Phase space methods in open quantum systems

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Abstract

In this work we extend the phase space approach of quantum mechanics to open quantum systems. Using the formalism of generalized coherent states and the time-dependent variational principle, phase space Langevin equations are derived for harmonic oscillator and spin systems. It is proved that the former is fully consistent with the quantum master equation. The latter, however, is an approximation that is accurate for large spin numbers or low temperatures.

Keywords: Quantum mechanics, phase space methods, coherent states, open quantum systems

Tiivistelmä

Tutkielmassani sovellan kvanttimekaniikan vaiheavaruusmenetelmiä avoimien kvanttisysteemien ongelmaan. Johdan nk. Langevin-yhtälöt vaiheavaruudessa harmoniselle värähtelijälle sekä spin-systeemeille hyödyntäen yleistettyjä koherentteja tiloja ja aikariippuvaa variaatioperiaatetta. Osoitan tämän menetelmän vastaavan täysin kvanttimekaanista master-yhtälöä harmonisen oskillaattorin tapauksessa. Spin-systeemeille saadaan approksimaatio, joka lähestyy tunnettuja tuloksia matalilla lämpötiloilla ja suurilla spin-luvuilla.

Avainsanat: Kvanttimekaniikka, vaiheavaruusmenetelmät, koherentit tilat, avoimet kvanttisysteemit

Contents

1 Introduction

The phase space approach to quantum mechanics is almost as old as quantum mechanics itself. In this formulation, the classical concept of phase space where a single point can describe the dynamical state of a system is taken as the foundation of quantum theory. However, the general description of a quantum state in phase space requires the introduction of *distribution functions* instead of single points as in classical mechanics. The phase space approach can be seen as an alternative and consistent formulation of quantum mechanics that discards the concepts of operators and Hilbert spaces. The history of this approach essentially begins in 1927 when Weyl published an article that related symmetrically-ordered operators to phase space functions. He believed at the time that this would be a quantization scheme of special importance: it would extend classical mechanics to the broader quantum theory. However, this quantization scheme was in fact only a change of representation from Hilbert space to phase space and it failed in the case of angular momentum [1].

Later in 1932 Wigner introduced his eponymous distribution function of position and momentum which links the quantum mechanical wavefunction in the Schrödinger equation to a probability-like distribution. Together with Weyl's publication these laid the foundations for a full phase space theory formalised by Moyal and Groenenwald around 1946. Notable physicists at the time, especially Dirac, objected that any distribution function is inherently incompatible with uncertainty principle. This misunderstanding arises from a misplaced interpretation of the uncertainty principle which states that one cannot determine simultaneously for instance the exact position and momentum of a particle. Thus, one could think, one cannot ascribe a probability-like weigth to positions and momentums at all. A similar argument was made against Feynman's path integral theory since a single path would be in contradiction with the uncertainty principle. These arguments follow from a misinterpretation of the theory: there are no physical paths in path integral theory nor does a distribution function necessarily imply that there is a certain probability to observe a given position and momentum of a particle. Indeed, both theories fulfill the uncertainty principle. For a historical and mathematical introduction, on which this overview is based, see [1].

The phase space formulation of quantum mechanics has been largely overshadowed by the canonical Hilbert space approach and path integral the-

ory. However, it has slowly been resurging since 1960's after Glauber introduced the field coherent states to describe optical coherence [2, 3]. These states form a basis that is more suitable than the so-called number state basis for the description of many optical fields and they are in a sense classical states of quantum harmonic oscillator. In the latter context these states were considered by Schrödinger already in 1926 [4]. The concept of coherent states was generalized independently by Gilmore and Perelomov around 1972 [5–7], extending the applicability of phase space theory to other systems than light as well. This group-theoretical and dynamical generalization made it possible to apply the theory of coherent states to a wide array of topics, for example [8]: quantum optics, nuclear physics, chemistry and statistical physics. An important and recent area of application is also quantum information with continuous variables [9].

The topic of this thesis is the application of phase space theory to open quantum systems. These systems have gathered a great deal of attention in the last 50 years. The term *open quantum system* refers to a quantum system that interacts with its environment. This interaction leads to dissipation, fluctuations and decoherence, the latter being a purely quantum mechanical property. The first two, dissipation and fluctations, arise also in the context of classical mechanics and thermodynamics. The last one, decoherence, means that the phase information which is essential to describe quantum superpositions is destroyed. Thus it explains why the underlying quantum nature of objects cannot usually be seen on a macroscopic level: it is lost in the interaction with the environment [10]. All these effects are captured by, for instance, the so-called quantum master equation (QME) and quantum Langevin equation (QLE) (also known as input-output formalism).

There are many methods that are not mentioned in this thesis but quite an extensive overview can be found in Ref. [11]. Some are mostly relevant in the historical sense, such as the approaches that alter either the commutation relations or the Schrödinger equation. The currently relevant approaches mainly start from the consideration of dynamics of the system and the environment. This includes both the QME and QLE. But for instance, path integral methods in real or imaginary time and non-equilibrium Green function methods are outside the scope of this thesis.

Open quantum systems are generally quite difficult to simulate numerically, and there is no algorithm that can simulate a general time-dependent open quantum system [11]. The theoretical tools discussed in this thesis,

the QME and QLE, are not straightforwardly transformed into a numerical method. For instance, the QME is a matrix differential equation for the quantum state's density matrix. In the case of a bosonic system this density matrix would be infinite-dimensional. Therefore the evaluation of the full quantum state itself is impossible. One can then either restrict the state space by some physical argument or try to find a closed set of equations for relevant observables. A more involved approach is to derive a Monte Carlo method that corresponds to the QME [12]. Using concepts of phase space theory, QMEs can be mapped to Fokker–Planck equations for distribution functions[1]. These can be then mapped to stochastic differential equations [13, 14] such as

$$\dot{\alpha}(t) = A(\alpha, t) + B(\alpha, t)\eta(t)$$

where η is a stochastic process. That is, η obtains values that obey a probability distribution. See e.g. [12, 15] for such a procedure. In general, it is possible to solve these equations in an efficient manner. This is the strength of phase space theory.

In this thesis, we try to use the concepts of phase space theory in a slightly different way. Starting from physical principles we derive phase space Langevin equations which are in connection with the aforementioned quantum Langevin equation. The naming convention follows from the work of Paul Langevin who introduced stochastic differential equations in 1908. He reframed the problem of Brownian motion, famously solved earlier in 1905 by Einstein, in terms of Newtonian mechanics and a fluctuating force. Nearly 40 years later, in 1952, a mathematical formalisation in terms of stochastic integrals was published by Itô. This mathematical ground is essential to this thesis as well as much of the literature that uses these mathematical tools. [13, 14]

The motivation to approach open quantum systems with the phase space theory comes from possibilities that a new approach can offer. There are many problems that could use this theoretical framework. For instance, it has been observed that squeezed light can be used to enhance cooling in optomechanical systems [16]. In general, this is connected to the concept of *reservoir engineering*. By controlling quantum systems coupling to the environment one could achieve e.g. to initialise a qubit for quantum computation or amplify signals efficiently [17].

[1]The Fokker–Planck equation is a certain kind of a partial differential equation that describes the time evolution of a probability distribution function.

The focus in the thesis is on two well-known classes of systems: harmonic oscillators and spin systems which interact with a thermal environment. These could correspond to, for instance, an electromagnetic field inside a cavity or non-interacting molecules in a liquid solution, respectively. From a theoretical standpoint these systems provide the necessary steps to more complicated physical systems.

This thesis is organized as follows: In Section 2 we introduce the theoretical background of this thesis. It is divided so that in Sections 2.1–2.3 we introduce the relevant building blocks of the phase space theory of quantum mechanics. Section 2.4 contains a brief overview to open quantum systems as well as the derivation of the QME in Section 2.4.1 and the QLE in Section 2.4.2. These concepts are then combined in a novel manner in Section 3 in which we focus on two examples, electromagnetic fields in Section 3.1 and linear spin systems in Section 3.2 in a thermal environment. Finally in Section 4, conclusions are drawn and the outlook discussed.

2 Theoretical background

In this section we review some theoretical concepts in quantum mechanics that are relevant for the thesis. First, we shortly discuss the operators and states related to harmonic oscillators and spin systems. Then, we go through the essential building blocks of phase space theory. These include the generalized coherent states, time-dependent variational principle and phase space distributions. As a convention throughout the thesis, we set $\hbar = 1$.

A suitable starting point is the quantization of the harmonic oscillator that can be found in any introductory text of quantum mechanics. The same concepts are found by quantising an electromagnetic (EM) field, see e.g. Ref. [12]. This leads to the introduction of the annihilation operator $\hat{a}$ and creation operator $\hat{a}^\dagger$ that obey the commutation relation

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1. \tag{2.1}$$

The dynamics of a quantum mechanical system is generated by its Hamiltonian. In the case of a harmonic oscillator (or a single-mode EM field) the Hamiltonian reads

$$\hat{H} = \omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \tag{2.2}$$

where ω is the eigenfrequency. The eigenstates of this Hamiltonian are the eigenstates of the operator $\hat{n} = \hat{a}^\dagger\hat{a}$ which is called the number operator. This means that there is a set of states $|n\rangle$ such that $\hat{n}\,|n\rangle = n\,|n\rangle$. These states are often called number or Fock states. By using the commutation relations (2.1) one can see that n can be considered as the number of excitations (e.g. photons) and that $\hat{a}$ ($\hat{a}^\dagger$) indeed annihilates (creates) one excitation

$$\hat{n}(\hat{a}\,|n\rangle) = \hat{a}^\dagger\hat{a}\hat{a}\,|n\rangle = \Big(\hat{a}\hat{a}^\dagger - 1\Big)\hat{a}\,|n\rangle = (n-1)\hat{a}\,|n\rangle\,.$$

Thus, it can be deduced that $\hat{a}\,|n\rangle = c_n\,|n-1\rangle$ with some constant c_n. Supposing that the states are normalised to unity, i.e. $\langle n|n\rangle = 1$, the constant can be found by evaluating the inner product

$$|c_n|^2 = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n \geq 0.$$

Thus, we can choose $c_n = \sqrt{n}$. A similar calculation can be made for the creation operator $\hat{a}^\dagger$. Gathering these results together we have

$$\begin{aligned} \hat{a}^\dagger |n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ \hat{a}\,|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned} \tag{2.3}$$

Note that when $n = 0$ the operation of the annihilation operator gives $\hat{a}\,|0\rangle = 0$. From a physical standpoint the state $|0\rangle$ corresponds to the lowest energy state.

Another important problem in quantum mechanics is that of spin and angular momentum. It is naturally related to physical particles (fermions and bosons) and atoms in a magnetic field, for instance. The relevant operators for this problem are spin (or total angular momentum) operators $\hat{J}_z, \hat{J}_x, \hat{J}_y$ for which the commutation relations are

$$\left[\hat{J}_z, \hat{J}_\pm\right] = \pm\hat{J}_\pm \quad \text{and} \quad \left[\hat{J}_+, \hat{J}_-\right] = 2\hat{J}_z \tag{2.4}$$

where $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$. These operators operate on spin states which are chosen to be the eigenstates of $\hat{J}_z$ and $\left|\hat{\vec{J}}\right|^2 = \hat{J}_4 = \hat{J}_z^2 + \hat{J}_x^2 + \hat{J}_y^2$ so that

$$\hat{J}_z\,|j,m\rangle = m\,|j,m\rangle\,, \qquad \hat{J}_\pm\,|j,m\rangle = \sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm 1\rangle\,.$$

Also, $\hat{J}_4\,|j,m\rangle = j(j+1)\,|j,m\rangle$. The quantum numbers can obtain values $j \in \{0, \frac{1}{2}, 1, \frac{3}{2}\dots\}$ and $m \in \{j, j-1, \dots, -j\}$. In this thesis, we call j simply *the spin number*.

The case $j = \frac{1}{2}$ corresponds to so-called *qubits* which play a crucial role in quantum computation [18]. As a physical realisation one can think of the spin state of an electron. Similarly to a bit in classical information theory, one can refer a spin-down state $\left|-\frac{1}{2}\right\rangle$ as 0 and spin-up state $\left|\frac{1}{2}\right\rangle$ as 1. Contrary to bits, qubits can also be in a superposition state $\alpha\left|-\frac{1}{2}\right\rangle + \beta\left|\frac{1}{2}\right\rangle$ where $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$. The probability to find the electron in spin-down (spin-up) state in this case is then $|\alpha|^2$ ($|\beta|^2$). Much of the power of quantum information lies in the clever usage of the superposition principle.

Larger spin numbers come up, for instance, when considering spin states of some atoms which naturally have $j > \frac{1}{2}$. They are also relevant when

working with an ensemble of systems with smaller spin numbers, e.g. a pair of qubits. Then, one can consider their collective behaviour such as the total spin value in the z-direction. If we introduce summed operators, e.g. $\hat{J}_z = \hat{J}_{z,1} + \hat{J}_{z,2}$ where subscripts 1 and 2 label the electrons, these follow the same commutation relations (2.4). Naively, one would think that all the eigenstates now have $j = 1$ but this is not the case. The eigenstates and their J_z and J_4 eigenvalues are (denoting $\left|\frac{1}{2}\right\rangle_1 \left|-\frac{1}{2}\right\rangle_2 = |+,-\rangle$)

Eigenstate	$\hat{J}_z$	$\hat{J}_4$
$\|+,+\rangle$	1	1
$\|-,-\rangle$	-1	1
$\frac{1}{\sqrt{2}}(\|+,-\rangle + \|-,+\rangle)$	0	1
$\frac{1}{\sqrt{2}}(\|+,-\rangle - \|-,+\rangle)$	0	0

There are three $j = 1$ states and one $j = 0$ state. This offers the possibility of considering the different j-subspaces when interested in the collective behaviour of spin systems.

2.1 Generalized coherent states

The phase space theory that is used in this thesis is formulated by using generalized coherent states. First, the concept of coherent states is introduced with field coherent states, and then the generalization is discussed in detail.

2.1.1 Field coherent states

The physical context of field coherent states is related to the quantum mechanical characterization of coherence in electromagnetic fields [2]. Even though the number states are the eigenstates of the free EM field's Hamiltonian (2.2), they are not very suitable for discussing other aspects of EM fields. For instance, the quantized electric field operator for a single mode can be written as $\hat{\vec{E}} = \vec{u}\hat{a}^\dagger + \vec{u}^*\hat{a}$ where $\vec{u} = i\sqrt{\frac{\omega}{2\epsilon_0 V}}\sum_\lambda \vec{\epsilon}^\lambda e^{i\vec{k}\vec{r}-i\omega t}$ is the position ($\vec{r}$) and time (t) dependent mode function [12]. Here, $\vec{k}$ is the wave

vector, $\vec{\epsilon}^{\lambda}$ the two unit polarization vectors that are perpendicular to $\vec{k}$, ϵ_0 the vacuum permittivity, and V is the volume in which the field is quantized. Therefore, $\langle n|\hat{\vec{E}}|n\rangle = 0$ for any n. A more suitable set of states are the field coherent states $|\alpha\rangle$ with $\alpha \in \mathbb{C}$ which can be defined in three distinct but equivalent ways [3]:

(i) as an eigenstate of the annihilation operator

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,, \tag{2.5}$$

(ii) as a state that can be obtained by applying a displacement operator $\hat{D}$ to the vacuum state

$$|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle = \exp\left(\alpha\hat{a}^{\dagger} - \alpha^{*}\hat{a}\right)|0\rangle\,, \tag{2.6}$$

and

(iii) as a minimum uncertainty state which saturates the lower limit of a Heisenberg uncertainty relation

$$\sigma_{\hat{q}}^2\sigma_{\hat{p}}^2 = \left|\frac{1}{2}\,\langle[\hat{q},\hat{p}]\rangle\right|^2 = \frac{1}{4} \tag{2.7}$$

where $\hat{q} = \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{a}^{\dagger}\right)$ and $\hat{p} = \frac{i}{\sqrt{2}}(\hat{a}^{\dagger} - \hat{a})$ are the so-called quadrature operators[2] that correspond to position and momentum operator, respectively. In this expression $\sigma_{\hat{A}}^2 = \left\langle (A - \langle A\rangle)^2 \right\rangle = \langle \hat{A}^2\rangle - \langle \hat{A}\rangle^2$ is the variance of an operator $\hat{A}$. For field coherent states $\sigma_{\hat{q}}^2 = \sigma_{\hat{p}}^2 = \frac{1}{2}$.

It is straightforward to prove that the definition (iii) follows from the definition (i)

$$\begin{aligned}\sigma_{\hat{q}}^2 &= \frac{1}{2}\left[\,\langle\alpha|\left(\hat{a} + \hat{a}^{\dagger}\right)^2|\alpha\rangle - \left(\,\langle\alpha|\left(\hat{a} + \hat{a}^{\dagger}\right)|\alpha\rangle\right)^2\right] \\ &= \frac{1}{2}\left[\,\langle\alpha|\left(\hat{a}^2 + \left(\hat{a}^{\dagger}\right)^2 + 2\hat{a}^{\dagger}\hat{a} + 1\right)|\alpha\rangle - (\alpha + \alpha^{*})^2\right] = \frac{1}{2}\end{aligned}$$

and similarly for $\sigma_{\hat{p}}^2$. Conversely, assuming the definition (iii) we can obtain the definition (i). The uncertainty relation in its general form follows from

[2]The factor $\frac{1}{\sqrt{2}}$ is chosen so that the quadrature operators obey $[\hat{q},\hat{p}] = i$. One can find alternative definitions from the literature, e.g. in Ref. [12].

the Cauchy–Schwartz inequality which reads in terms of operators $\hat{P} = \hat{p} - \langle \hat{p} \rangle$ and $\hat{Q} = \hat{q} - \langle \hat{q} \rangle$ [19]

$$\langle \psi | \hat{Q}^2 | \psi \rangle \ \langle \psi | \hat{P}^2 | \psi \rangle \geq \left| \langle \psi | \hat{Q}\hat{P} | \psi \rangle \right|^2 .$$

The Heisenberg uncertainty principle follows by writing the operator $\hat{Q}\hat{P}$ as a sum of commutator and anticommutator between $\hat{Q}$ and $\hat{P}$ and then noting that the anticommutator term gives only a positive contribution to the right-hand side. However, if we suppose that the lower bound is satisfied then necessarily the state $|\psi\rangle$ must be such that $\hat{Q}\,|\psi\rangle = \mu \hat{P}\,|\psi\rangle$ where $\mu \in \mathbb{C}$ is a constant [19]. This equation can be rearranged to an eigenvalue equation

$$(\hat{q} - \mu \hat{p})\,|\psi\rangle = (\langle \hat{q} \rangle - \mu \langle \hat{p} \rangle)\,|\psi\rangle \equiv \lambda\,|\psi\rangle\,. \tag{2.8}$$

The constant μ can be found by using the commutator relation $\left[\hat{Q}, \hat{P}\right] = [\hat{q}, \hat{p}] = i$

$$\sigma_{\hat{q}}^2 = \langle \psi | \hat{Q}^2 | \psi \rangle = \langle \psi | \mu \hat{Q}\hat{P} | \psi \rangle = \mu \langle \psi | \left(\left[\hat{Q}, \hat{P}\right] + \hat{P}\hat{Q} \right) | \psi \rangle = i\mu + \mu^2 \sigma_{\hat{p}}^2 .$$

If now $\sigma_{\hat{q}}^2 = \sigma_{\hat{p}}^2 = \frac{1}{2}$ we find that $\mu = -i$ and $\hat{q} - \mu\hat{p} = \sqrt{2}\hat{a}$. Thus Eq. (2.8) can be rearranged to exactly match the definition (i). Note that the value of μ can be found even if $\sigma_{\hat{q}}/\sigma_{\hat{p}} \neq 1$. These solutions correspond to the squeezed states.

One can obtain either from the definition (i) or (ii) the expression of a coherent state in the number state basis [3]. Let us focus on the definition (ii). Using the operator theorem [12]

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]} \quad \text{if} \quad \left[\left[\hat{A}, \hat{B}\right], \hat{A}\right] = \left[\left[\hat{A}, \hat{B}\right], \hat{B}\right] = 0 \tag{2.9}$$

we can decompose the displacement operator $\hat{D}(\alpha)$ when $\hat{A} = \alpha \hat{a}^\dagger$ and $\hat{B} = -\alpha^* \hat{a}$. Thus we find using the properties of the bosonic operators (2.3) that

$$|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle = e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* a}\,|0\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\,.$$

It is straightforward to show that this is equivalent with the definition (i). Consequently, the field coherent states are not orthogonal

$$\langle \beta | \alpha \rangle = e^{-\frac{1}{2}\left(|\alpha|^2 + |\beta|^2\right)} \sum_n \frac{(\alpha\beta^*)^n}{n!} = e^{-\frac{1}{2}\left(|\alpha|^2 + |\beta|^2\right) + \alpha\beta^*} .$$

Using the operator theorem (2.9) we can derive how the displacement operator acts on the field coherent states [12]

$$\hat{D}(\beta)\,|\alpha\rangle = \hat{D}(\beta)\hat{D}(\alpha)\,|0\rangle = e^{i\,\mathrm{Im}\{\alpha^*\beta\}}\hat{D}(\alpha+\beta)\,|0\rangle = e^{i\,\mathrm{Im}\{\alpha^*\beta\}}\,|\alpha+\beta\rangle\,.$$

Thus, the operation of the displacement operator $\hat{D}(\beta)$ to the state $|\alpha\rangle$ displaces the state in the complex plane from α to $\alpha+\beta$.

The field coherent states are a complete set. They are in fact *overcomplete* since the label of coherent states α is continuous and uncountable but the underlying number state basis is countable [7]. This means that the completeness relation is not unique. One useful expression of the completeness relation (and thus the identity operator $\hat{I}$) is [3]

$$\hat{I} = \sum_n |n\rangle\langle n| = \frac{1}{\pi}\int \mathrm{d}^2\alpha\,|\alpha\rangle\langle\alpha|\,.$$

The integration measure is defined as $\mathrm{d}^2\alpha = \mathrm{d}\,\mathrm{Re}\,\alpha\,\mathrm{d}\,\mathrm{Im}\,\alpha$ and the integration is over the whole plane.

