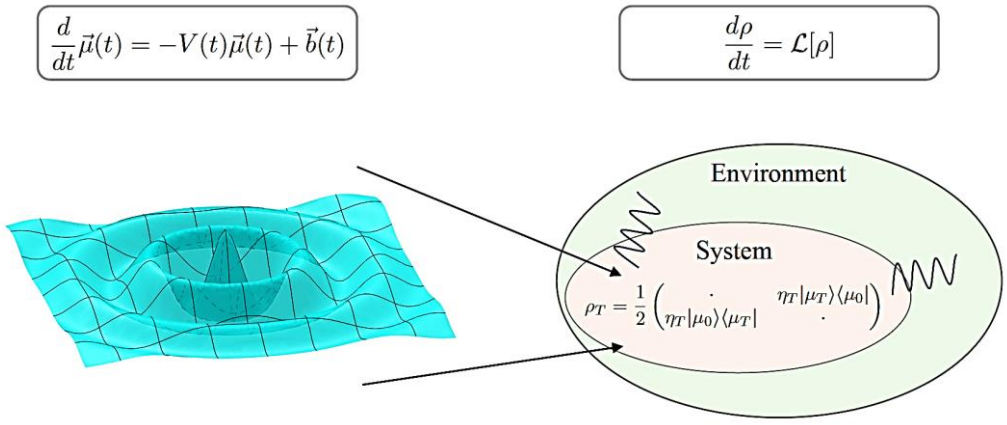


Fig. 12. High-level illustration of the algorithm [26].
[The dynamics of a linear ODE is embedded into the intrinsic non-unitary dynamics of a Lindbladian and the solution to the ODE is encoded into a non-diagonal block of the density matrix evolved according to the Lindbladian]

8. Quantum algorithms for open system simulation

The basic idea is to use high-order series expansion following the spirit of Duhamel's principle where the Lindbladian separated into two parts: the *jumping* part and the *drifting* part. The truncated expansion is then realized on quantum computers with the aid of linear combinations of unitaries (LCU) and oblivious amplitude amplification for isometry. A new quantum algorithm for linear ODEs is developed by combining the natural non-unitary dynamics of Lindbladians and a new technique called the non-diagonal density matrix encoding, the solution to a differential equation can be encoded into a non-diagonal block of a density matrix. With the aid of advanced Lindbladian simulation algorithms and the assumption of a plausible input model, we achieve near-optimal dependence on all parameters and outperform all existing methods.

8.1. Path integral control of open quantum systems

Let us now consider the state preparation problem. We want to prepare a quantum state from a given initial state in total time T, but want to do so by considering the interaction of the system with its environment. For this, we assume the system dynamics follows the Lindblad equation (21). One can formulate this as a finite horizon control problem where the Hamiltonian in (21) takes the form $H = H_0 + u_a H_a$ with H_a ($a = 1, \ldots, n_c$) a set of Hermitian operators and $u_a(a = 1, \ldots, n_c)$ real-valued control fields. Given the time interval $[0, T]$, we define the control objective as

$$C[u] = -\frac{Q}{2}\mathrm{F}\left(\rho_T\right) + \frac{1}{2}\int_0^T u_t^T R u_t dt \qquad (23)$$

where ρ_T represents the quantum state at the final time T, Q is a positive constant and R is a real symmetric positive $m \times m$ matrix. The objective is composed of two parts. The first term is the fidelity $\mathrm{F}\left(\rho_T\right) = \mathrm{Tr}\left(\rho_T \phi\phi^\dagger\right)$ of the final state ρ_T with respect to a target (pure) state ϕ. The second term is an energy constraint and it penalizes the accumulated magnitude of the different controls. We want to find the optimal control u^* that minimizes the objective function $u^* = \arg\min_u C[u]$.