The field coherent states were considered by Schrödinger in the very early days of quantum mechanics [4], albeit in the language of wave functions in position representation. He noted that these states are 'classical states' of a quantum harmonic oscillator which is described by a Hamiltonian $\hat{H} = \omega\hat{a}^\dagger\hat{a}$. If the initial state is a coherent state $|\alpha\rangle$, the state at a later time is given by the Schrödinger equation

$$e^{-i\hat{H}t}\,|\alpha\rangle = e^{-i\omega\hat{a}^\dagger\hat{a}t}\,|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_n \frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}\,|n\rangle = \left|\alpha e^{-i\omega t}\right\rangle. \qquad (2.10)$$

The state remains as a coherent state during time evolution. The physical picture Schrödinger was after is now clear: this quantum state follows a classical trajectory with $\langle\hat{q}\rangle = q_0\cos\omega t$ and $\langle\hat{p}\rangle = p_0\sin\omega t$ when $\alpha(t=0)$ is a real number. Furthermore, its wave packet is as localized as possible compatibly with the Heisenberg uncertainty relation (2.7). This does not change over time.

After the introduction of field coherent states one could ask if this idea can be applied to other systems with a different operator algebra such as spins. The definitions (i) and (iii) are unsuitable for a generalization: an eigenvalue equation for the lowering operator as Eq. (2.5) does not produce anything sensible if the Hilbert space is of finite dimension. On

the other hand, the minimum uncertainty states can be chosen in many different ways so the definition is not unique. A more detailed discussion of these problems can be found in Ref. [7].

On the other hand, definition (ii) can be formulated in a group-theoretical manner which can be generalized. With definition (ii) the time evolution (2.10) of a field coherent state with $\hat{H} = \omega\hat{n}$ can be rewritten as

$$e^{-i\hat{H}t}\hat{D}(\alpha)\,|0\rangle = \hat{D}(\alpha e^{-i\omega t})\,|0\rangle\,. \tag{2.11}$$

The operators of this equation are reminiscent of the group property closure[3] which states that the product of two group elements must also be an element of the same group.

At first glance, it is not easy to see what the group that contains both the time evolution and displacement operator is. This problem can be avoided by using the mathematical relationship between Lie groups and algebras [20]. In a quantum mechanical context, a Lie algebra can be defined as a vector space so that the commutator of two elements of the algebra is also an element. One can therefore only consider the commutators relevant to the Hamiltonian $\hat{H}$ instead of more complicated group elements. The relationship between Lie groups and algebras can be intuitively understood considering the Baker–Campbell–Hausdorff (BCH) formula

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\frac{1}{12}([\hat{A},[\hat{A},\hat{B}]]+[\hat{B},[\hat{A},\hat{B}]])+\ldots} \equiv e^{\hat{C}(\hat{A},\hat{B})}. \tag{2.12}$$

The series denoted by $\hat{C}(\hat{A},\hat{B})$ is infinite but depends only on the commutators of $\hat{A}$ and $\hat{B}$. Therefore, if $\hat{A}$ and $\hat{B}$ belong in the same algebra $\mathfrak{g}$ then also $\hat{C}(\hat{A},\hat{B})$ belongs in that algebra $\mathfrak{g}$. The corresponding group G can be defined to include all exponential maps of algebra's elements, that is

$$G = \left\{ e^{\hat{X}} \mid \hat{X} \in \mathfrak{g} \right\}. \tag{2.13}$$

It is now straightforward to find the group underlying Eq. (2.11). The operators in the exponentials are the Hamiltonian, essentially the number operator $\hat{n}$, and the expression $\alpha\hat{a}^\dagger - \alpha^*\hat{a}$ that defines the displacement operator. Since $[\hat{n},\hat{a}] = -\hat{a}$ and $\left[\hat{n},\hat{a}^\dagger\right] = \hat{a}^\dagger$ with $\left[\hat{a},\hat{a}^\dagger\right] = 1$, we note that the set $\left\{\hat{n},\hat{a}^\dagger,\hat{a},\hat{I}\right\}$ generates a Lie algebra whose general element is

[3]The other group axioms are associativity and the existence of the identity and the inverse element.

$z_1 + z_2\hat{a} + z_3\hat{a}^\dagger + z_4\hat{n}$ with $z_i \in \mathbb{C}$. This is the Weyl–Heisenberg algebra $\mathfrak{h}_4$ from which the corresponding group H_4 can be obtained through Eq. (2.13). Note that the Hamiltonian $\hat{H}$ was used to find the Weyl–Heisenberg algebra, so $\hat{H} \in \mathfrak{h}_4$. Consequently $\mathfrak{h}_4$ is called *the dynamical algebra of* $\hat{H}$.

Knowing that the Lie group H_4 corresponding to $\mathfrak{h}_4$ contains both the time evolution and displacement operator we can find the coherent state by reversing this process. Let us now take a general unitary group element[4] of H_4 and apply it to the ground state $|0\rangle$

$$e^{ix\hat{n}+ig\hat{I}+z\hat{a}-z^*\hat{a}^\dagger}|0\rangle = e^{\alpha\hat{a}^\dagger-\alpha^*\hat{a}}e^{iy\hat{n}+ig\hat{I}}|0\rangle = e^{ig}|\alpha\rangle\,. \tag{2.14}$$

Here, $x, g \in \mathbb{R}$ and $z \in \mathbb{C}$ are arbitrary and y, α are functions of these constants. The phase factor e^{ig} can be ignored as it is not an observable. The decomposition can be proved by using the properties of the displacement operator (2.6). Since the relations between the coefficients multiplying the operators are not of interest here, it can be schematically understood as an application of the BCH-formula (2.12) with $\hat{A} = \alpha\hat{a} - \alpha^*\hat{a}^\dagger$ and $\hat{B} = iy\hat{n}$. The right hand side of the BCH-formula can be formally written as $e^{ix\hat{n}+z\hat{a}-z^*\hat{a}^\dagger}$. This is the first equality in Eq. (2.14).

2.1.2 General definition of coherent states

Nearly ten years after Glauber's articles [2, 3] on field coherent states a group-theoretical generalization was developed independently by Gilmore [5] and Perelomov [6]. We will discuss Gilmore's algorithm but the differences to Perelomov's algorithm are minor [7].

All the elements of a general method for finding coherent states are present in Eq. (2.14). There are three important parts:

- the dynamical Lie algebra of $\hat{H}$ — denoted here by $\mathfrak{g}$ — and its corresponding Lie group G which determines the relevant unitary operator $\hat{g}$;
- a reference state $|\Omega\rangle$ on which the operator $\hat{g}$ acts;

[4] Unitarity of a group element is necessary to maintain the normalisation of the state. That is, for a unitary operator $\hat{U}$ we have $\langle\psi|\psi\rangle = \langle\Omega|\hat{U}^\dagger\hat{U}|\Omega\rangle = \langle\Omega|\Omega\rangle = 1$ assuming $|\Omega\rangle$ is normalized.

- the decomposition of the operator $\hat{g}$ so that physically irrelevant phase factors can be extracted and discarded.

The dynamical Lie algebra $\mathfrak{g}$ is the algebra spanned by the terms of Hamiltonian $\hat{H}$ so that $\hat{H} \in \mathfrak{g}$. This means that when $\hat{H} = \sum_i \lambda_i \hat{T}_i$ where $\hat{T}_i$ are operators and λ_i constants, the algebra is $\left\{\hat{T}_1, \hat{T}_2, \dots\right\}$. It must be closed by definition, i.e. $\left[\hat{T}_i, \hat{T}_j\right] = \sum_k f_{ijk} \hat{T}_k$. This can be always achieved by considering operators for which $\lambda_j = 0$. Such a trick was done in the case of harmonic oscillator as $\left\{\hat{a}^\dagger \hat{a}, I\right\}$ is a closed algebra by itself. The Lie group G is obtained from $\mathfrak{g}$ using Eq. (2.13), i.e. by exponentiating the algebra. Unitarity must be taken into account to preserve the normalisation of quantum states.

The choice for the reference state is, in principle, not unique. One could have chosen some $|n\rangle$ in Eq. (2.14) which would have lead to coherent states $\hat{D}(\alpha)|n\rangle$. However, choosing the vacuum state $|0\rangle$ clearly produces a more useful set of coherent states than any other state $|n\rangle$. The reference state can be fixed by demanding that it is the ground state of the unperturbed Hamiltonian. For instance, for an EM field this would be the ground state $|0\rangle$ of the Hamiltonian (2.2) and the perturbation could be of the form $\hat{H}_p = \lambda(\hat{a} + \hat{a}^\dagger)$. Similarly one can treat the interactions between two different modes as perturbations. We refer to the ground state as the *extremal state* of the system since there are no lower energy states [7].

In the last step a decomposition is needed so that every unitary $\hat{g} \in G$ can be written as $\hat{g} = \hat{D}\hat{h}$ and $\hat{h}|\Omega\rangle = e^{i\phi(\hat{h})}|\Omega\rangle$ where $\phi(\hat{h}) \in \mathbb{R}$ and $|\Omega\rangle$ is the reference state. The elements $\hat{h}$ which have this property form the maximum stability subgroup $H_0 \subset G$. The group G/H_0 in which $\hat{D}$ belongs is called the coset or quotient. The idea is to simply remove the total phase of the state which does not play any physical role. Indeed, since

$$\hat{g}|\Omega\rangle = \hat{D}\hat{h}|\Omega\rangle = e^{i\phi}\hat{D}|\Omega\rangle,$$

the generalized coherent states can be defined as $\hat{D}|\Omega\rangle$.

2.1.3 SU(2) coherent states

As an application of the general algorithm, we define the SU(2) (or atomic) coherent states. These are the coherent states related to the spin operators

$\hat{J}_z$ and $\hat{J}_\pm$. They are named after the SU(2) group because the commutation relations of spin operators (2.4) correspond exactly to the $\mathfrak{su}(2)$ algebra.

The most general Hamiltonian for such a system is $\hat{H} = \epsilon\hat{J}_z + g\hat{J}_+ - g^*\hat{J}_-$. A suitable reference state is $|j, -j\rangle$. Next, we note that a general element of the maximum stability subgroup H_0 is $e^{ix\hat{J}_z}$, $x \in \mathbb{R}$. The only missing part is now the decomposition of the general SU(2) group element $\exp\left(iy\hat{J}_z + z\hat{J}_+ - z^*\hat{J}_-\right)$, $y \in \mathbb{R}$.

By using the BCH-formula (2.12) one can show that

$$e^{iy\hat{J}_z + z\hat{J}_+ - z^*\hat{J}_-} = e^{\zeta\hat{J}_+ - \zeta^*\hat{J}_-}e^{ix\hat{J}_z}. \tag{2.15}$$

The most straightforward proof is provided by the so-called *faithful matrix representation* method [7]. Instead of evaluating the infinite series of commutators one can take this equation as an ansatz and evaluate both sides with a matrix representation of the spin operators. This is allowed by the fact that the BCH-formula (2.12) depends only on the commutation relations. Since these relations do not depend on j, it is possible to use a Pauli-like representation for the spin operators

$$S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{2.16}$$

and calculate all the exponential terms explicitly. These are related to the Pauli matrices by $2S_k = \sigma_k$ where $k = x, y, z$ and $S_\pm = \sigma_\pm$. It can be shown by using the properties of the Pauli matrices that the left hand side of Eq. (2.15) reads in this representation

$$e^{iyS_z + zS_+ - z^*S_-} = \begin{pmatrix} \cos r + iy\frac{\sin r}{2r} & z\frac{\sin r}{r} \\ -z^*\frac{\sin r}{r} & \cos r - iy\frac{\sin r}{2r} \end{pmatrix}$$

where $r = \sqrt{|z|^2 + y^2/4}$. The right hand side can be calculated similarly

$$e^{\zeta S_+ - \zeta^* S_-}e^{ixS_z} = \begin{pmatrix} e^{i\frac{x}{2}}\cos|\zeta| & \frac{\zeta e^{-i\frac{x}{2}}}{|\zeta|}\sin|\zeta| \\ -\frac{\zeta^* e^{i\frac{x}{2}}}{|\zeta|}\sin|\zeta| & e^{-i\frac{x}{2}}\cos|\zeta| \end{pmatrix}.$$

Now a comparison between these two matrices gives two complex equations which can be solved to give ζ and x in terms of z and y. The result is given by

$$|\zeta| = \arcsin\left(|z|\frac{\sin r}{r}\right),\ x = 2\arg\left(\cos r + iy\frac{\sin r}{2r}\right) \text{ and } v = \arg(z) + \frac{x}{2}$$

where $\arg(z)$ is the argument or phase of z. However, the exact relationship between the parameters is not as important as the fact that the decomposition exists.

In this manner the SU(2) coherent states are obtained

$$|j;\xi\rangle = e^{\zeta\hat{J}_+ - \zeta^*\hat{J}_-}\,|j,-j\rangle = \frac{e^{\xi\hat{J}_+}}{\Delta^j}\,|j,-j\rangle = \Delta^{-j}\sum_{m=-j}^{j} C_{j,m}\xi^{m+j}\,|j,m\rangle \quad (2.17)$$

where $C_{j,m} = \sqrt{\frac{(2j)!}{(j-m)!(j+m)!}} = \sqrt{\binom{2j}{j+m}}$ and $\Delta = 1+|\xi|^2$. The second equality is obtained by finding a decomposition

$$e^{\zeta\hat{J}_+ - \zeta^*\hat{J}_-} = e^{\xi\hat{J}_+}e^{\ln\left(1+|\xi|^2\right)\hat{J}_z}e^{-\xi^*\hat{J}_-}$$

where $\xi = \frac{\zeta}{|\zeta|}\tan|\zeta|$ with the faithful matrix representation method. The calculation of the decomposition can be found in Ref. [7]. Generally, ξ is used instead of ζ which appears in the displacement operator since it is calculationally easier to use.

The expectation values of $\hat{J}_z$ and $\hat{J}_\pm$ over the SU(2) coherent states can be now evaluated. The calculation is straightforward with the last form of the SU(2) coherent state given in the equation (2.17). One also needs the orthogonality of spin states $\langle j,m|j,m'\rangle = \delta_{m,m'}$. As an example we calculate the expectation value of $\hat{J}_z$

$$\begin{aligned}
\langle\hat{J}_z\rangle &= \langle j;\xi|\hat{J}_z|j;\xi\rangle = \sum_{m,n=-j}^{j}\Delta^{-2j}C_{j,n}C_{j,m}(\xi^*)^{j+n}\xi^{j+m}\,\langle j,n|\hat{J}_z|j,m\rangle \\
&= \Delta^{-2j}\sum_{m=-j}^{j}(C_{j,m})^2(|\xi|^2)^{m+j}(m+j-j) \\
&= -j+\Delta^{-2j}\sum_{m=-j}^{j}(C_{j,m})^2|\xi|^2\partial_{|\xi|^2}\left(\left(|\xi|^2\right)^{m+j}\right) \\
&= -j+\frac{|\xi|^2}{\Delta^{2j}}\partial_{|\xi|^2}\left(\Delta^{2j}\right) = j\frac{|\xi|^2-1}{|\xi|^2+1}.
\end{aligned}$$

In the second row we add a zero to use the relation $kx^k = x\partial_x x^k$. After that we use twice the binomial theorem that ensures the normalisation of the

SU(2) coherent state

$$\Delta^{2j} = \left(1 + |\xi|^2\right)^{2j} = \sum_{s=0}^{2j} \binom{2j}{s} (|\xi|^2)^s = \sum_{m=-j}^{j} (C_{j,m})^2 (|\xi|^2)^{m+j}.$$

The expectation value of $\hat{J}_\pm$ can be calculated similarly. The expectation values are

$$\langle \hat{J}_z \rangle = j \frac{|\xi|^2 - 1}{|\xi|^2 + 1} \quad \text{and} \quad \langle \hat{J}_- \rangle = \langle \hat{J}_+ \rangle^* = \frac{2j\xi}{|\xi|^2 + 1}. \tag{2.18}$$

Lastly we note that

$$\langle \hat{J}_z \rangle^2 + \langle \hat{J}_x \rangle^2 + \langle \hat{J}_y \rangle^2 = \langle \hat{J}_z \rangle^2 + \left| \langle \hat{J}_+ \rangle \right|^2 = j^2$$

which shows the semiclassical nature of these states. Also, it shows that the geometry of SU(2) is that of a sphere, and can be considered as a generalization of the Bloch sphere used for $j = \frac{1}{2}$ states [18].

2.1.4 Jordan–Schwinger map

Generalized coherent states can be approached from another direction for algebras that operate on finite-dimensional Hilbert spaces. In fact, they can be represented by field coherent states. This result is provided by the Jordan–Schwinger mapping. While, to the best of my knowledge, this aspect has not been previously discussed in the literature, the same algebra has been used in Ref. [21]. The interest to this topic arose from Ref. [22] where the idea is implicitly used but not in terms of generalized coherent states.

Following the general algorithm, suppose that operators $\hat{T}_i$ form an algebra and that there are (finite-dimensional) square matrices M_i that obey the same algebra, i.e. they constitute a representation of such algebra. That is, if $\left[\hat{T}_i, \hat{T}_j\right] = \sum_k f_{ijk} \hat{T}_k$ we suppose that the matrices $\left[M_i, M_j\right] = \sum_k f_{ijk} M_k$ exist with the same constants f_{ijk}. In this case one can utilize the Jordan–Schwinger map and replace

$$\hat{T}_i \longrightarrow \sum_{\alpha,\beta} \hat{a}^\dagger_\alpha M_i^{\alpha\beta} \hat{a}_\beta, \tag{2.19}$$

where $\hat{a}_\alpha$ are bosonic operators obeying the standard commutation relations $\left[\hat{a}_\alpha, \hat{a}_\beta^\dagger\right] = \delta_{\alpha\beta}$. This representation is valid because M_i obeys the same commutation relations as $\hat{T}_i$.

All bilinear operators $\hat{a}_i^\dagger \hat{a}_j$ preserve the total number of bosons N and they form an algebra, known as $\mathfrak{su}(r)$ for r modes [7]. One could already derive the coherent states starting at this point but instead we consider an extended algebra that also includes all the linear operators $\hat{a}_i^\dagger$ and $\hat{a}_j$. Note that this extended algebra is indeed an algebra, i.e. the commutation relations are closed

$$\begin{aligned}
&\left[\hat{a}_i^\dagger \hat{a}_j, \hat{a}_k^\dagger \hat{a}_l\right] = \delta_{jk} \hat{a}_i^\dagger \hat{a}_l - \delta_{il} \hat{a}_k^\dagger \hat{a}_j, \\
&\left[\hat{a}_i^\dagger \hat{a}_j, \hat{a}_k^\dagger\right] = \delta_{jk} \hat{a}_i^\dagger, \quad \text{and} \quad \left[\hat{a}_i^\dagger \hat{a}_j, \hat{a}_k\right] = -\delta_{ik} \hat{a}_j.
\end{aligned}$$

In terms of the general algorithm, this extension leads to the extremal state being the vacuum state $|0\rangle$ instead of the state $|N, 0, 0 \ldots\rangle$ which would be the ground state of a $\mathfrak{su}(r)$ Hamiltonian. Consequently, the maximum stability group for this extension is

$$H_0 = \left\{ \exp\left(i \sum_{j,k} y_{jk} \hat{a}_j^\dagger \hat{a}_k \right) \mid y_{jk} \in \mathbb{C}, y_{jk} = y_{kj}^* \right\}$$

whereas in the case of $\mathfrak{su}(r)$ the stability group would not contain terms $\hat{a}_j^\dagger \hat{a}_1$. The decomposition of a general group element can not be explicitly proved but by using a similar reasoning as with the field coherent states (2.14) and the BCH-formula (2.12) we have

$$e^{i \sum_{j,k} x_{jk} \hat{a}_j^\dagger \hat{a}_k + \sum_j \left(z_j \hat{a}_j^\dagger - z_j^* \hat{a}_j \right)} = e^{\sum_j \left(\alpha_j \hat{a}_j^\dagger - \alpha_j^* \hat{a}_j \right)} e^{i \sum_{j,k} y_{jk} \hat{a}_j^\dagger \hat{a}_k}.$$

Since all the different bosonic modes commute, the generalized displacement operator is just a product of displacement operators of different modes. Thus, the generalized coherent state is

$$|\alpha_1, \alpha_2 \ldots\rangle = \prod_i \hat{D}(\alpha_i) |0\rangle, \quad \text{with} \quad \hat{D}(\alpha_k) = e^{\alpha_k \hat{a}_k^\dagger - \alpha_k^* \hat{a}_k}. \tag{2.20}$$

Because the total boson number N related to the Jordan–Schwinger map (2.19) is conserved it must also be required that

$$\sum_i |\alpha_i|^2 = N. \tag{2.21}$$

The boson number N should then be related to a conserved quantity in the system.

The simplest example of Jordan–Schwinger map is the $\mathfrak{su}(2)$ algebra since the matrices M_i in Eq. (2.19) can be the spin matrices (2.16). Thus we have

$$\hat{J}_z \to \sum_{j=1}^{2}\sum_{k=1}^{2} \hat{a}_j^\dagger S_z^{jk} \hat{a}_k = \frac{1}{2}\left(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2\right),\ \hat{J}_+ \to \hat{a}_1^\dagger \hat{a}_2 \text{ and } \hat{J}_- \to \hat{a}_1 \hat{a}_2^\dagger. \quad (2.22)$$

Then, set $N = 2j$. By using Eqs. (2.20) and (2.21) we see that

$$\langle \hat{J}_z \rangle = \frac{1}{2}\left(|\alpha_1|^2 - |\alpha_2|^2\right) = \frac{N}{2}\frac{|\alpha_1|^2 - |\alpha_2|^2}{|\alpha_1|^2 + |\alpha_2|^2} \equiv j\frac{|\xi|^2 - 1}{|\xi|^2 + 1}$$

with $\xi \equiv \alpha_1/\alpha_2$ and similarly for $\hat{J}_\pm$. These results coincide with the expectation values over the SU(2) coherent state given in Eq. (2.18). Thus, the SU(2) coherent states can be replaced by field coherent states. This approach is useful when the Hilbert space size grows and the algebras become more complicated, e.g. in the case of SU(3).

Note that this method is different than simply taking the SU(2) coherent states and transforming them to a bosonic representation. For example, by using the representation (2.22) the SU(2) coherent state (2.17) would read $|\xi\rangle = \left(1 + |\xi|^2\right)^{-\frac{N}{2}} e^{\xi \hat{a}_1^\dagger \hat{a}_2} |0, 2N\rangle$.

2.2 Time-dependent variational principle

The time-dependent variational principle (TDVP) is a method that allows to find the exact quantum mechanical equations of motion in phase space. It can be regarded as a quantum mechanical equivalent of the Hamilton's principle in classical mechanics. The practical usefulness of the TDVP is that the equations of motion are simply (complex valued) differential equations which, for example, can be evaluated numerically. Also, there are many results from classical mechanics that can be used straightforwardly. First, we will derive the equations of motion generally. Then, we will discuss the important role of generalized coherent states in the TDVP.

2.2.1 Derivation

Let's consider a set of states $|\psi\rangle$ belonging to a Hilbert space $\mathcal{H}$, where ψ is an n-dimensional complex-valued parameter ($\psi \in \mathbb{C}^n$). Furthermore, we assume a time dependence for $\psi = \psi(t)$ and that $\langle\psi|\psi\rangle = 1$ for all times t. A similar proof with $\langle\psi|\psi\rangle \neq 1$ can be found in Ref. [23].

Let us consider a system that can be described by the Hamiltonian operator of the system $\hat{H}$. Now, define a Lagrangian function $\mathcal{L}$ and the action functional $\mathcal{S}$ by

$$\mathcal{S} = \int \mathcal{L}\,\mathrm{d}t = \int \mathrm{d}t\ \langle\psi(t)|\big(i\partial_t - \hat{H}\big)|\psi(t)\rangle\,. \tag{2.23}$$

Here, it is understood that the time derivative ∂_t operates always to the right. Note that the Lagrangian $\mathcal{L}$ is real-valued as long as $\hat{H}$ is hermitian. This can be proven by using the product rule of differentiation in the complex conjugate of $\mathcal{L}$

$$\begin{aligned}\mathcal{L}^* &= -i(\partial_t\,\langle\psi|)\,|\psi\rangle - \langle\psi|\hat{H}^\dagger|\psi\rangle \\ &= \partial_t(\langle\psi|\psi\rangle) + \langle\psi|\big(i\partial_t - \hat{H}\big)|\psi\rangle = \mathcal{L}\end{aligned}$$

since $\langle\psi|\psi\rangle = 1$.

Consider then an arbitrary variation of the action functional (2.23)

$$\delta\mathcal{S} = \int \delta\mathcal{L}\,\mathrm{d}t = \int \mathrm{d}t\,\left[\langle\delta\psi|\left(i\partial_t - \hat{H}\right)|\psi\rangle + \langle\psi|\left(i\partial_t - \hat{H}\right)|\delta\psi\rangle\right].$$

The variations $\langle\delta\psi|$ and $|\delta\psi\rangle$ can be considered independent. We can deduce that if $\delta\mathcal{S} = 0$ then both terms must vanish independently as the variations are arbitrary and independent. Thus, after integrating the latter term by parts we have

$$\big(i\partial_t - \hat{H}\big)\,|\psi\rangle = 0 \quad \text{and} \quad \langle\psi|\left(\overleftarrow{i\partial_t} + \hat{H}\right) = 0.$$

These are simply the Schrödinger equation and its adjoint. This proves that the quantum mechanical equations of motion are produced by the action (2.23). Also, it is well known from classical mechanics that the variational problem $\delta\mathcal{S} = 0$ is formally solved by the Euler–Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial\psi_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{\psi}_k} = 0. \tag{2.24}$$

2.2.2 Use of generalized coherent states

The formal proof of equivalence of the TDVP and the Schrödinger equation cannot be used to deduce what the state $|\psi\rangle$ that defines the Lagrangian $\mathcal{L}$ is. In fact, its existence was assumed in the beginning of the proof. For a practical application of TDVP the theory of generalized coherent states is needed. It provides the necessary parametric description of the Hilbert space and its group-theoretical foundation means that if the state is initially in a generalized coherent state of $\hat{H}$, it remains as such. Let us first outline this result. After that we discuss how TDVP can be used as an approximation if the generalized coherent states cannot be obtained.

Suppose that a system is in a state $|\psi_0\rangle$ and its dynamics is described by a Hamiltonian operator H that is time-independent, for simplicity. The formal solution of the Schrödinger equation can be now written as $|\psi_t\rangle = e^{-i\hat{H}t}|\psi_0\rangle$. If the initial state is in a generalized coherent state associated with the dynamical algebra of H it can be written as $|\psi_0\rangle = \hat{g}_0|\Omega\rangle$ where $\hat{g}_0$ is some element belonging to the dynamical Lie group and $|\Omega\rangle$ is a reference state. Now, the proof is simply an application of the group property: $\hat{g}_0$ and $e^{-i\hat{H}t}$ belong to the dynamical Lie group so their product $\hat{g}_t = e^{-i\hat{H}t}\hat{g}_0$ does too. Thus, the state at time t

$$|\psi_t\rangle = e^{-i\hat{H}t}|\psi_0\rangle = e^{-i\hat{H}t}\hat{g}_0|\Omega\rangle = \hat{g}_t|\Omega\rangle$$

is a generalized coherent state by definition. Therefore, only the parameters of the generalized coherent state evolve. The TDVP gives a formal method to find this time evolution. The proof follows similarly for a time-dependent Hamiltonian $\hat{H}_t$ as the time-ordered integral $T(e^{-\int i\hat{H}_t dt})$ appearing in the formal solution of the Schrödinger equation is an element of the dynamical Lie group.

It needs to be stressed that TDVP is exact only in the case that generalized coherent states are derived from the dynamical algebra of the system. If the algebraic structure of $\hat{H}$ is very complicated, this is practically impossible. As an approximative method one can choose a related algebra. For example, one could choose to analyze a spin Hamiltonian $\hat{H} = \epsilon\hat{J}_z + B\hat{J}_z^2$ by using SU(2) coherent states even though $\hat{J}_z^2 \notin \mathfrak{su}(2)$. This basically amounts to a mean-field approximation due to the structure of the coherent states. For instance,the expectation value of the nonlinear term $\hat{J}_z^2$ is

$$\left\langle \hat{J}_z^2 \right\rangle = \frac{j}{2} + \left(1 - \frac{1}{2j}\right)\langle \hat{J}_z \rangle^2 . \tag{2.25}$$

2.2.3 Example — spin precession

Let us now apply the formalism of generalized coherent states and the TDVP to a simple problem. Suppose a spin-j particle is in a magnetic field such that the Hamiltonian is given by $\hat{H} = \epsilon \hat{J}_z$. The algebra related to this physical system is $\mathfrak{su}(2)$. With this dynamical algebra we are able to solve the dynamics exactly by using SU(2) coherent states.

The first step is to calculate the Lagrangian $\mathcal{L} = \langle j;\xi|\left(i\partial_t - \hat{H}\right)|j;\xi\rangle$. Let's denote $K = \langle j;\xi|i\partial_t|j;\xi\rangle$ for brevity. It should be clear that only K depends on the derivatives of ξ. Thus, in the typical classical case K would correspond to a kinetic and $\langle \hat{H} \rangle$ to a potential term. With this notion we can write the Euler–Lagrange equation (2.24) as

$$0 = \frac{\partial \mathcal{L}}{\partial \xi^*} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{\xi}^*} = \frac{\partial K}{\partial \xi^*} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial K}{\partial \dot{\xi}^*}\right) - \frac{\partial \langle \hat{H} \rangle}{\partial \xi^*}. \tag{2.26}$$

Note that ξ and ξ^* can be treated as separate variables.

The term $\langle \hat{H} \rangle$ is given by Eq. (2.18). Its derivative is

$$\partial_{\xi^*} \langle \hat{H} \rangle = \partial_{\xi^*}\left[\epsilon j \frac{|\xi|^2 - 1}{|\xi|^2 + 1}\right] = 2j\epsilon \frac{\xi}{\left(1 + |\xi|^2\right)^2}. \tag{2.27}$$

The K-term can be calculated by using the second to last expression of the SU(2) coherent states in the Eq. (2.17)

$$K = \langle j,\xi|i\partial_t|j,\xi\rangle = i\langle j,\xi|\left(\dot{\xi}J_+ - j\frac{\dot{\xi}\xi^* + \dot{\xi}^*\xi}{1+|\xi|^2}\right)|j,\xi\rangle = ij\frac{\dot{\xi}\xi^* - \dot{\xi}^*\xi}{1+|\xi|^2}.$$

Consequently, the K-terms in the Euler–Lagrange equation contribute in total

$$\frac{\partial K}{\partial \xi^*} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial K}{\partial \dot{\xi}^*}\right) = i\frac{2j}{\left(1+|\xi|^2\right)^2}\dot{\xi}. \tag{2.28}$$

By substituting Eqs. (2.27) and (2.28) into Eq. (2.26), a simple dynamical equation is finally obtained

$$i\dot{\xi} = \epsilon\xi.$$

The solution to this equation is $\xi(t) = \xi_0 e^{-i\epsilon t}$ assuming that the initial state of the system is a SU(2) coherent state $\xi(0) = \xi_0$. Somewhat surprisingly,

considering the difference in algebras, the solution (and thus, the equation) corresponds exactly to the case of harmonic oscillator (2.10). This is due to the theory of generalized coherent states. However, the physical meaning is rather different. In terms of observables we obtain

$$\left\langle \hat{J}_z \right\rangle = \left\langle \hat{J}_z(0) \right\rangle, \left\langle \hat{J}_x \right\rangle = \left\langle \hat{J}_x(0) \right\rangle \cos(\epsilon t), \left\langle \hat{J}_y \right\rangle = \left\langle \hat{J}_y(0) \right\rangle \sin(\epsilon t)$$

where the initial values correspond to ξ_0 through the Eq. (2.18). This is the precession of the spin, also known as Larmor precession [18].

2.3 Phase space distributions

We established in the previous section that generalized coherent states and TDVP can describe the dynamics of quantum systems. However, this description is incomplete. What if the initial state of a quantum system is not a coherent state? In this case, there is the need to represent an arbitrary state as a collection of coherent states. This is achieved by defining a *phase space distribution* corresponding to the quantum state. Furthermore, in order to calculate any expectation value, a *symbol* must be defined accordingly.

There are multiple phase space distributions which differ in definitions. In this section, only the so-called P-representation and Wigner–Weyl representation will be discussed. Furthermore, we focus on distribution functions for bosonic systems. A more exhaustive overview of possible representations (Q, positive-P, R, etc.) can be found in Ref. [12]. Distribution functions of arbitrary systems are discussed in Ref. [7] using generalized coherent states.

In the following, we define a quantum state by its density matrix $\hat{\rho}$. It is defined as an operator

$$\hat{\rho} = \sum_j p_j \left|\psi_j\right\rangle\!\left\langle\psi_j\right|$$

where $p_j > 0$ and $\sum_j p_j = 1$. It describes a probabilistic collection of states $\left|\psi_j\right\rangle$ which are not necessarily orthogonal. In order to calculate expectation values one has to also define the trace operation over a complete basis (e.g. the number states)

$$\left\langle \hat{A} \right\rangle = \mathrm{tr}\left[\hat{\rho}\hat{A}\right] = \sum_n \langle n|\hat{\rho}\hat{A}|n\rangle = \sum_{j,n} p_j \left\langle \psi_j \middle| \hat{A} \middle| n \right\rangle \langle n|\psi_j\rangle = \sum_j p_j \left\langle \psi_j \middle| \hat{A} \middle| \psi_j \right\rangle .$$

The last equality follows from the completeness relation $\hat{I} = \sum_n |n\rangle\langle n|$. Note that the density matrix is normalized, i.e. $\mathrm{tr}[\hat{\rho}] = 1$. A useful property of the trace can be seen straight from the definition

$$\mathrm{tr}\left[\hat{A}\hat{B}\right] = \mathrm{tr}\left[\hat{B}\hat{A}\right]. \tag{2.29}$$

The probabilistic nature of the density matrix $\hat{\rho}$ can be characterized by the state's purity $\mathcal{P} = \mathrm{tr}\left[\hat{\rho}^2\right]$. If the purity equals unity then equivalently $\hat{\rho} = |\psi\rangle\langle\psi|$. This type of state is called *pure*. It is contrasted by a *mixed* state for which $\mathcal{P} < 1$. An important example of a mixed state is the thermal density matrix used in statistical physics to describe a quantum system in equilibrium at the temperature T

$$\hat{\rho}_{th} = \frac{1}{Z} e^{-\beta \hat{H}} = \frac{1}{Z} \sum_n e^{-\beta E_n} |\psi_n\rangle\langle\psi_n| . \tag{2.30}$$

Here, $\beta = \frac{1}{k_B T}$ where k_B is the Boltzmann constant, $|\psi_n\rangle$ is an eigenstate of $\hat{H}$ with energy E_n and $Z = \mathrm{tr}\left[e^{-\beta \hat{H}}\right]$ is the partition function ensuring normalisation.

2.3.1 P-representation

The P-representation was derived in connection with the field coherent states by Glauber [3]. It is the distribution function for a density matrix $\hat{\rho}$ that is diagonal in field coherent states

$$\hat{\rho} = \int \mathrm{d}^2\alpha \, P(\alpha) \, |\alpha\rangle\langle\alpha| . \tag{2.31}$$

This simple expression has a drawback: not all states have a well-behaved P-function. For instance, number states and squeezed states are tempered distributions, such as derivatives of delta functions [12]. Nevertheless, it is a useful calculational tool.

Even though the notation would suggest that the P-function is a probability distribution, this is not the case. It is properly normalized but it can have negative values so it is sometimes called a quasi-probability distribution. In any case, an important class is represented by states with Gaussian P-functions. These are the thermal states given by [12]

$$P(\alpha) = \frac{1}{\pi n_{th}} e^{-\frac{|\alpha|^2}{n_{th}}} . \tag{2.32}$$

Note that at the zero tempreature limit when the average bath population $n_{th} \to 0$, we obtain $P(\alpha) = \delta(\alpha)$ as the definition (2.31) would suggest.

Calculation of quantum mechanical expectation values gives the definition of a symbol [7]. When P-representation is used, we obtain the Q-symbol[5] of an operator. By using Eq. (2.31) the expectation value of an operator $\hat{A}$ is

$$\left\langle \hat{A} \right\rangle = \mathrm{tr}\left[\hat{A}\hat{\rho}\right] = \int \mathrm{d}^2\alpha \, P(\alpha) \, \langle \alpha | \hat{A} | \alpha \rangle \equiv \int \mathrm{d}^2\alpha \, P(\alpha) A_Q(\alpha). \tag{2.33}$$

In this expression A_Q is the Q-symbol of $\hat{A}$. The Q-symbol can be seen as a mapping between operators and phase space functions. For example, if $\hat{A}$ is normally-ordered, i.e. $\hat{A} = (\hat{a}^\dagger)^n \hat{a}^m$, a simple expression $A_Q = (\alpha^*)^n \alpha^m$ is obtained.

There are two choices available concerning the dynamical aspects of a quantum system. Either explicitly the distribution function P changes in time or the distribution simply depicts the initial state of the system. A classical analog can be found in fluid dynamics where either the fluid's velocity field can change in time (Eulerian description) or the individual fluid parcels starting at some initial positions can be followed in time (Lagrangian description). Since the dynamical equation of motion can be obtained from the TDVP method the latter one is our choice.

For a closed system, we can always write the time evolution of density matrix as $\hat{\rho}_t = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ where $\hat{U}$ is the unitary time evolution operator. Therefore, by substituting the initial state (2.31) we obtain

$$\hat{\rho}_t = \int \mathrm{d}^2\alpha_0 \, P(\alpha_0) \, |\alpha_t\rangle\langle\alpha_t| \, .$$

Here, α_t depends on α_0 via solution of corresponding TDVP equation. This leads to the symbol A_Q in Eq. (2.33) being time-dependent. There is a close parallel with classical mechanics. In the classical case the expectation value of position x, for instance, would be determined as an integral $\int \mathrm{d}x_0 \, P(x_0) x(t; x_0)$ where $x(t; x_0)$ obeys Newtonian dynamics.

[5] Conversely, P-symbol is used in Q-representation, essentially interchanging $\hat{\rho}$ and $\hat{A}$ in the definitions. That is, we define a Q-function $Q(\alpha) = \langle \alpha | \hat{\rho} | \alpha \rangle$ and a P-symbol $\hat{A} = \int \mathrm{d}^2\alpha \, A_P(\alpha) \, |\alpha\rangle\langle\alpha|$.

2.3.2 Wigner–Weyl representation

The origins of the Wigner–Weyl representation predates the invention of field coherent states [1]. Originally, its formulation was performed in terms of the position-momentum basis but it can also be transformed to the coherent state basis [24].

In the Wigner–Weyl representation, a Weyl transform of an arbitrary operator $\hat{A}$ is defined as a Fourier transform of a so-called characteristic function $\mathrm{tr}\big[\hat{A}\hat{D}(\eta)\big]$ where $\hat{D}$ is the displacement operator defined in Eq. (2.6) [24, 25]

$$\begin{aligned}\mathbb{W}[\hat{A}](\alpha) = A_W(\alpha) &= \frac{1}{\pi}\int \mathrm{d}^2\eta\, \mathrm{tr}\big[\hat{A}\hat{D}(\eta)\big] e^{\eta^*\alpha - \eta\alpha^*} \\ &= \frac{1}{2\pi}\int \mathrm{d}^2\eta\, \left\langle \alpha - \frac{\eta}{2}\middle|\hat{A}\middle|\alpha + \frac{\eta}{2}\right\rangle e^{\frac{1}{2}(\eta^*\alpha - \eta\alpha^*)}. \quad (2.34)\end{aligned}$$

The second form of this definition is similar to the original definition in the position-momentum basis and can be easier to use in calculations[6]. Again, A_W is called the Weyl symbol of the operator $\hat{A}$. However, in contrast to the P-representation, the phase space distribution is simply a Weyl symbol of a density matrix, denoted by $\mathbb{W}[\hat{\rho}](\alpha) = W(\alpha)$, and it is called the Wigner function.

Some properties of Wigner and P-functions are the same. For instance, Wigner functions are also quasi-probability distributions. The main difference is that Wigner functions are smoother than the corresponding P-functions. There are no delta functions involved: as an example we take the thermal state whose Wigner function is [12]

$$W(\alpha) = \frac{1}{\pi\left(n_{th} + \frac{1}{2}\right)} e^{-\frac{|\alpha|^2}{n_{th}+\frac{1}{2}}}. \quad (2.35)$$

Now, in the limit $n_{th} \to 0$ a non-singular Gaussian distribution is obtained. For illustrative purposes the Wigner functions of a pure state and a mixed state, whose density matrices are $\frac{1}{2}(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)$ and $\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ respectively, are plotted in Fig. 1. Note that the Wigner function of the pure quantum state is negative in a small region near the origin but the mixed state is positive everywhere.

[6]These two seemingly different definitions can be proven to be the same by using operator expansion $\hat{A} = \frac{1}{\pi}\int \mathrm{d}^2 z\, \mathrm{tr}\big[\hat{A}\hat{D}(z)\big]\hat{D}(-z)$ from Ref. [25] on the latter definition and calculating the inner product and resulting Gaussian integral.

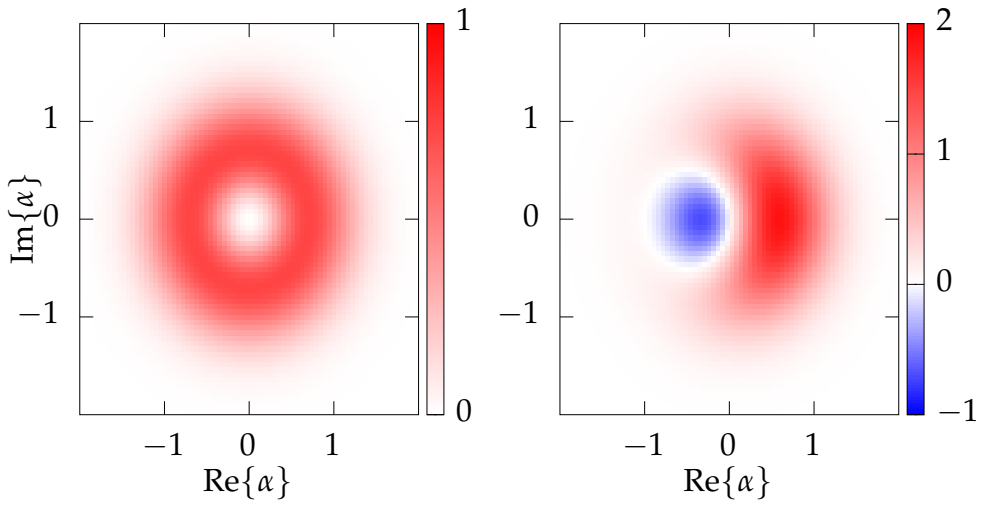


Figure 1: Wigner functions. On the left: $\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ with Wigner function $4|\alpha|^2 e^{-2|\alpha|^2}$. On the right: $\frac{1}{2}(|0\rangle + |1\rangle)(\langle 0| + \langle 1|)$ with Wigner function $(4|\alpha|^2 + 4\,\mathrm{Re}\{\alpha\})e^{-2|\alpha|^2}$.

Expectation values are calculated in the same manner as in P-representation, that is [25]

$$\langle \hat{A} \rangle = \mathrm{tr}\left[\hat{\rho}\hat{A}\right] = \frac{1}{\pi}\int \mathrm{d}^2\alpha\, W(\alpha) A_W(\alpha).$$

Note that the integral is taken over Weyl symbols whereas in P-representation one also needs to define the Q-symbol whose definition differs from the definition of the P-function. Consequently, the purity of a state $\mathcal{P} = \mathrm{tr}\left[\hat{\rho}^2\right]$ is found simply by integrating over W^2. By similar reasoning as with P-representation, one can interpret the integral to be taken over the initial distribution where as the symbol A_W depends on time.