Eqs. (21) and (23) define a deterministic control problem and the optimal control solutions u_a are state-independent functions. This is referred to as open-loop control and it can be approached by using for example the PMP method. Here instead, we propose to consider the stochastic optimal control problem based on the unravelings of the Lindblad equation. For this, consider the following cost functional $C = \left\langle -\frac{Q}{2}\mathrm{F}\left(\psi_T\right) + \frac{1}{2}\int_0^T u_t^T R u_t dt \right\rangle$ where ψ_t is the quantum state satisfying the SSE (22) and $F(\psi) = \mathrm{Tr}(\psi\psi^\dagger\phi\phi^\dagger)$. When the controls depend on the state, the problem is referred to as closed-loop/feedback control. These control problems can be solved using the PI control formalism when the Lindblad operators C_a can be transformed into anti-Hermitian operators $-iH_a$, while maintaining a real symmetric covariance matrix. When the transformation is possible, the unraveling is linear and norm-preserving and the SSE and SME take the form

$$\begin{aligned} d\psi &= -iH_0\psi dt - \frac{1}{2}\tilde{D}_{ab}H_aH_b\psi dt - iH_a\psi\left(u_a dt + d\tilde{W}_a\right), \quad \left\langle d\tilde{W}_a d\tilde{W}_b\right\rangle = \tilde{D}_{ab}dt \\ dP &= -i\left[H_0, P\right]dt + \mathrm{D}\left[\tilde{D}, H\right](P)dt - i\left(u_a dt + d\tilde{W}_a\right)\left[H_a, P\right]dt \end{aligned} \tag{24}$$

In addition, the transformation should leave the cost C invariant. The first term is invariant because $\left\langle \mathrm{Tr}\left(\psi_T\psi_T^\dagger Q\right)\right\rangle = \mathrm{Tr}\left(\rho_T Q\right)$ and ρ_T is invariant. The second term is generally not invariant, except when u is open loop, as there is no state dependence in that case. However, for feedback control, the optimal control formulation varies depending on the specific unraveling employed.

Example: Control of a noisy qubit. Consider a single-qubit system evolving according to the Lindblad equation (I.21) with $H = u_x H_x + u_y H_y$, where $H_x = \sigma_x$ and $H_y = \sigma_y$. The dissipation part is given by the two non-Hermitian operators $C_1 = \sigma^+$ and $C_2 = \sigma^-$, where $\sigma^\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$. This system is commonly used for modeling the emission and absorption of light quanta in a two-level system coupled to an electromagnetic field, e.g. a cavity resonator. Assume a diagonal noise matrix $D_{ab} = D\delta_{ab}$. The Lindblad equation is

$$\dot{\rho} = -i\left[H, \rho\right] + D\left(\sigma^+\rho\sigma^- + \sigma^-\rho\sigma^+ - \rho\right).$$

To propose an unraveling suitable for PI formulation, we transform the dissipators to a pair of anti-Hermitian operators. The unraveling becomes:

$$d\psi = -\tilde{D}\psi dt - i\sigma_a\psi\left(u_a dt + dW_a\right), \quad \tilde{D}_{ab} = \frac{1}{2}D\delta_{ab}, \quad a = x, y.$$

This unraveling preserves the norm of ψ. This implies that the stochastic trajectories generated by $d\psi$ lie on the Bloch sphere. We consider the state preparation problem from an initial state

$$\psi_0 = |X\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \text{ to a target state } \phi = |Y\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right).$$

Although the transformation $X \to Y$ can be realized by a simple σ_z rotation. This task is challenging, since σ_z is not one of the control primitives in H. Instead, σ_x, σ_y must coordinate so as to realize the desired rotation. As a result, the optimal trajectories do not lie on the equator.

In Fig. 13 (A) we show the adaptive importance sampling. In Fig. 13 (B) Optimal control solution $u_{x,y}(t)$ after convergence of the algorithm. In Fig. 13 (C) we show how the quality of the optimal control solution in

terms of asymptotic *ESS* depends on the number of pulses *K*. The *ESS* increases monotonically until reaching an asymptote at around $ESS \sim 0.21$, showing the sub-optimality of the open-loop control compared to the optimal feedback solution (for which $ESS = 1$).