From the definition of a Weyl symbol (2.34) one can derive an interesting formula for the Weyl symbol of a product of operators. It leads to the definition of star product [24]

$$\mathbb{W}[\hat{A}\hat{B}] = \mathbb{W}[\hat{A}] \star \mathbb{W}[\hat{B}] = \mathbb{W}[\hat{A}] \exp\left[\frac{1}{2}\left(\overleftarrow{\partial}_\alpha \overrightarrow{\partial}_{\alpha^*} - \overleftarrow{\partial}_{\alpha^*} \overrightarrow{\partial}_\alpha\right)\right] \mathbb{W}[\hat{B}], \tag{2.36}$$

where $\overleftarrow{\partial}$ ($\overrightarrow{\partial}$) operates to the left (right) and the exponential should be understood via its Taylor expansion. It provides a more useful method

for the calculation of some Weyl symbols than the definition given in Eq. (2.34). Evaluating $\mathbb{W}[\hat{a}] = \alpha$ we can straightforwardly obtain, for instance, $\mathbb{W}[\hat{a}^n] = \alpha^n$ and $\mathbb{W}[\hat{a}^\dagger a] = |\alpha|^2 - \frac{1}{2}$ by utilising star product. Note that there is no similar product formula in other representations and that there is no general connection between the symbols of P- and Wigner–Weyl-representation.

2.4 Open quantum systems

Most quantum systems interact with their environment at least to a small degree. Such systems are in general open in a thermodynamic sense: they can exchange energy, particles, and information with its environment. The distinction between system and environment is, however, arbitrary. It can be a useful idea theoretically because only a certain system is of interest and it offers a possibility to gauge the effects the environment has on the system. Sometimes there is also a separation in interaction strengths so that one has a strongly interacting system which is coupled weakly to a bath. In reality the system of interest cannot usually be accessed or measured by itself but rather via its environment [10].

A typical example is an optical cavity in which photons are confined between two reflecting mirrors. An experimentalist cannot make the mirrors so reflective that the photons would remain in the cavity forever but rather they leak through the mirrors. Even if it were a possibility, one could not observe anything from such a closed system. So in a measurement the dissipative environment is essential. On the other hand, photons can also enter the cavity from its environment, leading to fluctuations, dissipation, and decoherence.

The last term, decoherence, refers to the fact that quantum mechanical superpositions are destroyed in the interaction with the environment and only statistical mixtures are left in the system. A quantum mechanical description of thermalisation thus has to include this transition from a pure state to a mixed thermal state. This is aptly described by the density matrix formalism introduced in the beginning of Section 2.3 which was used to describe the thermal state in Eq. (2.30). The mixedness of a state can also be characterized in this formalism by the purity of a state $\mathcal{P} = \mathrm{tr}\left[\hat{\rho}^2\right]$. One can readily deduce using these tools that the dynamics of thermalisation must be non-unitary. If the dynamics were unitary one

could write the time evolution as $\hat{\rho}_t = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ which means that the purity does not change $\mathrm{tr}\left[\hat{\rho}_t^2\right] = \mathrm{tr}\left[\hat{U}\hat{\rho}_0\hat{U}^\dagger\hat{U}\hat{\rho}_0\hat{U}^\dagger\right] = \mathrm{tr}\left[\hat{\rho}_0^2\right]$. This contradicts the observation of decoherence in quantum systems so the dynamics of open quantum systems cannot generally be unitary.

A mathematical description of open quantum system is given by formally including the environment, usually referred as bath, to the Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{int} \tag{2.37}$$

where $\hat{H}_S$ describes the system alone, $\hat{H}_B$ the bath alone, and $\hat{H}_{int}$ the interaction between the system and the bath. The bath can be assumed to be a non-interacting set of bosonic or fermionic particles. Having in mind an environment of bosonic modes which we assume throughout the thesis the simplest coupling between system and environment is of bilinear form. The Hamiltonian with this prescription reads

$$\hat{H} = \hat{H}_S(\hat{c}_j, \hat{c}_j^\dagger) + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_j \sum_k g_{jk}\left(\hat{c}_j^\dagger \hat{b}_k + \hat{b}_k^\dagger \hat{c}_j\right)$$

where $\hat{H}_S$ is the thus far unspecified Hamiltonian of the system and $\hat{c}_k$ is some system operator.

2.4.1 Quantum master equation

The quantum master equation (QME) is one of the most used equation for analyzing weakly interacting open quantum systems. It describes the Markovian dynamics of an open quantum system in the density matrix formalism. Roughly, the idea is to consider the time evolution of the density matrix of the whole system and then trace out the bath degrees of freedom.

The QME can be derived in multitude of ways. For a physically motivated derivation, see e.g. Ref. [10] or [12]. The physical derivation relies on the assumption that the system and the environment interact weakly. Then the evolution of the density matrix can be written as a perturbative expansion and the higher order terms neglected. As a final step one must assume that the bath degrees of freedom are uncorrelated to obtain a closed equation for the density matrix. A general form of the equation can also be derived by mathematical considerations alone as first shown in Ref. [26]. We discuss this derivation briefly in a similar manner as in Preskill's lecture notes [27].

Let us start by supposing that the dynamics of an open quantum system are Markovian, i.e. memoryless. More precisely we suppose that there exists a map (or superoperator) $\hat{\mathcal{E}}$ that describes the infinitesimal time evolution of the system in the form $\hat{\rho}_S(t+dt) = \hat{\mathcal{E}}_{dt}(\hat{\rho}_S(t))$. This map should be linear and it should preserve the essential properties of a density matrix[7]. By expanding $\hat{\mathcal{E}}_{dt}$ to linear order in the time interval dt, $\hat{\mathcal{E}}_{dt} = \hat{I} + \hat{\mathcal{L}}dt$, we can express the dynamics as a first order differential equation

$$\dot{\hat{\rho}}(t) = \hat{\mathcal{L}}\hat{\rho}(t).$$

Consequently, $\hat{\mathcal{E}}_t(\hat{\rho}) = \exp(\hat{\mathcal{L}}t)\hat{\rho}$ if $\hat{\mathcal{L}}$ is time-independent.

To find the form of the QME, i.e. the superoperator $\hat{\mathcal{L}}$, we must consider both the system and the environment. The time evolution is determined by the Schrödinger equation and the Hamiltonian (2.37). Thus, it can be described by a unitary operator $\hat{U}$. If we assume that the environment has an orthonormal basis $|\mu\rangle_E, \mu \in \mathbb{N}$, and that initially the system and the environment are not coupled, i.e. in a product state $|\psi\rangle_S |\mu_0\rangle_E$, we can write

$$\hat{U}|\psi\rangle_S |\mu_0\rangle_E = \sum_\mu \hat{M}_\mu |\psi\rangle_S |\mu\rangle_E \tag{2.38}$$

where the operators $\hat{M}_\mu$ operate on the system state $|\psi\rangle_S$.

Since unitary operations conserve the normalisation of the state, a completeness relation for $\hat{M}_\mu$ can be obtained. At this point we drop the subscripts S and E for brevity. Now,

$$\langle\psi|\langle\mu_0|\hat{U}^\dagger\hat{U}|\mu_0\rangle|\psi\rangle = \sum_{\mu,\mu'} \langle\psi|\hat{M}^\dagger_{\mu'}\hat{M}_\mu|\psi\rangle \langle\mu'|\mu\rangle = \langle\psi|\sum_\mu \hat{M}^\dagger_\mu\hat{M}_\mu|\psi\rangle = 1$$

and thus

$$\sum_\mu \hat{M}^\dagger_\mu\hat{M}_\mu = \hat{I}. \tag{2.39}$$

Let us then consider the density matrix of the system and its evolution. We can find it by tracing out the bath degrees of freedom from the total density matrix that evolves unitarily as in Eq. (2.38)

$$\hat{\rho}_S(t) = \mathrm{tr}_E(\hat{\rho}_{SE}) = \sum_{\mu,\mu',\mu''} \langle\mu|\hat{M}_{\mu'}|\mu'\rangle|\psi\rangle\langle\psi|\langle\mu''|\hat{M}^\dagger_{\mu''}|\mu\rangle = \sum_\mu \hat{M}_\mu\hat{\rho}_S(0)\hat{M}^\dagger_\mu. \tag{2.40}$$

[7]It must be Hermitian, positive definite ($\langle\psi|\hat{\rho}|\psi\rangle \geq 0$ for all $|\psi\rangle$) and its trace must be unity. In fact, the map $\hat{\mathcal{E}}$ should strictly be *completely positive*, meaning that every extension of the map in the form $\hat{\mathcal{E}} \otimes \hat{I}$ is also positive.

This is the so-called *operator-sum (or Kraus) representation* of the mapping $\mathcal{E}_t$. Note that it indeed has the the properties mentioned earlier (linearity, preserves trace, positivity and hermiticity).

If we consider again the infinitesimal time evolution of the system, remembering that $\hat{\mathcal{E}}_{dt} = \hat{I} + \hat{\mathcal{L}}dt$, we may write a specific form for the operators $\hat{M}_\mu$ so that we can separate the terms that are up to linear order in dt. Because of the form of Eq. (2.40) we have two types of terms which we may suppose to be

$$\begin{aligned} \hat{M}_0 &= \hat{I} + (-i\hat{H}_S + \hat{K})dt \\ \hat{M}_a &= \hat{L}_a\sqrt{dt}, \quad a \in \mathbb{N}, a \neq 0. \end{aligned} \tag{2.41}$$

where both $\hat{H}_S$ and $\hat{K}$ are hermitian. In this expression we have chosen to include all operators of the order dt in $\hat{M}_0$ and without the loss of generality the operator can be written by using its hermitian and anti-hermitian components, $\hat{K}$ and $\hat{H}_S$ respectively. The operators $\hat{L}_a$ are called Lindblad or quantum jump operators and they are specified later. Each $\hat{M}_a$ describes a possible quantum jump of the system induced by the environment that can happen during the time interval dt. The operator $\hat{K}$ is in fact related to these quantum jump operators and it can be determined with the help of the completeness relation (2.39)

$$\hat{I} = \sum_\mu \hat{M}_\mu^\dagger \hat{M}_\mu = \hat{I} + \left(2\hat{K} + \sum_a \hat{L}_a^\dagger \hat{L}_a\right)dt + \mathcal{O}\left(dt^2\right)$$

so that when retaining only the linear terms in dt we obtain

$$\hat{K} = -\frac{1}{2}\sum_a \hat{L}_a^\dagger \hat{L}_a. \tag{2.42}$$

Finally, the superoperator $\hat{\mathcal{L}}$ can be deduced by using the operator-sum representation (2.40) with the operators (2.41) and (2.42). The general form of the QME in the Lindblad form is thus

$$\begin{aligned} \dot{\hat{\rho}} &= -i\left[\hat{H}_S, \hat{\rho}\right] + \sum_a \left(\hat{L}_a\hat{\rho}\hat{L}_a^\dagger - \frac{1}{2}\left(\hat{L}_a^\dagger\hat{L}_a\hat{\rho} + \hat{\rho}\hat{L}_a^\dagger\hat{L}_a\right)\right) \\ &= -i\left[\hat{H}_S, \hat{\rho}\right] + \sum_a \hat{\mathcal{D}}\left[\hat{L}_a\right]\rho. \end{aligned}$$

The first term of the equation can be identified as producing the dynamics of the closed system, so $\hat{H}_S$ is the Hamiltonian of the closed system. The

second term arises from the system's interaction with the environment and it can be condensed into a single superoperator $\hat{\mathcal{D}}$ that is often called *the Lindblad superoperator*. In this superoperator, the term $\hat{L}_a\hat{\rho}\hat{L}_a^\dagger$ describes a possible interaction, e.g. the system can dissipate energy into the environment or the environment can excite the system, and the other two terms are to preserve the properties of the density matrix $\hat{\rho}$.

Let us then consider the QME of a bosonic system. If the system dissipates to the bath then $\hat{L}_1 \propto \hat{a}$ as this corresponds to the system giving up one excitation. Conversely, if the bath can excite the system then $\hat{L}_2 \propto \hat{a}^\dagger$. The full QME can now be written as [12]

$$\dot{\hat{\rho}} = -i\big[\hat{H}_S, \hat{\rho}\big] + \gamma(n_{th}+1)\hat{\mathcal{D}}[\hat{a}]\hat{\rho} + \gamma n_{th}\hat{\mathcal{D}}[\hat{a}^\dagger]\hat{\rho} \tag{2.43}$$

where γ is the dissipation rate and n_{th} describes the mean number of quanta in the bath. If the bath is in thermal equilibrium and $H_S = \omega\hat{n}$ then $n_{th} = \left(e^{\frac{\omega}{k_B T}} - 1\right)^{-1}$. It provides that the stationary solution is indeed the thermal density matrix (2.30) with the correct Boltzmann weights.

A master equation can be derived in a similar manner for spin systems [10]. This is usually done only for spin-half systems but there is no reason why higher spins $j > 1/2$ should be excluded. However, in the process of moving from two-level system to a multilevel system with $2j+1$ levels we implicitly assume that all the levels couple to the bath in the same way. Following the same reasoning as in the bosonic case, the spin QME is

$$\dot{\hat{\rho}} = -i\big[\hat{H}_S, \hat{\rho}\big] + \frac{\gamma}{2j}(n_{th}+1)\hat{\mathcal{D}}\big[\hat{J}_-\big]\rho + \frac{\gamma}{2j}n_{th}\hat{\mathcal{D}}[\hat{J}_+]\hat{\rho}. \tag{2.44}$$

The factor $(2j)^{-1}$ is needed to obtain the correct limit. If $j \to \infty$, corresponding to infinitely many levels in the system, we should obtain the bosonic QME (2.43). This can be understood by using Holstein–Primakoff realisation of $\mathfrak{su}(2)$

$$\hat{J}_z = \hat{a}^\dagger\hat{a} - j, \qquad \hat{J}_+ = \hat{a}^\dagger\sqrt{2j - \hat{a}^\dagger\hat{a}}, \quad \text{and} \quad \hat{J}_- = \sqrt{2j - \hat{a}^\dagger\hat{a}}\hat{a} \tag{2.45}$$

where $\hat{a}$ is a bosonic operator, operating on Fock states $|n\rangle$ with $n \in [0, 2j]$. If we choose only states $j \gg n$, the spin ladder operators are approximated by $\hat{J}_+ \approx \sqrt{2j}\hat{a}^\dagger$ and $\hat{J}_- \approx \sqrt{2j}\hat{a}$. Now, by taking $j \to \infty$ and ignoring the 'offset' in $\hat{J}_z$ we have $\{\hat{J}_z, \hat{J}_+, \hat{J}_-\} \to \{\hat{a}^\dagger\hat{a}, \sqrt{2j}\hat{a}^\dagger, \sqrt{2j}\hat{a}\}$.

The QME in the Lindblad form is important in the fact that it can be taken as the definition of a quantum Markov process. In classical physics, Markovianity can be described in simple terms: a particles position at different

times is a Markov process if only initial distribution and transition probability between any two positions and times needs to be specified. This means essentially that the system has no memory. This definition does not transfer naturally to quantum mechanics because these probability distributions cannot be described. However, there are alternative methods for characterizing non-Markovianity. One can think about the information flow between the system and the environment; non-Markovianity is essentially information backflow from the environment to the system. [28]

2.4.2 Quantum Langevin equation

The quantum Langevin equation[8] (QLE) is essentially a counterpart to the QME. Whereas the QME is formulated in the Schrödinger picture, the QLE is formulated in the Heisenberg picture where operators depend on time.

The idea behind QLE is the following [29]: consider the Hamiltonian

$$\hat{H} = \hat{H}_S + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k g_k \left(\hat{c}^\dagger \hat{b}_k + \hat{b}_k^\dagger \hat{c} \right)$$

where $\hat{H}_S$ is the Hamiltonian of the system and $\hat{c}$ is some system operator which describes the interaction between system and a bath. It is not necessary to specify what the operator $\hat{c}$ is but $\hat{b}_k$ is again supposed to be a bosonic operator. Now, the Heisenberg equations of motion for a system operator $\hat{a}$ and the bath operator $\hat{b}_k$ are

$$\dot{\hat{a}} = i\big[\hat{H}, \hat{a}\big] = i\big[\hat{H}_S, \hat{a}\big] + i \sum_k g_k \Big(\Big[\hat{c}^\dagger, \hat{a}\Big] \hat{b}_k + \hat{b}_k^\dagger [\hat{c}, \hat{a}] \Big) \tag{2.46}$$

$$\dot{\hat{b}}_k = i\Big[\hat{H}, \hat{b}_k\Big] = -i\omega_k \hat{b}_k - i g_k \hat{c}. \tag{2.47}$$

Equation (2.47) can be formally solved with an initial condition at $t = 0$, giving

$$\hat{b}_k(t) = \hat{b}_k(0) e^{-i\omega_k t} - i g_k e^{-i\omega_k t} \int_0^t e^{i\omega_k \tau} \hat{c}(\tau) \mathrm{d}\tau.$$

[8] Sometimes it is called the quantum stochastic differential equation technique or simply the input-output formalism.

Then, this can be substituted into equation (2.46) which leads to

$$\begin{aligned}\dot{\hat{a}} =& i\big[\hat{H}_S, \hat{a}\big] + i\sum_k g_k\Big(\Big[\hat{c}^\dagger, \hat{a}\Big]\hat{b}_k(0)e^{-i\omega_k t} + \hat{b}_k^\dagger(0)e^{i\omega_k t}[\hat{c}, \hat{a}]\Big) \\ &+ \sum_k g_k^2 e^{-i\omega_k t}\left(\Big[\hat{c}^\dagger, \hat{a}\Big]\int_0^t e^{i\omega_k \tau}\hat{c}(\tau)\mathrm{d}\tau - \left(\int_0^t e^{-i\omega_k\tau}\hat{c}^\dagger(\tau)\mathrm{d}\tau\right)[\hat{c}, \hat{a}]\right).\end{aligned}$$

This is as far as one can reach without any assumptions. If it is supposed that the system-bath interaction is independent of frequency of a bath mode, one can make a significant simplification. This is called *the first Markov assumption* as it will lead to time-local dissipation [29]. So, let us suppose that $g_k^2 = \frac{\gamma}{2\pi}D$ where D is the density of modes, i.e. $\omega_k = kD$. In the last term we can write $\sum_k e^{iD(t-\tau)k} = \frac{2\pi}{D}\delta(t-\tau)$ assuming infinite number of modes k. The resulting integral is somewhat problematic as it requires the evaluation of the Dirac delta function at the integration limit. If we consider delta function to be a product of limiting procedure in which, for instace, the variance of Gaussian distribution is taken to zero we have

$$\int_{t_0}^{t} f(\tau)\delta(t-\tau)\mathrm{d}\tau = \int_{t}^{t_1} f(\tau)\delta(t-\tau)\mathrm{d}\tau = \frac{1}{2}f(t)$$

when $t_0 < t < t_1$ and f is a smooth function [29]. It is a reasonable interpretation in this case since it produces the same result even if we were to integrate backwards in time. Finally, we arrive at the QLE

$$\dot{\hat{a}} = i\big[\hat{H}_S, \hat{a}\big] + \Big[\hat{c}^\dagger, \hat{a}\Big]\Big(\frac{\gamma}{2}\hat{c} + \sqrt{\gamma}\hat{a}_{in}\Big) - \Big(\frac{\gamma}{2}\hat{c}^\dagger + \sqrt{\gamma}\hat{a}_{in}^\dagger\Big)[\hat{c}, \hat{a}] \tag{2.48}$$

with the definition

$$\hat{a}_{in} = -i\sqrt{\frac{D}{2\pi}}\sum_k \hat{b}_k(0)e^{-i\omega_k t}. \tag{2.49}$$

The operator $\hat{a}_{in}$ is called an input operator because the Heisenberg equations are solved forward in time, i.e. with some initial condition $\hat{b}_k(0)$. Similarly one can solve the equation backwards in time which essentially changes only $\gamma \to -\gamma$ and $\hat{a}_{in} \to \hat{a}_{out}$. The output operator is defined similarly. The input and output are related by $\sqrt{\gamma}\hat{a} = \hat{a}_{out} - \hat{a}_{in}$ from which the naming convention follows [29].

The formal connection between the QLE and the QME was provided by Gardiner and Collett [29]. Essentially, one needs to define and recognize $\hat{a}_{in}$ as a quantum stochastic process.

3 TDVP for open quantum systems

The concepts of phase space theory can be applied to open quantum systems. One possibility is to start from the QME and derive an equation for the phase space distribution function by using the properties of the different phase space representations. For instance, one can apply the Weyl transform (2.34) to the QME or use the definition of the P-function (2.31) in the QME to find an equation for the Wigner function or $P-function$, respectively. This approach is chosen for instance in Refs. [12, 15] and it is briefly discussed in Section 3.1.2. We choose a different approach that is independent of the QME and based on the TDVP.

The most straightforward approach is to formally consider the Hamiltonian (2.37) which generates the dynamics of the system and the bath and then to self-consistently eliminate the bath as in the derivation of QLE. In this case, however, the general algebraic approach of generalized coherent states and TDVP is not feasible, since the algebraic structure is often intractable due to the coupling term $\hat{H}_{SB}$. Therefore, one cannot derive the generalized coherent states. As an approximation we choose the generalized coherent states of the system $\hat{H}_S$ and the bath $\hat{H}_B$ separately. If the bath is bosonic as we assume, these bath states are field coherent states.

This approach leads to the phase space version of the QLE. As example, we derive the phase space Langevin equations for the harmonic oscillator and a spin system which obey the Weyl–Heisenberg and the $\mathfrak{su}(2)$ algebra, respectively. The first part of this section focuses on the derivation of the TDVP method for an open system and the inclusion of a thermal environment. Then, analytical results for the harmonic oscillator are shown, e.g. in section 3.1.2 it is shown that the TDVP method produces exactly the same results as the QME. Spin systems are considered in Section 3.2 both analytically and numerically. For spin systems the TDVP method is not exact and does not correspond to the QME but is a good approximation in certain cases.

3.1 Electromagnetic field — Weyl–Heisenberg algebra

Let us first consider a harmonic oscillator coupled to a bosonic bath, for instance a single electromagnetic (EM) mode inside an optical cavity. The

dynamics of the cavity mode without the bath is described by the Hamiltonian $\hat{H}_S = \omega \hat{a}^\dagger \hat{a}$ where ω is the cavity resonance frequency. The bath consists of free EM modes outside of the cavity. We describe the interaction between the system and the environment by a number-conserving bilinear Hamiltonian. The total Hamiltonian is given by

$$\hat{H} = \omega \hat{a}^\dagger \hat{a} + \sum_k \omega_k \hat{b}_k^\dagger b_k + \sum_k g_k \left(\hat{a}^\dagger \hat{b}_k + \hat{a} \hat{b}_k^\dagger \right). \tag{3.1}$$

The cavity mode can exchange photons with the bath which in terms of the mode's dynamics alone seems like that there is dissipation and fluctuations in the system. Due to this reason the cavity mode is often called a damped harmonic oscillator. It can be considered a prototypical system in quantum mechanics in the same manner as a Brownian particle is in classical mechanics. The damped harmonic oscillator is one of few open systems that is well understood and can be solved analytically [13]. Therefore it provides a good test case.

Next, let us use the TDVP method. As discussed earlier, we choose the Lagrangian $\mathcal{L} = \left\langle \alpha, \vec{\beta} \right| (i\partial_t - \hat{H}) \left| \alpha, \vec{\beta} \right\rangle$ where $\left| \vec{\beta} \right\rangle = |\beta_1, \beta_2, \ldots\rangle$ is a tensor product of field coherent states and $\hat{b}_k |\beta_k\rangle = \beta_k |\beta_k\rangle$. In this case, actually, the argument made in Section 2.1.4 in relation with the Jordan–Schwinger map holds[9] and the state $\left| \alpha, \vec{\beta} \right\rangle$ is indeed a generalized coherent state of $\hat{H}$ given by Eq. (3.1).

We will go through the derivation explicitly following the derivation of the QLE in Section 2.4.2. The starting point is the calculation of the Lagrangian $\mathcal{L}$. Since the displacement operator $\hat{D}$ satisfies

$$\partial_t \hat{D}(\alpha) = \partial_t \left(e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} \right) = -\frac{1}{2}(\dot{\alpha}\alpha^* + \dot{\alpha}^*\alpha) + \dot{\alpha}\hat{a}^\dagger \hat{D}(\alpha) - \dot{\alpha}^* \hat{D}(\alpha)\hat{a}$$

the Lagrangian is

$$\begin{aligned} \mathcal{L} &= i \left\langle \alpha, \vec{\beta} \right| \partial_t \left| \alpha, \vec{\beta} \right\rangle - \left\langle \alpha, \vec{\beta} \right| \hat{H} \left| \alpha, \vec{\beta} \right\rangle \\ &= \frac{i}{2}(\dot{\alpha}\alpha^* - \dot{\alpha}^*\alpha) + \frac{i}{2} \sum_k \left(\dot{\beta}_k \beta_k^* - \dot{\beta}_k^* \beta_k \right) \\ &\quad - \omega |\alpha|^2 - \sum_k \omega_k |\beta_k|^2 - \sum_k g_k (\alpha^* \beta_k + \alpha \beta_k^*). \end{aligned}$$

[9] Note that if there were only r bath modes in the Hamiltonian $\hat{H}$ in Eq. (3.1) then $\hat{H} \in \mathfrak{su}(r)$. In this case we consider the limit $r \to \infty$.

The Euler-Lagrange equations for the whole system are simply

$$i\dot{\alpha} = \omega\alpha + \sum_k g_k\beta_k, \tag{3.2}$$

$$i\dot{\beta}_k = \omega_k\beta_k + g_k\alpha. \tag{3.3}$$

The derivation follows now exactly the same steps as in Section 2.4.2. We arrive at the Weyl–Heisenberg phase space Langevin equation

$$\dot{\alpha} = -i\omega\alpha - \frac{\gamma}{2}\alpha + \sqrt{\gamma}\alpha_{in} \tag{3.4}$$

with the definition that is similar to Eq. (2.49)

$$\alpha_{in} = -i\sqrt{\frac{D}{2\pi}}\sum_k \beta_k(0)e^{-i\omega_k t}. \tag{3.5}$$

In this equation, dissipation of the system and input of the bath are clearly separated into two different terms. This fact is extremely helpful for the analysis of damped harmonic oscillator as it essentially makes solving this equation possible.

The derivation is essentially the same for the quantum Langevin equation for operators since the Heisenberg equations corresponding to Eqs. (3.2) and (3.3) are linear. Thus, it is clear that Eq. (3.4) corresponds exactly to the QLE for the operator $\hat{a}$. The only difference is that the operators are replaced by coherent state labels, i.e. complex numbers. Formally, we could have just written the QLE and taken the expectation value over field coherent states and arrive at the same result. The Weyl–Heisenberg algebra is a special case in this sense and generally the phase space Langevin equations obtained with this method do not correspond to the expectation value of the QLE over generalized coherent states.

Even though the phase space distributions were not mentioned even once during the derivation of the phase space Langevin equation they play an important role. Without their existence one could only use Eq. (3.4) to describe the time evolution of a coherent state. One can again think that there is an initial distribution in phase space and then the phase space Langevin equation determines the dynamics in that space. Next we will show how this underlying structure of distribution functions affects the interpretation of Eq. (3.4) in the case of a thermal bath.

3.1.1 Thermal environment

The Weyl–Heisenberg phase space Langevin equation (3.4) can be used to describe the dynamics of thermalisation. However, the bath term (3.5) must be discussed first. It clearly requires interpretation so that the equation (3.4) is of practical use. Generally, the initial bath coherent state labels $\beta_k(0)$ have a corresponding phase space distribution.

The definition of the bath input (3.5) in phase space formalism is thus that of a *stochastic process* [13]. That is, α_{in} is a function of time and variables $\beta_k(0)$ that obey a probability distribution. The quasi-probability nature of P-functions does not play a role since the P-functions of thermal states (2.32) are positive on the whole complex plane.

Let us then investigate the properties of α_{in}. Suppose that every bath degree of freedom is in a thermal state without any correlations among modes. The total P-function then factorizes into a product of P-functions given by Eq. (2.32)

$$P(\beta_1, \beta_2 \dots) = P(\vec{\beta}) = \prod_k P_k(\beta_k) = \prod_k \frac{1}{\pi n_k} e^{-\frac{|\beta_k|^2}{n_k}}$$

where the bath population for mode k is n_k. Now, the bath input correlation function $\left\langle \hat{a}_{in}^\dagger(t_1)\hat{a}_{in}(t_2)\right\rangle$ is

$$\begin{aligned}\left\langle \hat{a}_{in}^\dagger(t_1)\hat{a}_{in}(t_2)\right\rangle &= \mathbb{E}_P[\alpha_{in}^*(t_1)\alpha_{in}(t_2)] = \int P(\vec{\beta}_0)\alpha_{in}^*(t_1)\alpha_{in}(t_2)\,\mathrm{d}^2\vec{\beta}_0 \\ &= \frac{D}{2\pi}\sum_k \mathbb{E}_{P_k}[\beta_k^*(0)\beta_k(0)]e^{i\omega_k(t_1-t_2)} = \frac{D}{2\pi}\sum_k n_k e^{i\omega_k(t_1-t_2)}.\end{aligned} \tag{3.6}$$

The statistical expectation value $\mathbb{E}_P[\cdot]$ over a symbol is defined in the second equality of this expression. The equality on the second row is obtained by using the factorization assumption of the P-function and the relation given by Eq. (3.5). If $t_1 = t_2$ the sum seems to diverge when the bath is in thermal equilibrium, assuming infinite amount of modes and no frequency cutoff. On the other hand, if $t_1 - t_2 \neq 0$, the terms in the sum oscillate in different phases, mostly cancelling each other. Thus the input correlation function is proportional to the delta function $\delta(t_1 - t_2)$.

Instead of using the definition (3.5) of α_{in} and the individiual bath distributions, we can simplify the discussion by defining the input term α_{in} to be

white noise following the example of the Eq. (3.6). This model entails that α_{in} has the following properties: it is Gaussian with vanishing mean and with complex autocorrelation function

$$\mathbb{E}_P\left[\alpha_{in}^*(t)\alpha_{in}(t')\right] = C_P\delta(t-t') \tag{3.7}$$

where $\mathbb{E}_P[\cdot]$ was defined in Eq. (3.6). The bath can be in a thermal coherent state if the system is driven but this drive can be absorbed in the definition of the Hamiltonian. We also suppose that there are no phase dependent correlations so that $\mathbb{E}_P[\alpha_{in}(t)\alpha_{in}(t')]$ vanishes. This would not be the case if the bath is in a squeezed state. Note that due to the Gaussian nature of white noise only one number is needed to describe the bath. The higher moments of α_{in} are determined by the following property: If the mean of Gaussian variables X_i vanishes, the odd moments also vanish and the even moments factorize

$$\mathbb{E}\left[\prod_i X_i\right] = \sum_{i_k} \mathbb{E}\left[X_{i_1}X_{i_2}\right]\mathbb{E}\left[X_{i_3}X_{i_4}\right]\cdots \tag{3.8}$$

where the summation is taken over all the different subdivisions of the original product into pairs [13].

What if we used the Wigner–Weyl representation in the example (3.6)? The end result must remain the same so that the expectation values of operators are independent of representation. As mentioned in Section 2.3.2 the Weyl symbol of $\hat{a}_{in}^\dagger(t_1)\hat{a}_{in}(t_2)$ is $\alpha_{in}^*(t_1)\alpha_{in}(t_2) - \frac{1}{2}$. This difference is also at the last equality so that $\mathbb{E}_{W_k}\left[\beta_k^*(0)\beta_k(0) - \frac{1}{2}\right] = n_k$. The generalization to white noise must be similar to the one in the P-representation, i.e.

$$\mathbb{E}_W\left[\alpha_{in}^*(t)\alpha_{in}(t')\right] = C_W\delta(t-t') \tag{3.9}$$

since $\mathbb{E}_W\left[\frac{1}{2}\right] = \frac{1}{2}$. The factor $\frac{1}{2}$ difference between the symbols in different representations leads to the relation $C_P = C_W + \frac{1}{2}$. We will derive the value of C_P and thus C_W more formally but in order to do that some mathematical tools are needed.

Since the input is considered to be stochastic, the phase space Langevin equations are generally stochastic differential equations (SDEs). We will now discuss some operationally necessary aspects of SDEs. Some additional information can be found in the appendix A.

Even though the phase space Langevin equation are SDEs there is still a problem known as the Itô–Stratonovich dilemma. It means that SDEs can

be interpreted in two different ways which alters the results. Mainly, it is related to how one defines an integral $\int G(t)\eta(t)\,\mathrm{d}t$ where G is a function and η is a white noise process. The definition has an effect on the transformation rules of SDEs and the evaluation of expectation values [14].

The Stratonovich approach to SDEs, Stratonovich SDEs in short, can be interpreted using ordinary rules of calculus. Following the notation of Ref. [14] where differential notation is used, $\mathrm{d}W(t) = \eta(t)\,\mathrm{d}t$ and Einstein summation convention[10] is assumed, it means that if a Stratonovich SDE system is

$$\mathrm{d}x_i = A_i(\vec{x})\,\mathrm{d}t + B_{ij}(\vec{x})\,\mathrm{d}W_j(t) \tag{3.10}$$

then the differential of a function $f(\vec{x}, t)$ is simply

$$\begin{aligned}\mathrm{d}f &= \frac{\partial f}{\partial t}\,\mathrm{d}t + \frac{\partial f}{\partial x_i}\big(A_i(\vec{x})\,\mathrm{d}t + B_{ij}(\vec{x})\,\mathrm{d}W_j(t)\big) \\ &= \frac{\partial f}{\partial t}\,\mathrm{d}t + (\boldsymbol{\nabla} f)^T\Big(\vec{A}(\vec{x})\,\mathrm{d}t + B(\vec{x})\,\mathrm{d}\vec{W}(t)\Big).\end{aligned}$$

Despite the simplicity of the transformation rule in the Stratonovich interpretation, its application is problematic since there is no general rule to determine the expectation value $\mathbb{E}\big[\int B_{ij}\,\mathrm{d}W_j(t)\big]$.

The Itô interpretation provides a much easier calculational tool since it is defined so that $\mathbb{E}\big[\int B_{ij}\,\mathrm{d}W_j(t)\big]$ generally vanishes. Also, one has for the second moment that $\mathbb{E}\Big[\big(\int B_{ij}\,\mathrm{d}W_j(t)\big)^2\Big] = \int B_{ij}^2\,\mathrm{d}t$. However, the simple definition of the Itô stochastic integral comes with a caveat. A special rule is needed to transform variables which is often called Itô's lemma or formula. The transformation of the Itô SDE (3.10) to the SDE of a function $f(x, t)$ reads

$$\begin{aligned}\mathrm{d}f &= \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_i}A_i + \frac{1}{2}B_{ki}\frac{\partial^2 f}{\partial x_k \partial x_j}B_{ji}\right)\mathrm{d}t + \frac{\partial f}{\partial x_i}B_{ij}\,\mathrm{d}W_j \\ &= \left(\frac{\partial f}{\partial t} + (\boldsymbol{\nabla} f)^T\vec{A} + \frac{1}{2}\operatorname{tr}\Big(B^T H_f B\Big)\right)\mathrm{d}t + (\boldsymbol{\nabla} f)^T B\,\mathrm{d}\vec{W}\end{aligned} \tag{3.11}$$

where H_f is the Hessian matrix of f.

There is a connection between the two seemingly different interpretations. A multidimensional Stratonovich equation (3.10) corresponds to the fol-

[10] If a term has two or more of the same index the sum is taken over that index.

lowing Itô equation

$$\mathrm{d}x_i = \left(A_i(\vec{x}) + \frac{1}{2} \sum_{j,k} B_{kj} \partial_k B_{ij} \right) \mathrm{d}t + \sum_j B_{ij}(\vec{x}) \, \mathrm{d}W_j(t) \, . \tag{3.12}$$

It should be noted that the phase space Langevin equations are presumably Stratonovich SDEs. This is due to the white noise approximation in which the autocorrelation time of the bath is set to zero. If it is assumed that this is an approximation of some small but finite autocorrelation time, it can be proven that this limiting procedure leads to Stratonovich SDE [14]. In fact, the Itô interpretation cannot even be formulated for a stochastic process with a non-vanishing autocorrelation time. Another argument in favor of the Stratonovich interpretation is that the definition of the Itô and Stratonovich stochastic integrals (see Appendix A) imply that the Itô interpretation is not symmetrical with respect to time. That is, one cannot derive an Itô SDE with a final condition. This is not the case for Stratonovich SDE. Finally we note that the QLE (2.48) obeys a quantum mechanical version of the Stratonovich interpretation [29]. Since we wish to average over the bath input that is assumed to be white noise, we need to therefore use the relation (3.12) connecting Stratonovich and Itô SDEs so that the average over the term $\sum_j B_{ij}(\vec{x}) \, \mathrm{d}W_j(t)$ vanishes.

The mathematical process is ideally that we first solve the Weyl–Heisenberg phase space Langevin equation (3.4) for α. Naturally, this solution depends on the initial conditions of α given by some distribution and on the bath variables. Then, we can find the symbol of any observable in terms of α_t. Taking the statistical expectation value corresponds to tracing out the bath. For example, if $\hat{A}$ is some system operator then according to Eq. (2.33) its expectation value is

$$\left\langle \hat{A}(t) \right\rangle = \int P(\alpha_0, \vec{\beta}_0) A_Q(\alpha_t(\alpha_0, \vec{\beta}_0)) \, \mathrm{d}^2\alpha_0 \, \mathrm{d}^2\vec{\beta}_0 = \mathbb{E}_P\big[A_Q(\alpha_t)\big]. \tag{3.13}$$

It is almost always supposed that the intial states of the system and bath are uncorrelated so that $P(\alpha_0, \vec{\beta}_0) = P(\alpha_0)P(\vec{\beta}_0)$, similarly to the case of the QME. This assumption can be made since the interaction between the system and the environment correlates them and one can choose the initial condition so that the correlations are not yet relevant [28]. Then with the white noise approximation we can essentially forget the underlying bath distributions and treat α_{in} as a stochastic process with known mean and autocorrelation function. The possiblity of using the TDVP method to

explicitly describe initial correlations between the system and the bath — which is inherently a non-Markovian property as it is incompatible with the QME [28] — seems a very interesting possibility.

Let us now consider the calculation of observables using the Weyl–Heisenberg phase space Langevin equation (3.4). First, we write it in an explicitly two-dimensional form without specifying the representation

$$\partial_t \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} = \begin{pmatrix} -(i\omega + \frac{\gamma}{2})\alpha \\ (i\omega - \frac{\gamma}{2})\alpha^* \end{pmatrix} + \sqrt{\frac{\gamma}{2}C} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}. \tag{3.14}$$

It is easy to see that the construction $\alpha_{in} = \sqrt{\frac{C}{2}}(\eta_1 + i\eta_2)$ leads to correct autocorrelators when $\mathbb{E}\left[\eta_i(t_1)\eta_j(t_2)\right] = \delta_{ij}\delta(t_1 - t_2)$. Here, C is the constant factor of the autocorrelator given in Eqs. (3.7) and (3.9) that is to be determined. Since the matrix multiplying the stochastic vector $(\eta_1, \eta_2)^T$ (B in Eq. (3.10)) is constant there is no difference between the Itô and Stratonovich SDEs according to Eq. (3.18). We can now calculate the expectation value of $|\alpha|^2$ using the Itô's lemma for transformation of variables (3.11). Since the expectation value of the stochastic terms vanishes in the Itô interpretation we obtain without specifying the representation

$$\partial_t \mathbb{E}\left[|\alpha|^2\right] = -\gamma\Big(\mathbb{E}\left[|\alpha|^2\right] - C\Big). \tag{3.15}$$

This equation is very similar to what we would obtain from the quantum master equation (2.43) for number operator $\hat{n} = \hat{a}^\dagger\hat{a}$ by using $\partial_t \langle\hat{n}\rangle = \mathrm{tr}\left[\hat{n}\dot{\hat{\rho}}\right]$ and Eq. (2.29)

$$\partial_t \langle\hat{n}\rangle = -\gamma(\langle\hat{n}\rangle - n_{th}). \tag{3.16}$$

Now the representation can be specified. In the P-representation, $|\alpha|^2$ corresponds to the number operator $\hat{n}$, i.e. $A_Q = |\alpha|^2$. Therefore, we have

$$\partial_t \mathbb{E}_P\left[|\alpha|^2\right] = -\gamma\Big(\mathbb{E}_P\left[|\alpha|^2\right] - C_P\Big).$$

The identification (3.13) implies that $\mathbb{E}_P\left[|\alpha|^2\right] = \langle\hat{n}\rangle$. Therefore, a direct comparison with (3.16) implies that $C_P = n_{th}$. On the other hand, in Wigner–Weyl representation the symbol corresponding to the number operator is $\mathbb{W}[\hat{n}] = |\alpha|^2 - \frac{1}{2}$. Thus, by a simple manipulation of Eq. (3.15) we obtain

$$\partial_t \mathbb{E}_W\left[|\alpha|^2 - \frac{1}{2}\right] = -\gamma\left(\mathbb{E}_W\left[|\alpha|^2 - \frac{1}{2}\right] - C_W + \frac{1}{2}\right).$$

As expected, we obtain $C_W = n_{th} + \frac{1}{2}$ by a similar reasoning since $\langle \hat{n} \rangle = \mathbb{E}_W \left[|\alpha|^2 - \frac{1}{2} \right]$. Therefore, the symbol of the input operator $\hat{a}_{in}^\dagger \hat{a}_{in}$ in different representations effectively implies that one needs to choose the noise according to the representation.

One important difference between P- and Weyl–Wigner representation must be noted. At zero temperature, when $n_{th} = 0$, the stochastic input term vanishes in the P-representation as $C_P = 0$. Thus, the dynamical equation is not a SDE but a deterministic equation. This is contrasted by Weyl–Wigner representation where $C_W \geq \frac{1}{2}$ and the theory of SDEs is always needed. This is due to the difference between thermal distributions in P- and Wigner–Weyl representation, Eqs. (2.32) and (2.35) respectively. The singularity of the P-function that is $\delta(\alpha)$ in zero temperature means that the symbols of input operators (e.g. Eq. (3.6)) are always strictly zero. This is not the case in Wigner–Weyl representation as the Wigner function is a non-singular Gaussian function.

3.1.2 Equivalence with the quantum master equation

In Section 3.1.1 we found a description of the noise such that the expectation value of the number operator obeys the same equation whether it is derived from QME or TDVP. In fact, the Weyl–Heisenberg phase space Langevin equation (3.4) with the white noise approximation is equivalent to the QME (2.43). The equivalences between different methods discussed in this thesis are presented in Fig. 2. The equivalence of the QME and QLE was proven by Gardiner and Collett [29] and it was already briefly mentioned in the end of Section 3.1 that the Weyl–Heisenberg phase space Langevin equation corresponds to the expectation value of the QLE over field coherent states. Now we wish to show that the QME and the Weyl–Heisenberg phase space Langevin equation are also connected by the Fokker–Planck equation. This can be proven by using the connection between Fokker–Planck equations and SDEs. First, we transform the phase space Langevin equation to a Fokker–Planck equation. Then we show that the QME can be transformed into a Fokker–Planck equation as well. This is done also in Ref. [12] for different representations.