Figure I13 (D) shows quantum trajectories on the Bloch sphere under optimal control.

Remark. We plot the average fidelity over trajectories F_{avg}, the worst-case fidelity over trajectories $F_{\min}$ and the average control cost *C* versus IS steps. In addition, we plot the effective sample size *ESS*, which is a sensitive measure of the quality of the optimal control solution. The *ESS* indicates how close the control solution is to the optimal (feedback) control, for which $ESS = 1$. We observe that while the fidelity and control cost converge fast to constant values, the ESS still increases indicating that the quality of the control solution is still improving (shaded region). We observe that the control solution becomes smoother in these later IS iterations. The asymptotic average fidelity for $K = 128$ is $F^* = 0.9759 \pm 0.0006$.

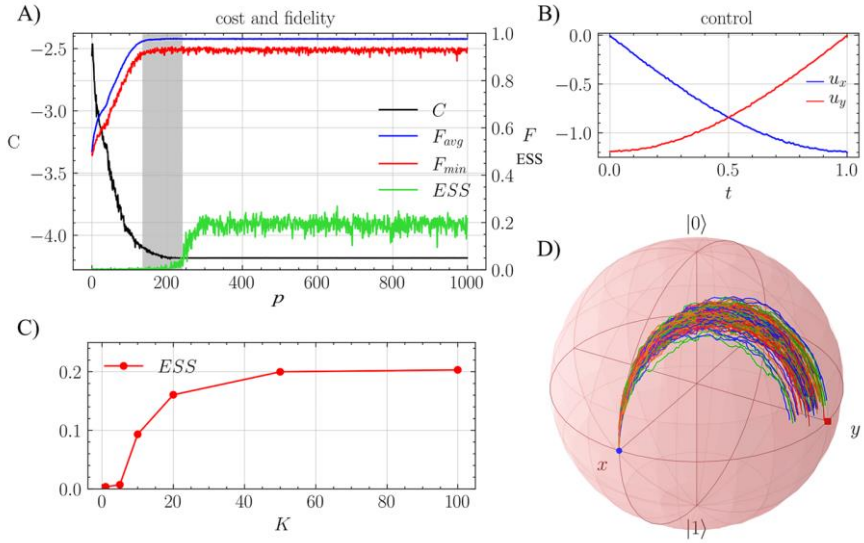


Fig. 13. Control of a noise qubit from $X \rightarrow Y$ [27]
[(A) Average fidelity F_{avg}, minimal fidelity F_{min}, effective sample size ESS and cost C versus importance sampling iterations p. The converged average fidelity is $F^* = 0.9759 \pm 0.0006$. (B) Optimal control solution $u_{x,y}(t)$ after convergence of the algorithm. The optimal solution is two-fold degenerate. The two solutions are related by a global sign $u_{x,y} \rightarrow -u_{x,y}$. (C). Dependence of the quality of the optimal control, measured by the ESS, on the number of pulses K. (D). Optimally controlled trajectories on the Bloch sphere. Parameters: horizon time $T = 1$, noise coupling $D = 0.005$, control weight $R = 1$, fidelity weight $Q = 10$, number of pulses $K = 128$, number of trajectories $n_{traj} = 400$ per IS step, maximum number of importance sampling (IS) steps $n_{IS} = 1000$ and time discretization $dt = T/N$ with $N = 128$. IS smoothing window $w = 40$]

The feedback controller requires information about the quantum state through measurement. Since the quantum state is only partially observable through measurement, the control problem becomes what is known as a partial observable control problem. A unique quantum feature, not present in classical systems, is that measurement will *disrupt the quantum state by projecting the state* onto one of the measurement eigenstates (quantum back-action). A compromise between information gain and minimal disruption of the quantum state is given by the so-called weak or continuous measurement. Weak measurement can be elegantly formalized by the so-called hybrid dynamics, which describes the simultaneous time evolution of the quantum state and the classical observation(s). The issue of partial observability and measurement is not so important for LQG control problems, because of a property called certainty equivalence, which essentially states that the optimal control depends on the expected latent state only. However, partial observability and the correct treatment of measurement becomes important for stochastic optimal control problems beyond the LQG regime.

8.2. Optimal feedback control of a continuously monitored spin

The spin interacts weakly with an optical mode (laser) along the *z*-axis. The cavity is used to control the strength of that interaction. Then, a continuous measurement is performed on the laser using a technique known as homodyne detection. This provides an indirect continuous measurement of the *z*-component of the spin

angular momentum in such a way that the state of the system does not collapse to an eigenstate of S_z (a so-called non-demolition measurement). A magnetic field in the *y*-direction is applied for control purposes.

Figure 14 is a schematic representation of an experimental set-up for continuous measurement and control of a spin. The dynamics of the continuously monitored spin system is described by a quantum stochastic differential equation (QSDE).

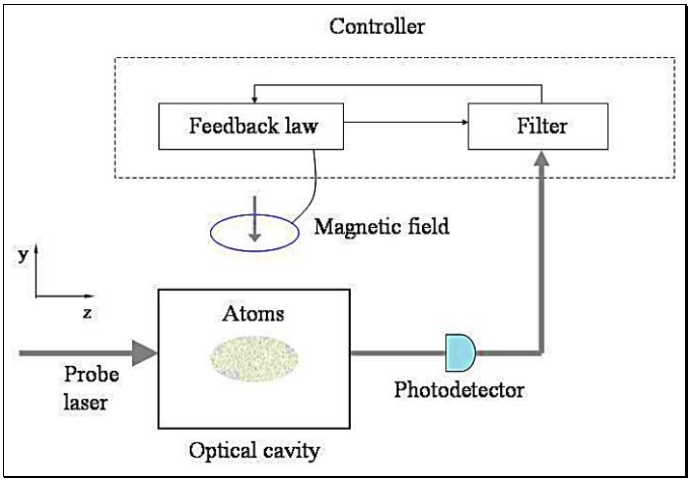


Fig. 14. Schematic of an experiment for continuous measurement and control of a spin [28]. [The spin interacts with a probe laser, which is measured continuously using photodetectors. A magnetic field is used for feedback]

The proper mathematical framework for QSDEs is the non-commutative analog of the Ito stochastic calculus that was developed by Hudson and Parthasarathy. There is also a corresponding observation process for a field observable of the laser probe. At this point, we should recall that it is impossible to measure all components of the state because they are non-commuting observables. Hence, any measurement can provide only partial information about the state of the system [29].

The situation is analogous with that of classical partially observed stochastic systems. As in the classical case, one can derive a quantum filtering equation which is the equivalent of the Kushner-Stratonovich equation in classical nonlinear filtering theory. The quantum filtering equation is a classical Ito SDE for the conditional expectation of the density matrix $\hat{\rho}_t$ (conditioned on the measurement record up to time *t*). The important property of the filtering equation is that the expectation value of any system observable at time *t* is the same whether it is computed from the corresponding QSDE or from $\hat{\rho}_t$, even with feedback control that depends on the measurement record. This is a great simplification, since it allows us to circumvent the dynamical QSDE and use the filtering equation (or Belavkin equation) for control design. Moreover, an output feedback control problem has been converted into a state feedback control problem for the conditional expectation of the state $\hat{\rho}_t$.

The starting point of the analysis will be the spin filtering equation. It has the following form:

$$d\hat{\rho}_t = \left(iu(t)\left[S_y, \hat{\rho}_t\right] + M\left(S_z\hat{\rho}_t S_z - \frac{1}{2}\left(S_z^2\hat{\rho}_t + \hat{\rho}_t S_z^2\right)\right)\right)dt + \sqrt{\eta M}\left(S_z\hat{\rho}_t + \hat{\rho}_t S_z - 2\mathrm{Tr}\left(S_z\hat{\rho}_t\right)\hat{\rho}_t\right)dW_t$$

where the innovations process W_t is a Wiener process that describes the difference between the measured value of S_z at time *t* and its expected value.