The Fokker–Planck equation describes the time evolution of a probability distribution or more generally a phase space distribution. The general

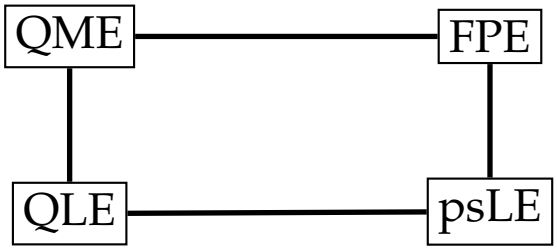


Figure 2: Equivalences between different equations. Here, psLE refers to the Weyl–Heisenberg phase space Langevin equation and FPE to Fokker–Planck equation.

form of the Fokker–Planck equation for a distribution P is [13, 14]

$$\partial_t P(\vec{x},t) = \left[-\sum_k \partial_{x_k} A_k(\vec{x}) + \frac{1}{2}\sum_{i,j} \partial_{x_i}\partial_{x_j} D_{ij}(\vec{x}) \right] P(\vec{x},t) \tag{3.17}$$

where D is often called the diffusion matrix. It can be proven that this corresponds to the multidimensional Itô SDE [13, 14]

$$\dot{x}_k = A_k(\vec{x}) + \sum_j B_{kj}(\vec{x})\eta_j \tag{3.18}$$

where η_j is white noise, $\mathbb{E}\left[\eta_i(t_1)\eta_j(t_2)\right] = \delta_{ij}\delta(t_1 - t_2)$, when $D = B^T B$. The A, B and thus D related to the Weyl–Heisenberg phase space Langevin equation can be identified from Eq. (3.14)

$$A = \begin{pmatrix} -(i\omega + \frac{\gamma}{2})\alpha \\ (i\omega - \frac{\gamma}{2})\alpha^* \end{pmatrix},\ B = \sqrt{\frac{\gamma}{2}}\mathrm{C}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix},\ D = \gamma \mathrm{C}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.19}$$

Next we discuss how the QME (2.43) can be transformed to a Fokker–Planck equation (3.17). In P-representation the proof relies on the properties of coherent states and partial integration [12]. First, it can be noted[11] that

$$e^{\frac{|\alpha|^2}{2}} \hat{a}^\dagger |\alpha\rangle = \sum_n (n+1) \frac{\alpha^n}{\sqrt{(n+1)!}} |n+1\rangle = \partial_\alpha \left(e^{\frac{|\alpha|^2}{2}} |\alpha\rangle \right)$$

[11] The unnormalized states $e^{\frac{|\alpha|^2}{2}} |\alpha\rangle$ are called Bargmann states.

so that for instance

$$\begin{aligned}\hat{a}^\dagger\hat{a}\rho &= \int \mathrm{d}^2\alpha\, P(\alpha)\hat{a}^\dagger\hat{a}\,|\alpha\rangle\langle\alpha| = \int \mathrm{d}^2\alpha\, P(\alpha)\alpha e^{-\frac{|\alpha|^2}{2}}\partial_\alpha\left(e^{\frac{|\alpha|^2}{2}}\,|\alpha\rangle\right)\langle\alpha| \\ &= \int \mathrm{d}^2\alpha\, P(\alpha)\alpha e^{-|\alpha|^2}\partial_\alpha\left(e^{|\alpha|^2}\,|\alpha\rangle\langle\alpha|\right) \\ &= -\int \mathrm{d}^2\alpha\,\partial_\alpha\left(P(\alpha)\alpha e^{-|\alpha|^2}\right)e^{|\alpha|^2}\,|\alpha\rangle\langle\alpha| \\ &= \int \mathrm{d}^2\alpha\,\left[(\alpha^* - \partial_\alpha)\alpha P(\alpha)\right]|\alpha\rangle\langle\alpha|\,.\end{aligned}$$

When $\hat{H}_S = 0$, which corresponds to working in the interaction picture of the closed system $\hat{\rho} \leftarrow e^{-i\hat{H}_S t}\hat{\rho}_I e^{i\hat{H}_S t}$ where ρ_I is the density matrix in the interaction picture, every term in the QME (2.43) can be written as an integral over $|\alpha\rangle\langle\alpha|$ by similar manipulations. The final result is the Fokker-Planck equation

$$\partial_t P(\alpha) = \left[\frac{\gamma}{2}(\partial_\alpha\alpha + \partial_{\alpha^*}\alpha^*) + \gamma n_{th}\partial_\alpha\partial_{\alpha^*}\right]P(\alpha). \tag{3.20}$$

In Wigner–Weyl representation one can use the properties of the characteristic function $\mathrm{tr}\left(\hat{\rho}\hat{D}(\eta)\right)$ to derive a similar equation [12]. An alternative method is provided by the Weyl transform (2.34) and star product (2.36). For instance, since $\mathbb{W}[\hat{a}^\dagger\hat{a}] = |\alpha|^2 - \frac{1}{2}$, applying the Weyl transform to the term $\hat{a}^\dagger\hat{a}\hat{\rho}$ gives

$$\begin{aligned}\mathbb{W}[\hat{a}^\dagger\hat{a}] \star \mathbb{W}[\hat{\rho}] &= \left(|\alpha|^2 - \frac{1}{2}\right)\exp\left[\frac{1}{2}\left(\overleftarrow{\partial}_\alpha\overrightarrow{\partial}_{\alpha^*} - \overleftarrow{\partial}_{\alpha^*}\overrightarrow{\partial}_\alpha\right)\right]W(\alpha) \\ &= \left(|\alpha|^2 - \frac{1}{2}\right)\left[1 + \frac{1}{2}\left(\overleftarrow{\partial}_\alpha\overrightarrow{\partial}_{\alpha^*} - \overleftarrow{\partial}_{\alpha^*}\overrightarrow{\partial}_\alpha\right) - \frac{1}{2}\overleftarrow{\partial}_\alpha\overleftarrow{\partial}_{\alpha^*}\overrightarrow{\partial}_\alpha\overrightarrow{\partial}_{\alpha^*}\right]W(\alpha) \\ &= \left(|\alpha|^2 - \frac{1}{2}\right)W(\alpha) + \frac{1}{2}(\alpha^*\partial_{\alpha_*} - \alpha\partial\alpha)W(\alpha) - \frac{1}{2}\partial_\alpha\partial_{\alpha^*}W(\alpha).\end{aligned}$$

The other terms in the QME (2.43) can be calcuated similarly. These terms can be rearranged to give a Fokker–Planck equation

$$\partial_t W = i\{W, H_W\}_{MB} + \left[\frac{\gamma}{2}(\partial_\alpha\alpha + \partial_{\alpha^*}\alpha^*) + \gamma\left(n_{th} + \frac{1}{2}\right)\partial_\alpha\partial_{\alpha^*}\right]W. \tag{3.21}$$

It is now easy to see that the Fokker–Planck equations Eqs. (3.20) and (3.21) correspond exactly to the Fokker–Planck equation (3.17) with the constants

given in Eq. (3.19) both in P- and Wigner–Weyl representations when $C_P = n_{th}$ and $C_W = n_{th} + \frac{1}{2}$ respectively. This establishes the equivalence of the phase space Langevin equation and QME in the bosonic case.

3.1.3 Full solution and some examples

The Weyl–Heisenberg phase space Langevin equation (3.14) is known in the mathematical literature as the two-dimensional Orstein–Uhlenbeck process whose solution is generally known [14]. This solution can be used to show, for instance, that the phase space Langevin equation produces the correct thermal density matrix, and how the purity of a state evolves in time.

The solution of Eq. (3.14) can be found from Eq. (3.4) as well. By substituting $z = \alpha e^{\left(i\omega + \frac{\gamma}{2}\right)t}$ the equation reads

$$\dot{z}_t = \sqrt{\gamma C} e^{\left(i\omega + \frac{\gamma}{2}\right)t} \eta \equiv \eta_\theta$$

where $\theta = C\left(e^{\gamma t} - 1\right)$ is a result of deterministic time change[12] and refers to the variance of the noise. The complex factor can be neglected. By integration the final result is obtained

$$\alpha_t = \alpha_0 e^{-\left(i\omega + \frac{\gamma}{2}\right)t} + e^{-\frac{\gamma}{2}t} B_\theta. \tag{3.22}$$

Here, B_θ is a complex Wiener process [14]. This entails Gaussianity and $\mathbb{E}\left[|B_\theta|^2\right] = \theta$. Again, $\mathbb{E}[B_\theta] = 0$.

With the full solution we can calculate almost any expectation value we are interested in. Let us first focus on finding the stationary density matrix. A somewhat confusing aspect of phase space quantum mechanics is that the coherent state label describes both the state and observables since a label directly relates to expectation values. The distinction between Schrödinger and Heisenberg picture is therefore moot. For instance, the elements of density matrix in the number basis can be expressed in P-representation as

$$\rho_{nm} = \langle n|\hat{\rho}|m\rangle = \mathrm{tr}[\hat{\rho}\,|m\rangle\langle n|] = \int \mathrm{d}\alpha_0\, P(\alpha_0) e^{-|\alpha_t|^2} \frac{(\alpha_t^*)^n \alpha_t^m}{\sqrt{n!m!}}.$$

[12] See Appendix A for details.

Let us then calculate for a later convenience the expectation value of $|\alpha_t|^{2n}$ in the stationary limit $t \to \infty$ using Eq. (3.22) in P-representation where $C = C_P = n_{th}$

$$\mathbb{E}\left[|\alpha_t|^{2n}\right] = \mathbb{E}\left[\left|\alpha_0 e^{-\left(i\omega+\frac{\gamma}{2}\right)t} + e^{-\frac{\gamma}{2}t}B_\theta\right|^{2n}\right] = e^{-\gamma n t}\mathbb{E}\left[\left|\alpha_0 e^{-i\omega t} + B_\theta\right|^{2n}\right]$$

$$\to e^{-\gamma n t}\mathbb{E}\left[|B_\theta|^{2n}\right] = e^{-n\gamma t} n!\theta^n = n! n_{th}^n (1 - e^{-\gamma t})^n \to n! n_{th}^n. \tag{3.23}$$

On the second row we employ the Gaussian property of the Wiener process for moments (3.8) to obtain $\mathbb{E}\left[|B_\theta|^{2n}\right] = n!\theta^n$. Since $\theta^n \propto e^{\gamma n t}$ the initial value α_0 vanishes in the limit $t \to \infty$. In the case $n = 1$ we obtain the same result as in Eq. (3.15). Note that the expectation values of $\alpha^m|\alpha|^{2n}$ are all zero in the stationary limit unless $m = 0$ due to the vanishing mean and the Gaussianity of B_θ.

Then, suppose that the initial state is a coherent state. In the stationary limit $t \to \infty$ using Eq. (3.23) the elements of the density matrix are

$$\begin{aligned}\rho_{nm} &= \mathbb{E}\left[e^{-|\alpha_t|^2}\frac{(\alpha_t^*)^n \alpha_t^m}{\sqrt{n!m!}}\right] = \sum_{k=0}^{\infty}\frac{(-1)^k}{k!\sqrt{n!m!}}\mathbb{E}\left[(\alpha_t^*)^n \alpha_t^m |\alpha_t|^{2k}\right] \\ &= \begin{cases} 0, & n \neq m \\ \sum\limits_{k=0}^{\infty}(-1)^k \frac{(n+k)!}{n!k!} n_{th}^{(n+k)}, & n = m \end{cases}\end{aligned}$$

It can be easily verified that $\rho_{nn} = \frac{1}{1+n_{th}}\left(\frac{1}{1+n_{th}}\right)^n$ which proves that the system thermalizes to the correct thermal state [12].

It is established that the formalism developed in the last section is equivalent to QME. However, there is a variable that is more readily obtained by using the phase space methods than the operator methods. This is the time evolution of a state's purity, defined as $\mathcal{P} = \mathrm{tr}\left[\hat{\rho}^2\right]$, for which one cannot obtain a differential equation with the QME. Using the P-representation

$$\begin{aligned}\mathrm{tr}\left[\hat{\rho}_t^2\right] &= \int \mathrm{d}^2\alpha_0\, \mathrm{d}^2\beta_0\, P(\alpha_0)P(\beta_0)|\langle\alpha_t|\beta_t\rangle|^2 \\ &= \int \mathrm{d}^2\alpha_0\, \mathrm{d}^2\beta_0\, P(\alpha_0)P(\beta_0)e^{-|\alpha_t-\beta_t|^2}.\end{aligned}$$

Let us suppose that initially the system is in a coherent state $|\alpha'\rangle$, i.e. $P(\alpha_0) = \delta(\alpha_0 - \alpha')$. By using the solution (3.22) the time evolution of

state's purity is obtained

$$\mathcal{P} = \mathbb{E}\left[\mathrm{tr}\left[\hat{\rho}_t^2\right]\right] = \mathbb{E}\left[e^{-e^{-\gamma t}\left|B_\theta^a - B_\theta^b\right|^2}\right] = \sum_{k=0}^{\infty} \frac{\left(-e^{-\gamma t}\right)^k}{k!} \mathbb{E}\left[\left|B_\theta^a - B_\theta^b\right|^{2k}\right]$$
$$= \sum_{k=0}^{\infty} \frac{\left(-e^{-\gamma t}\right)^k}{k!} k!(2\theta)^k = \frac{1}{1 + 2n_{th}(1 - e^{-\gamma t})}.$$

Here, a and b refer to independent Wiener processes in the solutions α_t and β_t. The expectation value of $\left|B_\theta^a - B_\theta^b\right|^{2k}$ can be calculated by using the fact that $B_\theta^a - B_\theta^b$ is also a Wiener process so the Gaussian property (3.8) holds and

$$\mathbb{E}\left[\left|B_\theta^a - B_\theta^b\right|^2\right] = \mathbb{E}\left[\left|B_\theta^a\right|^2\right] + \mathbb{E}\left[\left|B_\theta^b\right|^2\right] = 2\theta.$$

Also, the geometric series is formally identified in the last equality. The same result is derived in Ref. [30] albeit in a more general manner using Wigner–Weyl representation and QME which allows the analysis of squeezed states.

3.2 Spin systems — $\mathfrak{su}(2)$ algebra

Let us consider a spin system in a bosonic bath with a coupling term $\sum_k g_k\left(\hat{J}_+\hat{b}_k + \hat{J}_-\hat{b}_k^\dagger\right)$. As a physical setting one could think of e.g. an atom that interacts with light or a collection of molecules in an liquid solution modeled as a collection of bosonic modes [10, 12, 18] as mentioned in the introduction. The TDVP formalism can be used to find the collective dynamics of such systems in a certain j-subspace since

$$\sum_k \hat{J}_{z,k}, \qquad \sum_k \hat{J}_{+,k}, \quad \text{and} \quad \sum_k \hat{J}_{+,k}$$

also obey the $\mathfrak{su}(2)$ algebra [7].

Let us focus on three systems: First, consider a collection of non-interacting spins in a magnetic field. The Hamiltonian is in this case $H_S = \mu\vec{B}\cdot\hat{\vec{J}}$ where μ is the gyromagnetic ratio and B the magnetic field. The second case to be considered is a classically driven atom with two relevant electronic states would be described as $\hat{H}_S = \omega_a\hat{J}_z + \frac{\lambda}{2}\left(\hat{J}_+e^{-i\omega_L t} + \hat{J}_-e^{i\omega_L t}\right)$. Here, ω_a is the energy difference between two levels and ω_L the frequency of the optical

drive. By moving to the interaction frame of the optical drive[13], this can be reduced to $\hat{H}_S = \epsilon \hat{J}_z + \lambda \hat{J}_x$ with $\epsilon = \omega_a - \omega_L$ being the detuning [12]. The third case is superconducting qubits that can be described by the same Hamiltonian. They are currently studied extensively since they might be useful in the implementation of a physical quantum computer. At the time of writing, Martinis' group has been able to build a working quantum computer up to 9 qubits [31] but there are already plans to build up to 50 qubits. We won't concentrate on the physics of superconducting qubits but detailed descriptions can be found from e.g. [18, 32] and Girvin's lecture notes from the Les Houches summer school [33].

For now, let us keep the system Hamiltonian $\hat{H}_S$ arbitrary but suppose still that the environment is bosonic. Following similar steps as in the bosonic case we choose the SU(2) coherent states for the system and field coherent states for the environment. The total Lagrangian is

$$\begin{aligned}\mathcal{L} = ij\frac{\dot{\xi}\xi^* - \dot{\xi}^*\xi}{1+|\xi|^2} + \frac{i}{2}\sum_k (\dot{\beta}_k\beta_k^* - \dot{\beta}_k^*\beta_k) \\ - \langle \hat{H}_S \rangle - \sum_k \omega_k |\beta_k|^2 - \sum_k g_k \frac{2j}{1+|\xi|^2}(\xi^*\beta_k + \xi\beta_k^*).\end{aligned}$$

The derivation follows the same steps, except we set $g_k^2 = \frac{\gamma}{2j}\frac{D}{2\pi}$. We obtain the $\mathfrak{su}(2)$ phase space Langevin equation

$$\dot{\xi} = -i\frac{\left(1+|\xi|^2\right)^2}{2j}\partial_{\xi^*}\langle \hat{H}_S \rangle - \frac{\gamma}{2}\xi + \sqrt{\frac{\gamma}{2j}}\left(\alpha_{in} + \xi^2\alpha_{in}^*\right). \tag{3.24}$$

The different choice with respect to the bosonic case for the damping constant, i.e. the factor $\frac{1}{2j}$, is related to the fact that in the limit $j \to \infty$, the SU(2) coherent states $|j,\xi\rangle$ approach a field coherent state $|\alpha\rangle$ with $\alpha = \sqrt{2j}\xi$. This can be proven by using the Holstein–Primakoff realization (2.45) of $\mathfrak{su}(2)$.

The $\mathfrak{su}(2)$ phase space Langevin equation (3.24) looks very similar to the Weyl–Heisenberg one (3.4) except for the nonlinear term $\xi^2\alpha_{in}^*$. Despite the similarity, the dissipation term is problematic. This problem is apparent

[13]This can be done in TDVP by noting that $\{\hat{J}_z, \hat{J}_+ e^{-i\omega_L t}, \hat{J}_- e^{i\omega_L t}\}$ is in fact a realisation of $\mathfrak{su}(2)$ so that the generalized coherent state is $|j,\xi'\rangle = |j,\xi e^{i\omega_L t}\rangle$.

when the equation for $\langle \hat{J}_z \rangle$ is evaluated for $\hat{H}_S = \epsilon \hat{J}_z$

$$\partial_t \langle \hat{J}_z \rangle = -\frac{\gamma}{2j} \langle \hat{J}_+ \rangle \langle \hat{J}_- \rangle + \sqrt{\frac{\gamma}{2j}} (\langle \hat{J}_+ \rangle \alpha_{in} + \langle \hat{J}_- \rangle \alpha_{in}^*).$$

When compared to the QLE (2.48) for $\hat{J}_z$ (with $\hat{a} = \hat{J}_z$ and $\hat{c} = \hat{J}_-$) [29]

$$\partial_t \hat{J}_z = -\frac{\gamma}{4j} \{ \hat{J}_+, \hat{J}_- \} + \sqrt{\frac{\gamma}{2j}} \left(\hat{J}_+ \hat{b}_{in} + \hat{J}_- \hat{b}_{in}^\dagger \right)$$

we see that the dissipation term represents a mean-field approximation. This follows from the fact that $|j, \xi\rangle \left| \vec{\beta} \right\rangle$ is not a generalized coherent state for the total Hamiltonian. Also, in the case of the damped harmonic oscillator the Heisenberg equation of motion (2.46)–(2.47) are linear whereas in the spin case they are nonlinear. These two facts lead to a mean-field approximation at the level of the equations of motion which in turn affects the dissipation term.

3.2.1 Thermalization

The SU(2) equation (3.24) represents only an approximation to the dynamics of a spin system. However, there are two important limits in which the SU(2) equation coincides with known results. First, in the limit of large spins the SU(2) equation approaches the Weyl–Heisenberg equation (3.4). The spin QME (2.44) approaches similarly the bosonic QME (2.43) which was proved to be equivalent with the Weyl–Heisenberg equation. Second, it is known that without the coupling to the bath the TDVP equation is exact as long as the Hamiltonian is an element of $\mathfrak{su}(2)$ algebra.

Let us choose for definiteness the Hamiltonian $H_S = \epsilon \hat{J}_z + \lambda \hat{J}_x$ which can represent any of the three systems mentioned in the earlier section. Using Eqs. (2.18) and (3.24) we have

$$\dot{\xi} = -i\epsilon\xi - i\frac{\lambda}{2}\left(1 - \xi^2\right) - \frac{\gamma}{2}\xi + \sqrt{\frac{\gamma}{2j}}\left(\alpha_{in} + \xi^2 \alpha_{in}^*\right). \tag{3.25}$$

This equation seems not to be a trivially solvable SDE. As it is often the case, we must resort to either numerics or special cases and approximations. Numerical simulations will be discussed in the next section. In both cases we focus on the expectation values of $\hat{J}_z$ and $\hat{J}_z^2$ even though any quantity could be calculated using the SU(2) coherent states.

Analytically one can find the stationary value of $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ using the SU(2) equation (3.25) in P-representation. The simplest approach is to employ the corresponding Fokker–Planck equation. Therefore the connection between equations (3.18) and (3.17) is needed. First, a transformation must be made as the equation (3.25) is a Stratonovich SDE. It also seems helpful to write $\xi = e^{i\phi} \tan \frac{\theta}{2}$ with $\theta \in [0, \pi]$. By utilizing Itô's lemma (3.11) we obtain

$$\dot{\theta} = -\lambda \sin\phi - \frac{\gamma}{2}\left(\sin\theta - \frac{n_{th}}{j}\cot\theta\right) + \sqrt{\gamma\frac{n_{th}}{j}}\eta_\theta \tag{3.26}$$

$$\dot{\phi} = -\epsilon - \lambda \cot\theta \cos\phi + \sqrt{\gamma\frac{n_{th}}{j}}\cot(\theta)\eta_\phi \tag{3.27}$$

with $\eta_\theta = \cos(\phi)\eta_1 + \sin(\phi)\eta_2$ and $\eta_\phi = -\sin(\phi)\eta_1 + \cos(\phi)\eta_2$. The full calculation can be found in Appendix A.1. These noises can be treated as white noise since there is no correlation between $\phi(t)$ and $\eta_i(t)$ in the Itô picture. Thus, it is an orthogonal transformation on the noise which does not affect the diffusion matrix. This property does not hold for Stratonovich SDEs so using Itô calculus is essential [14].

Let us first consider a non-driven system, i.e. set $\lambda = 0$. In this case we can find the exact value value of $\langle \hat{J}_z \rangle$ by using the thermal density matrix (2.30) with $\hat{H}_S = \epsilon \hat{J}_z$

$$\langle \hat{J}_z \rangle_S = \frac{\mathrm{tr}\left[\hat{J}_z e^{-\beta \hat{H}_S}\right]}{\mathrm{tr}\left[e^{-\beta \hat{H}_S}\right]} = \frac{\sum_{k=-j}^{j} k e^{-k\beta\epsilon}}{\sum_{k=-j}^{j} e^{-k\beta\epsilon}} \tag{3.28}$$

where $\beta = \frac{1}{k_B T}$ which is related to the thermal population $n_{th} = \left(e^{\beta\epsilon} - 1\right)^{-1}$. The calculation is similar for $\langle \hat{J}_z^2 \rangle$, replacing $k \to k^2$ in the numerator.