The measurement strength *M* is determined by the properties of the cavity and the probe laser and effectively determines the time-scale of the measurement process. The parameter $\eta \in [0, 1]$ is the detection efficiency of the photodetectors and $u(t)$ is the amplitude of the magnetic field applied in the *y*-direction. By defining $\tau = Mt$, $V_\tau = \sqrt{M}W_t$ (so that $\left(dV_\tau\right)^2 = M\left(dW_t\right)^2 = Mdt = d\tau$) and $\tilde{u} = \frac{1}{M}u$, we can set $M = 1$, which we do from now on.

For the case of a spin-1/2 system, we use the Bloch vector representation of ρ_t introduced in Chapter 1,

$$\hat{\rho}_t = \frac{1}{2}\left(I_2 + x_t\sigma_x + y_t\sigma_y + z_t\sigma_z\right) = \frac{1}{2}\begin{pmatrix} 1+z_t & x_t - iy_t \\ x_t + iy_t & 1-z_t \end{pmatrix}$$

in terms of which, the spin filtering equation becomes the following system of SDEs:

$$dx_t = -\left(u(t)z_t + \frac{1}{2}x_t\right)dt - \sqrt{\eta}x_t z_t dW_t,\ dy_t = -\frac{1}{2}y_t dt - \sqrt{\eta}y_t z_t dW_t,\ dz_t = u(t)x_t dt + \sqrt{\eta}\left(1-z_t^2\right)dW_t$$

We seek to design optimal feedback strategies for this objective. Certainly, one may design feedback laws for the filter dynamics based on some objective but they will not necessarily be optimal for the system. What is needed is an appropriate Separation Principle, that is, a statement that under appropriate conditions the optimal feedback control designed based on the filter dynamics remains optimal for the system (with the same objective). Then, the optimal feedback is a separated strategy. The associated state space will now be the disk $0 \le x^2 + z^2 \le 1$.

To the analysis let us use polar coordinates (r, θ) for the state space defined by $x = r\sin\theta$ and $z = r\cos\theta$. It is a simple application of Ito 's rule to obtain the following SDEs for them:

$$\begin{aligned} dr_t &= \frac{1}{2}\left(\frac{\eta}{r_t} - r_t\right)\sin^2\theta_t dt + \sqrt{\eta}\left(1-r_t^2\right)\cos\theta_t dW_t, \\ d\theta_t &= \left[-u(t) + \left(\frac{\eta}{r_t^2} - \eta - \frac{1}{2}\right)\sin\theta_t\cos\theta_t\right]dt - \sqrt{\eta}\frac{\sin\theta_t}{r}dW \end{aligned} \tag{25}$$

Let us pose now the following optimization problem: Suppose that at time t the state of the system is (r, θ). Let $u(s)$, $s \in [t, T]$ (T is the time at which the experiment terminates) be a square integrable function. We define the following expected cost-to-go

$$J\left(t, r, \theta, u(s)\right) = \mathrm{E}_{(r,\theta)}\left[\int_0^T\left(\frac{1}{2}u^2(s) + U\left(r_s, \theta_s\right)\right)ds\right],$$

where the expectation value is taken with respect to every possible sample path that starts at (r, θ) at time t. We seek the control law u that minimizes J. The expected cost-to-go of the optimal law is called the value function: $V(t, r, \theta) = \min_{u(s)} J\left(t, r, \theta, u(s)\right)$.

Bellman's principle of optimality and dynamic programming lead to the following Bellman equation for the value function: $\min_u\left\{\frac{u^2}{2} + U + \frac{\partial V}{\partial t} + \mathrm{L}V\right\} = 0$.