The assumption $\lambda = 0$ provides a great simplification as the equations (3.26)–(3.27) fully decouple. The Fokker-Planck equation corresponding to the SDE (3.26) is

$$\partial_t P(\theta) = \frac{\gamma}{2}\partial_\theta\left[\left(\sin\theta - \frac{n_{th}}{j}\cot\theta\right)P(\theta)\right] + \frac{\gamma n_{th}}{2j}\partial_\theta^2 P(\theta). \tag{3.29}$$

The stationary distribution is found when the time derivative vanishes. By rearranging we obtain

$$\partial_\theta\left(\partial_\theta P(\theta) - \left[\cot\theta - \frac{j}{n_{th}}\sin\theta\right]P(\theta)\right) \equiv \partial_\theta J(\theta) = 0. \tag{3.30}$$

Therefore $J(\theta) = J$ is a constant. The function $J(\theta)$ is related to the so-called probability current [14]. Since $\theta \in [0, \pi]$ and $P(\theta)$ is normalized to unity we must require that $J(\theta)$ vanishes at the boundaries $\theta = 0$ and $\theta = \pi$ which in turn means that $J = 0$. Then

$$\partial_\theta \ln P(\theta) = \cot\theta - \frac{j}{n_{th}} \sin\theta, \tag{3.31}$$

implying that

$$P(\theta) = \frac{\frac{j}{n_{th}}}{2\sinh\left(\frac{j}{n_{th}}\right)} e^{\frac{j}{n_{th}}\cos\theta} \sin\theta, \tag{3.32}$$

where the prefactor follows from the normalization of P-functions.

With the stationary distribution any expectation value can now be calculated using Eq. (2.33). For instance, since $\langle \hat{J}_z \rangle = j\frac{|\xi|^2-1}{|\xi|^2+1} = -j\cos\theta$, the stationary expectation value of $\hat{J}_z$ is

$$\langle \hat{J}_z \rangle_S = -j \int_0^\pi P(\theta) \cos\theta \, \mathrm{d}\theta = n_{th} - j \coth\left(\frac{j}{n_{th}}\right) \tag{3.33}$$

by straightforward integration. In a similar manner we obtain for $\hat{J}_z^2$ (using Eq. (2.25))

$$\begin{aligned} \left\langle \hat{J}_z^2 \right\rangle_S &= \frac{j}{2} + j\left(j - \frac{1}{2}\right)\left[1 + 2\left(\frac{n_{th}}{j}\right)^2 - 2\frac{n_{th}}{j}\coth\left(\frac{j}{n_{th}}\right)\right] \\ &= j^2 + 2n_{th}\left(1 - \frac{1}{2j}\right)\langle \hat{J}_z \rangle_S . \end{aligned} \tag{3.34}$$

The stationary values of $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ from TDVP (3.33) and (3.34) are compared to the exact thermal values from the equation (3.28) in Figs. 3 and 4. The two bath populations are chosen so that they are relevant for superconducting qubits. This entails frequency scales from 1 GHz to 10 GHz and temperature around 20 mK [32], resulting roughly in $n_{th} \in \left[10^{-10}, 0.1\right]$. At very low bath populations the TDVP results are indistinguishable from the exact results. For $n_{th} = 10^{-4}$ the difference between the results is below 10^{-7} when $\langle \hat{J}_z \rangle \approx -1$. Some discrepancy is found at higher bath populations but the difference vanishes as j increases.

A peculiar property of the equation (3.26) is that in the limit $n_{th} = 0$, there is no more j dependence. In fact, the whole equation is simply $\dot{\theta} = -\frac{\gamma}{2}\sin\theta$

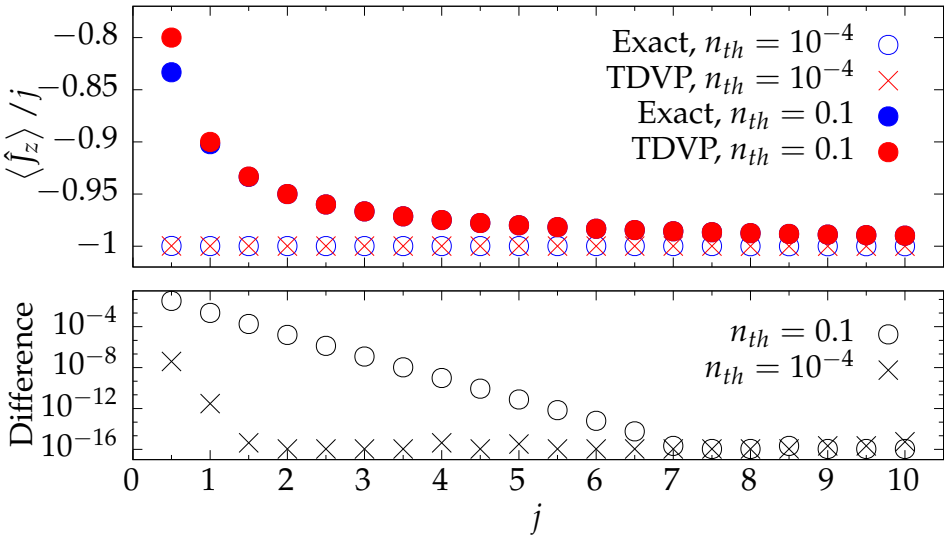


Figure 3: Stationary normalized values of $\langle \hat{J}_z \rangle$ calculated using the exact result (3.28) and the TDVP result (3.33) and their difference for two different bath populations. The differences near 10^{-16} seem to be limited by the numerical accuracy.

meaning that both $\theta = 0$ and $\theta = \pi$ are stationary solutions. This would correspond to spin-down and spin-up states, respectively. However, the P-function (3.32) approaches the delta function $\delta(\theta)$ which corresponds to a spin-down state. This is a fairly interesting contradiction which is probably caused by the improper handling of the limit $n_{th} \to 0$ since it is also a limit between an ordinary and stochastic differential equation. Using Wigner functions might avoid this problem since the mathematical 'transition' is missing.

The method of solving the stationary case shown in Eqs. (3.29) and (3.31) can be in principle used also if $\lambda \neq 0$ when one has to include in the Fokker–Planck equation terms related to ϕ. It is known as the method of potential conditions [14] as it leads to a gradient equation $\boldsymbol{\nabla} \ln P(\theta, \phi) = \vec{v}(\theta, \phi)$ where $\boldsymbol{\nabla} P = (\partial_\theta P, \partial_\phi P)^T$. A solution exists only if $\boldsymbol{\nabla} \times \vec{v} = 0$ since $\boldsymbol{\nabla} \times \boldsymbol{\nabla} \ln P = 0$, but unfortunately this is not the case discussed here. The method fails apparently since the probability currents similar to J in Eq. (3.30) do not vanish even if the periodicity of ϕ in $P(\theta, \phi)$ is taken into account.

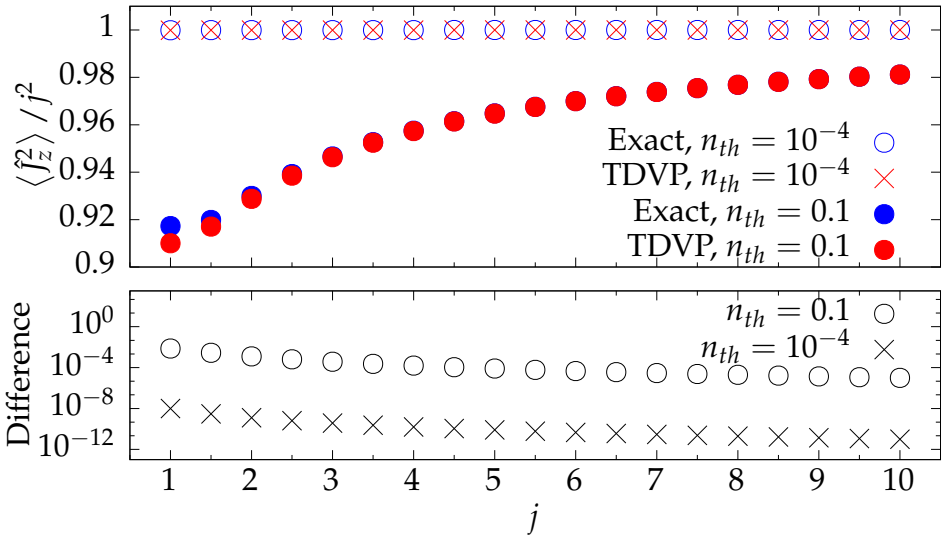


Figure 4: Stationary normalized values of $\langle \hat{j}_z^2 \rangle$ calculated using the exact resut and the TDVP result (3.34) and their difference for two different bath populations.

Let us then focus on a special case of $n_{th} = 0$ which corresponds to zero temperature. This assumption holds for resonance fluorescence of atomic systems since at optical wavelengths $\hbar\omega_a \gg k_B T$. Resonance fluorescence occurs when an atom is driven with a laser so that the frequency of the laser is near to the frequency associated with the energy difference of two electronic levels of the atom [12]. The atom is excited from its ground state by this process and then it can decay by releasing a photon. Note that the thermal population is evaluated at the atomic frequency ω_a rather than detuning ϵ which is the frequency in the interaction frame. Let us set $\epsilon = 0$ which corresponds driving the system exactly on resonance. If $n_{th} = 0$ Eqs. (3.26)–(3.27) are ordinary differential equations. There is no analytical solution available but the nature of the solution can be understood by analysing the fixed points of the system. That is, constant solutions of Eqs. (3.26)–(3.27) so that $\dot{\theta} = \dot{\phi} = 0$. The equations can now be rewritten as

$$\sin\phi = -\frac{\gamma}{2\lambda}\sin\theta$$
$$0 = \cot\theta\cos\phi.$$

There are multiple solutions depending on the value of $\frac{\gamma}{2\lambda}$. In the region $\frac{\gamma}{2\lambda} \leq 1$ the solution is $\theta = \frac{\pi}{2}$ and $\phi = \arcsin\left(-\frac{\gamma}{2\lambda}\right)$. When $\frac{\gamma}{2\lambda} \geq 1$, the

fixed points are $\phi = \frac{3\pi}{2}$, $\theta = \arcsin\left(\frac{2\lambda}{\gamma}\right)$ and $\theta = \frac{\pi}{2} + \arcsin\left(\frac{2\lambda}{\gamma}\right)$. Further investigations reveal that only $\theta = \arcsin\left(\frac{2\lambda}{\gamma}\right)$ is a stable fixed point to which every dynamical solution tends. This corresponds to the stationary value $\langle \hat{J}_z \rangle_S = -j\sqrt{1 - \frac{4\lambda^2}{\gamma^2}}$. When $\frac{\gamma}{2\lambda} < 1$ there are no such stable states so the solutions oscillate.

A similar analysis can be made by using the spin quantum master equation (2.44) for $j = \frac{1}{2}$. This is done for example in Ref. [12]. Let us see why this analysis can not be generalized to higher spins. We wish to derive differential equations for the expectation values of $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_\pm \rangle$. Since $\partial_t \langle \hat{J}_z \rangle = \mathrm{tr}\left[\hat{J}_z \dot{\hat{\rho}}\right]$ we can use the spin QME (2.44) with $\hat{H}_S = \lambda \hat{J}_x$ and $n_{th} = 0$, the commutation relations (2.4), and the trace property (2.29) to obtain

$$\partial_t \langle \hat{J}_z \rangle = -i\frac{\lambda}{2}\left(\langle \hat{J}_+ \rangle - \langle \hat{J}_- \rangle\right) - \frac{\gamma}{2j}\langle \hat{J}_+ \hat{J}_- \rangle$$
$$\partial_t \langle \hat{J}_+ \rangle = -i\lambda \langle \hat{J}_z \rangle + \frac{\gamma}{2j}\langle \hat{J}_+ \hat{J}_z \rangle .$$

The last terms in these equations are generally nonlinear and it is impossible to find a closed set of equations. However, if $j = \frac{1}{2}$ then all the operators can be expressed in a linear form. In this case $\hat{J}_+\hat{J}_- = \frac{1}{2} + \hat{J}_z$ and $\hat{J}_+\hat{J}_z = -\hat{J}_+$. Then, we can manipulate the equations to write a single second order equation

$$\left(\partial_t^2 + \frac{3}{2}\gamma\partial_t + \lambda^2 + \frac{\gamma^2}{2}\right)\langle \hat{J}_z \rangle = -\frac{\gamma^2}{4}.$$

We now find in a stark contradiction to TDVP that there is always a stable fixed point $\langle \hat{J}_z \rangle_S = -\frac{1}{2+4(\lambda/\gamma)^2}$. The solutions are damped oscillations when $\frac{\gamma}{\lambda} < 16$. This oscillation corresponds to fluorescence as the system relaxes after emitting a photon. In conclusion, the solutions obtained with TDVP and QME when $j = \frac{1}{2}$ differ greatly in their dynamical behaviour due to the nonlinearity of the underlying equations of motion.

3.2.2 Numerical simulation of a driven system

Numerical methods can be used to evaluate Eqs. (3.26)–(3.27). Since SDEs are used also in other contexts than physics there are many methods available. For the scope of this work we have chosen to implement the simplest

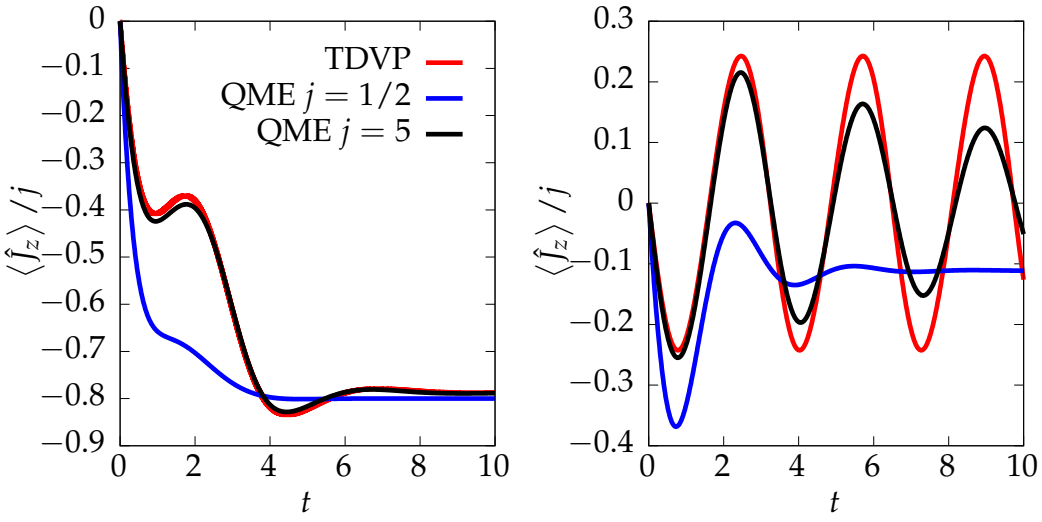
algorithm which is the so-called Euler–Maruyama algorithm [14]. Details can be found in Appendix B.1.

The spin QME (2.44) is straightforward to simulate. Since the density matrices are of finite dimension one can treat the QME as a matrix-valued ordinary differential equation. Then, one must solve a matrix representation for spin operators in a general dimension. The result is shown in Eq. (B.1). The implementation in Mathematica can also be found in Appendix B.2.

The dynamics of the resonance fluorescence is graphed in Fig. 5 by using Eqs. (3.26)–(3.27) and QME. The numerical parameters in the Fig. 5a are chosen roughly according to experimental parameters from Ref. [34]. The system is driven off-resonance in this case. Due to the short lifetime of the excited state, $\gamma = 289\,\mathrm{MHz}$ is twice as large as the detuning ϵ. However, this number is very small compared to the atomic frequency ω_a since it is in optical regime, i.e. of the order 100 THz. Therefore, the quantum master equation should apply [10]. Again, it can be seen that for $j = 5$ that the methods agree considerably well but not for $j = \frac{1}{2}$. In the figure 5b the system is driven on-resonance. The difference of the dynamics, as discussed at the end of the section 3.2.1, is quite notable as the QME result oscillates with a strong damping where as the TDVP result is not damped at all. However, TDVP and QME produce coinciding results for short timespans. Interestingly, the higher the spin number j, the more pronounced oscillations are. It is reasonable to assume that in the limit $j \to \infty$ the non-damped oscillation is obtained.

Next we focus on superconductive qubits for which the dissipation rate is small. In fact, when the transition frequency is of the order 10 GHz, the dissipation rate is in the regime $\gamma \approx 10\,\mathrm{MHz}$ or even smaller [32]. The simulations of QME and TDVP for typical parameters in such a system can be seen in Fig. 6. For small dissipation rates γ the simulations of QME and TDVP agree well because the TDVP equations are exact without the coupling to the bath. The effects of dissipation are made more pronounced by using γ that is larger by a factor of 100 in Fig. 7. This also pronounces the discrepancy between the QME and TDVP simulations. Qualitatively, one can see comparing Figs. 7a and 7b that the difference is inversely proportional to j, i.e. the larger j, the smaller difference, and comparing Figs. 7a and 7c that n_{th} does not seem to affect it at all. Fig. 7d shows how the dissipation rate γ affects the dynamics of $\langle \hat{J}_z^2 \rangle$ which is very intricate compared to the dynamics shown in Fig. 6.

The complexity of the numerical algorithm to evaluate the quantum master equation grows at least quadratically in j since the size of the corresponding Hilbert space is $(2j+1)^2$. This is in stark contrast with the evaluation of phase space Langevin equations for which j is an external parameter. In fact, since the noise term scales with $\sqrt{\frac{n_{th}}{j}}$ it can be argued that a smaller statistical sample can be taken for larger j if the statistical error is kept fixed. Therefore, larger the j the better in terms of efficiency. If $\frac{n_{th}}{j} \approx 0$, only a single evaluation is needed in the P-representation.



(a) $\gamma/2 = \lambda = \epsilon = 1$ *(b)* $\epsilon = 0, \gamma = \lambda/2 = 1$

Figure 5: Comparison of the dynamics of driven system both off- and on-resonance ($\epsilon = 1$ and $\epsilon = 0$ respectively) when $n_{th} = 0$ with TDVP and master equation approach. Note that TDVP equations do not depend on j.

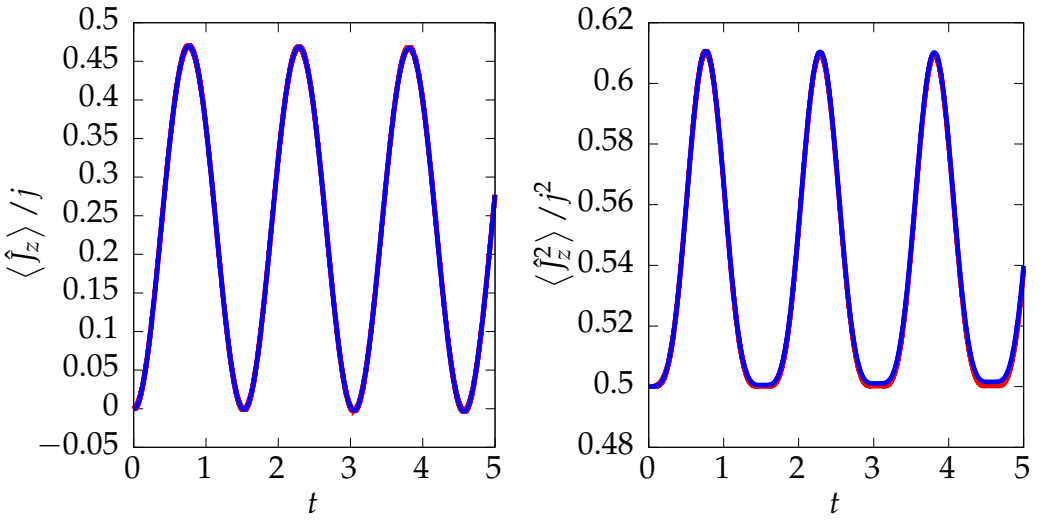
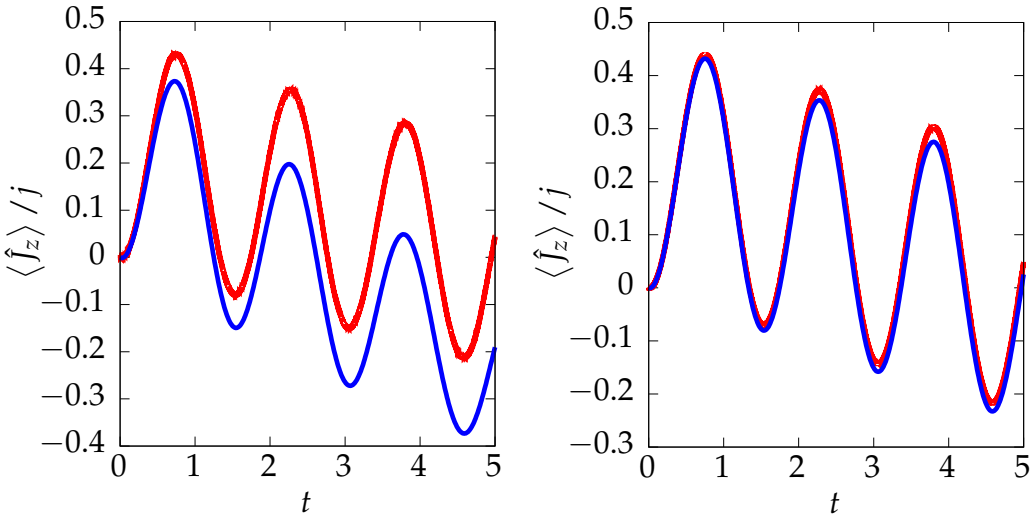
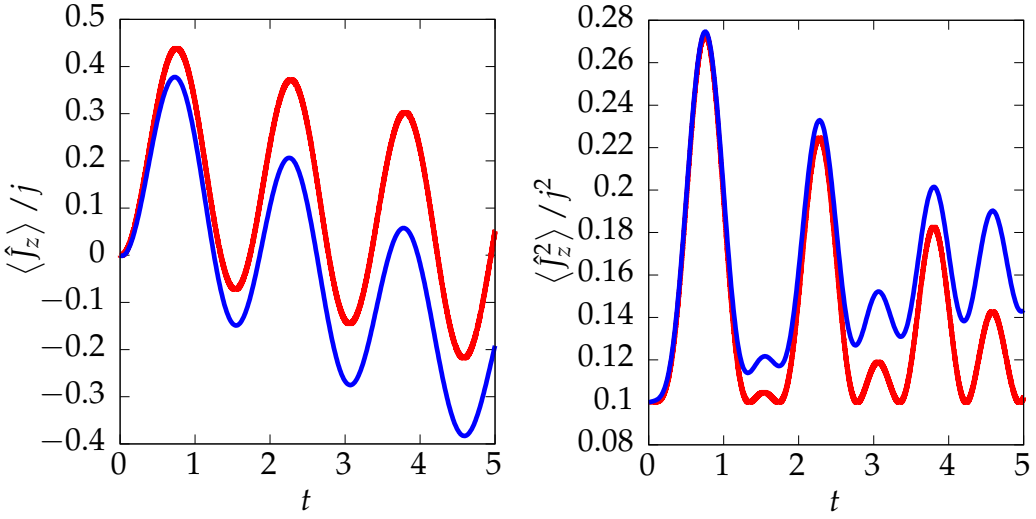


Figure 6: Dynamics of $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ in a spin system with $j = 1$ and $n_{th} = 0.1$. Blue is evaluated using QME and red using TDVP. In every plot $\epsilon = 4, \lambda = 1$, and $\gamma = 0.001$. The initial state is chosen so that $\langle \hat{J}_x \rangle = j$. TDVP is averaged over 1000 realisations with a time step of 10^{-4}.