The stochastic generator L of the SDE system acts on V as follows:

$$\begin{aligned} \mathrm{L}(V) = \frac{1}{2}\left(\frac{\eta}{r} - r\right)\sin^2\theta\frac{\partial V}{\partial r} + \left[-u + \left(\frac{\eta}{r^2} - \eta - \frac{1}{2}\right)\sin\theta\cos\theta\right]\frac{\partial V}{\partial\theta} + \frac{1}{2}\eta\left(1-r^2\right)^2\cos^2\theta\frac{\partial^2 V}{\partial r^2} \\ + \frac{1}{2}\eta\frac{\sin^2\theta}{r^2}\frac{\partial^2 V}{\partial\theta^2} - \eta\left(\frac{1}{r} - r\right)\sin\theta\cos\theta\frac{\partial^2 V}{\partial r\partial\theta} \end{aligned}.$$

For the case of *perfect* detector efficiency ($\eta = 1$), it is possible provide such a boundary condition and hence obtain a solution to the problem.

Letting the initial value of r equal to 1 ($r_0 = 1$)

$$dr_t = \frac{1}{2}\left(\frac{\eta}{r_t} - r_t\right)\sin^2\theta_t dt + \sqrt{\eta}\left(1 - r_t^2\right)\cos\theta_t dW_t,$$

we see that $dr_0 = 0$ and hence $r_t = 1$, $\forall\ t \geq 0$. Hence, $r = 1$ is a forward invariant set of the stochastic dynamics. Physically, this means that if the detection is perfect, a pure state of the system will remain pure for all time. Let us rewrite dynamics on the invariant set $r = 1$:

$$d\theta_t = -\left(u(t) + \frac{1}{2}\sin\theta_t\cos\theta_t\right)dt - \sin\theta_t dW_t.$$

This stochastic system is the reduction of the full system whose state space is the disk $0 \leq r \leq 1$, on the boundary $r = 1$ which is a forward invariant set of the full dynamics.

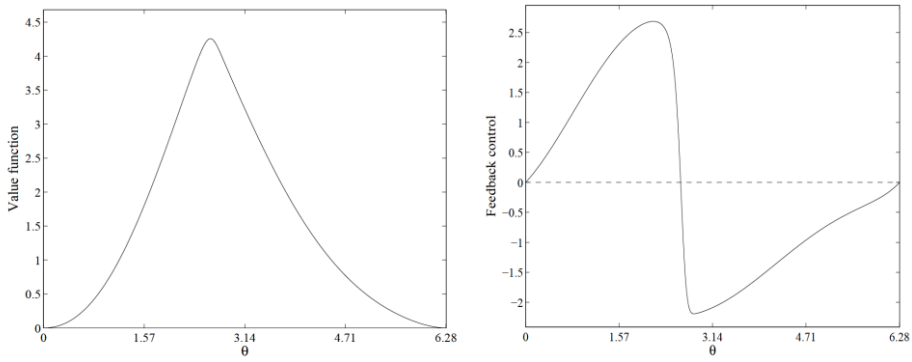
Figures 15 (a,b) represent the value function and the optimal feedback for the infinite-horizon problem on the boundary of the state space.

Figures 16 (a,b) represent the value function and the optimal feedback on the whole disk.

The asymmetry between the left and right side of the disk is obvious in all figures.

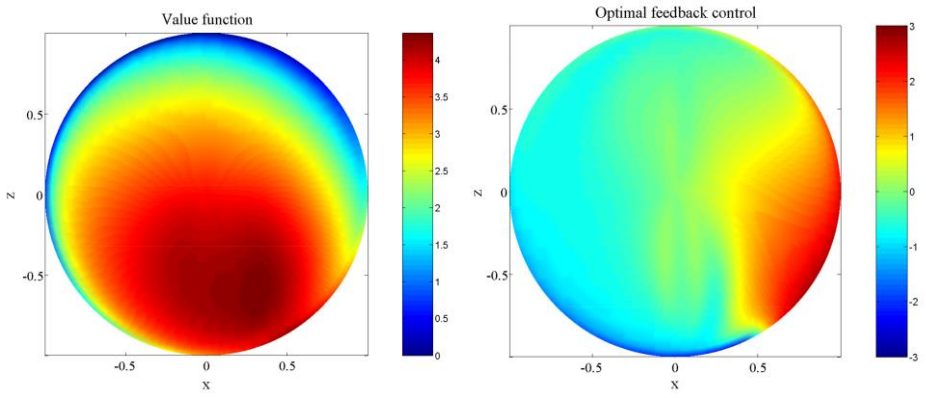
To elucidate the action of the control on the system, we portray, in Fig. 17(a), the vector field $(-u(x, z)z, u(x, z)x)$.

This vector field is the part of the dynamics that depends on the control. The fact that there are lines on which this field vanishes should not be alarming: The action of the rest of the dynamics, the deterministic dissipative part and the stochastic part, "throws" the system off these points. Finally, Fig. 17(b) demonstrates some typical trajectories of the closed-loop system.



(a) (b)

Fig. 15. (a) Steady-state value function V on the boundary; (b) Optimal feedback on the boundary



(a) (b)

Fig. 16. (a) Steady-state value function V on the disk; (b) Optimal feedback on the disk

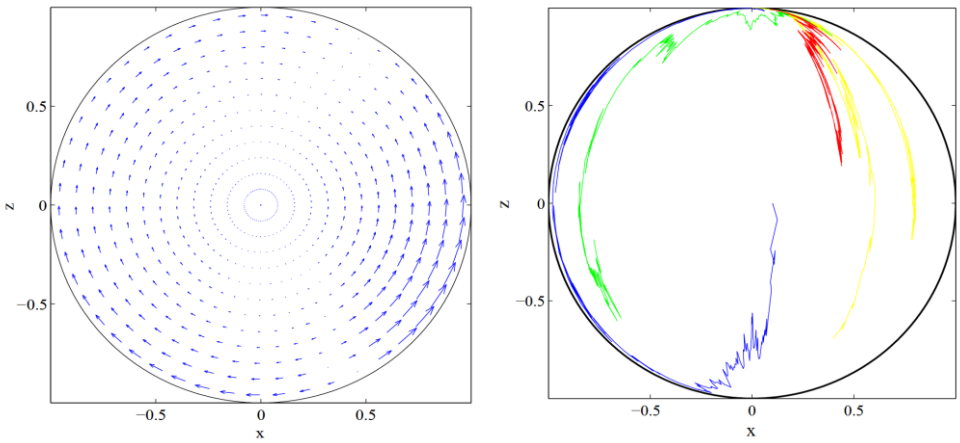


Fig. 17. (a) Vector field generated by the feedback control; (b) Typical trajectories of the closed-loop system

Thus, it is possible to construct corresponding “averaged” systems and optimal transfer problems that capture the long time-scale dynamics and in which the contribution of the short time-scale natural dynamics is averaged out. These reduced problems off er great conceptual and computational simplifications to the solution of the original ones. For example, the solution to an optimal feedback stabilization problem for an eigenstate of a continuously monitored spin-1/2 system in the case of perfect detection.

Practical examples of quantum optimal control in [30] are described.

Conclusions

The results obtained in the field of quantum computer science clearly demonstrate the high technological potential of quantum technologies.

A cryptanalytically significant quantum computer can threaten the functioning of various systems. The article [1] formulates the main provisions of the Concept of ensuring the sustainability of national digital platforms and blockchain ecosystems in the context of a new quantum security threat. When developing this concept, the results obtained in the works of well-known Russian scientists on quantum information technologies, as well as the results obtained in the works of the authors of this article and other members of the Technologies for Countering Previously Unknown Quantum Cyber Threats group from the Scientific Center for Information Technology and Artificial Intelligence of the Sirius University of Science and Technology, were summarized, systematized and comprehensively rethought.

The lack of teaching staff and objective assessments of the necessity of industry and science for quantum engineering personnel only increased the difficulties in the development of quantum engineering. In this article, we have reviewed only the basics necessary for a deeper study of quantum computing, quantum information technology, quantum strong artificial intelligence and quantum resilience of information systems.

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