(a) $n_{th} = 0.1, j = \frac{1}{2}$.

(b) $n_{th} = 0.1, j = 5$.



(c) $n_{th} = 10^{-10}, j = \frac{1}{2}$.

(d) $n_{th} = 10^{-10}, j = 5$.

Figure 7: Dynamics of $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ in different spin systems. Blue is evaluated using QME and red using TDVP. In every plot $\epsilon = 4, \lambda = 1$, and $\gamma = 0.1$. The initial state is chosen so that $\langle \hat{J}_x \rangle = j$. TDVP is averaged over 1000 realisations with a time step of 10^{-4}.

4 Conclusions

In this thesis we have studied the phase space theory of quantum mechanics. We have focused in particular on the dynamical aspects of the phase space theory. These concepts have been used to construct a phase space Langevin equation that has been used to analyse certain open quantum systems.

In the case of the damped harmonic oscillator we obtain exact equivalence with the bosonic quantum master equation in the limit of white noise. The mathematical connection has been made e.g. in Ref. [12] but the TDVP method studied here gives a physical justification for this. Several calculational examples are given; one notable example being the evolution of the system state purity.

The phase space Langevin equation for spin systems proved not to be exact. However, it works well as an approximation in many cases. Qualitatively, the approximation is the better the lower the dissipation rate and temperature is and the larger the spin number is. As a concrete example this was shown with parameters that describe superconducting qubits. However, one should be aware of systems that exhibit parametric transitions where the dynamical properties of the system can change with a change in parameters. This can be observed in the case of resonance fluorescence.

There are many types of systems that have not been discussed in the literature for which the TDVP method would work straightforwardly. The only limitation is in principle that the generalized coherent states for the closed system exists. This rules out some interesting systems since the generalized coherent states of, for instance, optomechanical or Jaynes–Cummings Hamiltonian, which describe light-matter interaction, have not been found. However, in these cases a mean-field approximation might be possible also for the system.

The phase space approach to quantum mechanics, in the sense described in this thesis, provides dynamical equations which are straightforward and efficient to simulate numerically. Even in the case of large or infinite Hilbert space, as is the case with Weyl–Heisenberg algebra, only a single complex equation is needed to determine the dynamics. For the SU(2) case, the spin quantum number j enters the equations only as an parameter. Due to the stochastic nature of the phase space Langevin equations, however, a

statistical sample is needed.

There are many possible directions that can be explored along the lines discussed here. One could add to the total Hamiltonian a phase decaying term (e.g. $\hat{J}_z(\hat{b}_k + \hat{b}_k^\dagger)$) and try to analyze the decoherence times T_1 and T_2. As earlier noted, of theoretical interest might be to investigate non-Markovianity, especially initially correlated states. Also, it would be mathematically easy to set a finite autocorrelation time instead of white noise which is relevant if the bath cannot be assumed to be infinite. In addition to these purely theoretical interests, one could try to apply this formalism to different physical setups.

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A Stochastic differential equations

This appendix is mostly based on the books by Gardiner [14] and van Kampen [13]. The main results related to SDEs, such as Itô's lemma, can be found in the main text of the thesis so the role of this appendix is to provide some additional information that can help to understand for instance the Itô–Stratonovich dilemma.

A general first order SDE system reads

$$\dot{x}(t) = A(x,t) + B(x,t)\eta(t) \tag{A.1}$$

where $\eta(t)$ is a stochastic process. It is an extension of the concept of a stochastic variable Y whose values are associated with a probability density function P_Y so that $\eta(t) \equiv \eta_t = f(Y,t)$. The expectation value or the average of η is determined by

$$\mathbb{E}[\eta_t] = \int P_X(x)\eta_t(x)\,\mathrm{d}x\,.$$

Here $\eta_t(y) = f(y,t)$ refers to a realisation of the stochastic process. Note that we can always assume that $\mathbb{E}[\eta_t] = 0$ since if $\mathbb{E}[\eta_t] \neq 0$ then we can replace $\eta_t \to \eta_t - \mathbb{E}[\eta_t]$ and $A(x,t) \to A(x,t) + B(x,t)\mathbb{E}[\eta_t]$. Generally, x, A, and η are vectors and B is a matrix. Let us however mainly discuss the one-dimensional case without loss of generality. Let us denote for brevity $x(t) = x_t$, $A(x,t) = A(x_t)$ and $B(x,t) = B(x_t)$.

Equation (A.1) is not well defined. A somewhat intuitive explanation for this is that there are multiple ways to evaluate the term $B(x_t)\eta_t$. For instance, in a single and very small time step Δt

$$x_{t+\Delta t} - x_t = A(x_t)\Delta t + B(x_\tau)\int_t^{t+\Delta t} \eta_{t'}\,\mathrm{d}t'$$

with $\tau \in [t, t+\Delta t]$. Now, the choice of τ is important. If $\tau = t$ it seems clear that the value of $B(x_t)$ is independent of the stochastic variable. Therefore the expectation value of x follows deterministic motion

$$\mathbb{E}[x_{t+\Delta t}] = \mathbb{E}[x_t + A(x_t)\Delta t].$$

If $\tau = t + \Delta t$ this interpretation is does not work as one would assume that the value $B(x_{t+\Delta t})$ is affected by the stochastic integral. This can be remedied by considering the corresponding integral equation

$$x_{t_1} - x_{t_0} = \int_{t_0}^{t_1} A(x_t)\,\mathrm{d}t + \int_{t_0}^{t_1} B(x_t)\eta_t\,\mathrm{d}t$$

and providing the interpretation of the stochastic integral.

The theory of SDEs is formulated often for white noise meaning that η is a Gaussian process with a vanishing mean and autocorrelation function $\mathbb{E}[\eta_{t_1}\eta_{t_2}] = \delta(t_1 - t_2)$. The delta correlation represents an idealisation that the noise varies very rapidly and its effects are instantaneous and uncorrelated. Higher moments can be obtained by using the Gaussian property mentioned in Eq. (3.8).

The integral $W_t = \int_0^t \eta_\tau \, \mathrm{d}\tau$ plays an important role in the mathematical formulation of the stochastic integral and SDEs. One can straightforwardly find that $\mathbb{E}[W_t] = 0$ and that W_t is also a Gaussian process using the properties of η. Its autocorrelation function is derived by a short calculation

$$\begin{aligned}\mathbb{E}[W_{t_1}W_{t_2}] &= \int_0^{t_1}\int_0^{t_2} \mathbb{E}[\eta_{\tau_1}\eta_{\tau_2}] \, \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \\ &= \int_0^{t_1}\int_0^{t_2} \delta(\tau_1 - \tau_2) \, \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 = \min(t_1, t_2). \end{aligned} \tag{A.2}$$

The integral process W is the *Wiener process* which has been used, for instance, to describe the position of Brownian particle. The Wiener process is a continuous Markov process which, even though defined as an integral, is not differentiable. This again shows the ill-defined nature of SDE (A.1). It can also be proven that if instead of the Gaussianity of white noise one assumes the continuity of the Wiener process, then η must be a Gaussian process [14, ch. 4]. Especially in mathematical context the notation $\mathrm{d}W_t = \eta_t \, \mathrm{d}t$ is used as it represents the stochastic integral in a sensible manner.

There are two popular choices for the definition of stochastic integral. These are called Itô and Stratonovich integrals. They are both defined as a kind of stochastic Riemann–Stieltjes integrals. That is,

$$\int_{t_0}^{t_1} B(x_t) \, \mathrm{d}W_t = \lim_{n\to\infty} \sum_i^n B(x_{\tau_i}) \Delta W_i$$

where $\Delta W_i = W_{t_i} - W_{t_{i-1}}$. The choice $\tau_i = t_{i-1}$ corresponds to Itô integral. The Stratonovich integral is obtained by replacing x_{τ_i} with $\frac{1}{2}\left(x_{t_i} + x_{t_{i-1}}\right)$.

The Itô integral's definition is mathematically very simple to use and some general results are easy to find. In context of a SDE we can suppose that $B(x_{t_1})$ and W_{t_2} are statistically independent when $t_1 \leq t_2$. That is, we

suppose that there is a causality in the sense that the value of the Wigner process in the future (t_2) cannot affect the past value of x_{t_1}. This makes $B(x)$ a non-anticipating function. Now, we find that

$$\mathbb{E}\left[B(x_{t_{i-1}})\Delta W_i\right] = \mathbb{E}\left[B(x_{t_{i-1}})\right]\mathbb{E}[\Delta W_i] = 0 \tag{A.3}$$

since $\mathbb{E}[\Delta W_i] = 0$. This result implies that the mean of an Itô integral vanishes. The second moment of an Itô integral follows an equally simple formula

$$\begin{aligned}\mathbb{E}\left[\left(\int_{t_i}^{t_f} B(x_t)\,\mathrm{d}W_t\right)^2\right] &= \lim_{n\to\infty}\sum_{i,j}^{n}\mathbb{E}\left[B_iB_j\Delta W_i\Delta W_k\right] \\ &= \lim_{n\to\infty}\left[\sum_{i}^{n}\mathbb{E}\left[B_i^2\Delta W_i^2\right] + \sum_{i\neq j}^{n}\mathbb{E}\left[B_iB_j\Delta W_i\Delta W_j\right]\right] \\ &= \lim_{n\to\infty}\sum_{i}^{n}B_i^2(t_i - t_{i-1}) = \int_{t_i}^{t_f} B(x_t)^2\,\mathrm{d}t\,.\end{aligned}$$

In this calculation we denoted $B_i = B(x_{t_i})$. The third equality follows from the same argument that was used in Eq. (A.3), that is if $i > j$ then ΔW_i is independent of $B_iB_j\Delta W_j$, and $\mathbb{E}\left[\Delta W_i^2\right] = t_i - t_{i-1}$ follows from Eq. (A.2). This can be transcribed to a formal rule $(\mathrm{d}W_t)^2 = \mathrm{d}t$ when using a shorthand notation where the integral signs are dropped. In higher dimensions we have $\mathbb{E}\left[\eta_{i,t_1}\eta_{j,t_2}\right] = \delta_{ij}\delta(t_1 - t_2)$ which leads to $\left(\mathrm{d}W_{i,t}\,\mathrm{d}W_{j,t}\right)^2 = \delta_{ij}\,\mathrm{d}t$. Using this rule and the Taylor expansion we obtain the Itô's lemma (3.11) when higher order terms, e.g. $\mathrm{d}t^2$ and $\mathrm{d}t\,\mathrm{d}W_t$, are dropped.

The Stratonovich integrals do not possess such a simple qualities. For instance, in the evaluation of the average of a Stratonovich integral we have

$$\mathbb{E}\left[B\left(\frac{1}{2}\left[x_{t_i} + x_{t_{i-1}}\right]\right)\left(W_{t_i} - W_{t_{i-1}}\right)\right].$$

The different terms here are not independent since the value of $W_{t_{i-1}}$ can affect the value of x_{t_i}. Therefore, there is a correlation and so the average does not generally vanish. Due to this reason they are somewhat impractical to use.

Lastly, we discuss deterministic time change in an Itô integral. It is essentially a change of variables in a stochastic integral. Let $f > 0$ be a integrable

deterministic function of time. Then it holds that

$$\mathbb{E}\left[\left[\int_{t_0}^{t_1}\sqrt{f(t)}\,\mathrm{d}W_t\right]^2\right] = \int_{t_0}^{t_1} f(t)\,\mathrm{d}t = F(t_1) - F(t_0)$$
$$= \mathbb{E}\left[\left[\int_{F(t_0)}^{F(t_1)}\mathrm{d}W_F\right]^2\right]$$

where F is the integral function of f and the subscripts of stochastic processes refer to their variance. This is enough to prove that

$$\sqrt{f(t)}\,\mathrm{d}W_t = \mathrm{d}W_F$$

due to the vanishing mean and Gaussianity of Wiener process. Scaling with a constant is a special case of this formula since $F = \int c\,\mathrm{d}t = ct$. The substitution made in the main text is now easy: $\sqrt{f(t)} = \sqrt{\gamma C}e^{\frac{\gamma}{2}t}$ so the time change is obtained by an integral

$$F(t) = \theta = \gamma C\int_0^t e^{\gamma t'}\,\mathrm{d}t' = C(e^{\gamma t} - 1).$$

A.1 Example about Itô's lemma — polar transformation

We now show explicitly the steps between Eq. (3.25) and Eqs. (3.26)–(3.27). First, we write the equation (3.25) in terms of independent Wiener processes. Also, we separete the real and imaginary parts of ξ and write $\xi = x + iy$. The SDEs are

$$\begin{aligned}\mathrm{d}\begin{pmatrix}x\\y\end{pmatrix} =& \epsilon\begin{pmatrix}y\\-x\end{pmatrix}\mathrm{d}t + \frac{\lambda}{2}\begin{pmatrix}-2xy\\x^2-y^2-1\end{pmatrix}\mathrm{d}t - \frac{\gamma}{2}\begin{pmatrix}x\\y\end{pmatrix}\mathrm{d}t\\ &+\sqrt{\frac{\gamma n_{th}}{4j}}\begin{pmatrix}x^2-y^2+1 & 2xy\\ 2xy & -x^2+y^2+1\end{pmatrix}\begin{pmatrix}\mathrm{d}W_1\\\mathrm{d}W_2\end{pmatrix}\end{aligned} \tag{A.4}$$

from which A and B of the general formula given in Eq. (3.10) can be inferred.

To apply the polar transformation properly as explained in the main text we must first have an Itô SDE. We thus utilize the connection between Stratonovich SDE (3.10) and Itô SDE (3.12). The relevant transformation

terms are

$$\frac{1}{2}\sum_{j,k=1}^{2} B_{kj}\partial_k B_{1j} = \frac{\gamma n_{th}}{2j}x, \quad \text{and} \quad \frac{1}{2}\sum_{j,k=1}^{2} B_{kj}\partial_k B_{2j} = \frac{\gamma n_{th}}{2j}y.$$

The effect of the transformation is simply $\gamma \to \gamma\left(1 - \frac{n_{th}}{j}\right)$ in the first row of Eq. (A.4).

We choose to write the polar form of $\xi = x + iy$ as $\xi = e^{i\phi}\tan(\theta/2)$ where $\phi \in [0, 2\pi]$ and $\theta = [0, \pi]$. Now we will work to find the Itô equations in terms of these polar parameters θ and ϕ. Inverting the polar form we have in terms of x and y that $\theta = 2\arctan\left(\sqrt{x^2+y^2}\right)$ and $\phi = \arctan(y/x)$. At this point, only simple calculus is needed. For the gradients of this transformation reads

$$\boldsymbol{\nabla}\theta = \frac{2}{(|\xi|^2+1)|\xi|}\begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \boldsymbol{\nabla}\phi = \frac{1}{|\xi|^2}\begin{pmatrix} -y \\ x \end{pmatrix}.$$

The Hessian matrices are

$$H_\theta = \frac{2}{|\xi|^3(1+|\xi|^2)^2}\begin{pmatrix} y^4+y^2-x^2y^2-2x^4 & xy(3|\xi|^2+1) \\ xy(3|\xi|^2+1) & x^4+x^2-x^2y^2-2y^4 \end{pmatrix}$$

$$H_\phi = \frac{1}{|\xi|^4}\begin{pmatrix} 2xy & y^2-x^2 \\ y^2-x^2 & -2xy \end{pmatrix}.$$

Now the Itô's lemma (3.11) can be used for $\theta(x,y)$ and $\phi(x,y)$

$$\begin{aligned} \mathrm{d}\theta = &-\lambda\frac{y}{|\xi|}\,\mathrm{d}t - \gamma\left[\frac{|\xi|}{1+|\xi|^2} + \frac{n_{th}}{2j}\frac{|\xi|^4-1}{2|\xi|(1+|\xi|^2)}\right]\mathrm{d}t \\ &+ \sqrt{\frac{\gamma n_{th}}{j}}\left(\frac{x}{|\xi|}\,\mathrm{d}W_1 + \frac{y}{|\xi|}\,\mathrm{d}W_2\right) \\ \mathrm{d}\phi = &\left[-\epsilon + \frac{\lambda}{2}\frac{x}{|\xi|}\left(|\xi| - \frac{1}{|\xi|}\right)\right]\mathrm{d}t \\ &+ \left(|\xi| - \frac{1}{|\xi|}\right)\sqrt{\frac{\gamma n_{th}}{4j}}\left(\frac{y}{|\xi|}\,\mathrm{d}W_1 - \frac{x}{|\xi|}\,\mathrm{d}W_2\right) \end{aligned}$$

We arrive at Eqs. (3.26)–(3.27) by utilising $x = \tan\left(\frac{\theta}{2}\right)\cos\phi, y = \tan\left(\frac{\theta}{2}\right)\sin\phi$ and a set of trigonometric identities, e.g.

$$\frac{1}{2}\left(\tan\left(\frac{\theta}{2}\right) - \cot\left(\frac{\theta}{2}\right)\right) = -\cot\theta \quad \text{and} \quad \frac{\tan\left(\frac{\theta}{2}\right)}{1+\tan^2\left(\frac{\theta}{2}\right)} = \frac{1}{2}\sin\theta.$$

B Numerical methods

B.1 Simulation of SDEs

Numerical simulation of SDEs is a large field and there are many methods. However, as far as I understand, there are not as many resources available but MATLAB and Mathematica do contain some methods. Fortunately, the most simple algorithm called the Euler–Maruyama algorithm is very straightforward to construct. I chose to implement it in MATLAB. Suppose one wants to simulate the Itô SDE $\dot{x}_t = A(x_t) + B(x_t)\,\mathrm{d}W$. The steps of the algorithm [29] are:

1. Choose initial conditions for x, draw from initial distribution if necessary.
2. Time propagation is calculated as $x_{t+dt} = x_t + A(x_t)dt + B(x_t)\Delta W$ where $\Delta W \sim \sqrt{dt}N(0,1)$. Here, $N(0,1)$ is the standard normal distribution with a vanishing mean and unity variance so that ΔW represents white noise.
3. Calculate relevant observables and gather enough statistics for averaging.

The only difference to the Euler algorithm for ordinary differential equations (ODE) is the noise term $B(x_t)\Delta W$. In general, one can use the same method even for vector-valued equations.

Compared to simulation of ODEs a major difference is numerical stability related to the noise term. This issue is very relevant: in fact, the SU(2) phase-space Langevin equation (3.25) could not be straightforwardly simulated. The stability problems are apparently caused by the nonlinear stochastic term $\xi^2\beta^*_{in}$.

The equations (3.26) and (3.27) are more numerically stable. There is a problem with the fact that θ should range between $[0,\pi]$. It is possible for the noise to set the value of θ negative. A small numerical error is introduced when this is prohibited. It effectively correlates the noise to the state of the system which means that the noise is not truly white. This happens however very rarely when the variance of the noise is small, i.e. n_{th}/j is small.

B.2 Simulation of QME with Mathematica

To simulate the spin QME (2.44) the matrix representations of spin operators, denoted here by $S_z, S_\pm$, must be solved. One possible representation is

$$[S_z]_{nm} = \delta_{n,m}(j+1-n), \qquad [S_+]_{nm} = \delta_{n,m-1}\sqrt{n(2j+1-n)}. \tag{B.1}$$

where $n, m \in \{1, \ldots, 2j+1\}$ and naturally $S_- = S_+^T$. In this representation, the eigenstate of J_z with eigenvalue j is the vector $(1, 0, \ldots 0)^T$. It is easy to check that these indeed fulfill the commutation relations of $\mathfrak{su}(2)$ algebra.

The simulation of QME (2.44) with $\hat{H} = \epsilon \hat{J}_z + \lambda \hat{J}_x$ can be implemented by the following Mathematica code (note that $g = \gamma$, $e1 = \epsilon, l1 = \lambda$ in the code)

```
(*Definitions of the spin matrices*)
sz[j_] := Table[KroneckerDelta[n, m] (j + 1 - n),
          {n, 1, 2 j + 1}, {m, 1, 2 j + 1}];
sp[j_] := Table[KroneckerDelta[n, m - 1] Sqrt[n (2 j + 1 - n)],
          {n, 1, 2 j + 1}, {m, 1, 2 j + 1}];
sm[s_] := Transpose[sp[s]];
sx[s_] := 1/2 (sp[s] + sm[s]);

(*Constants*)
tmax = 10;
g = 0.1;
e1 = 3;
l1 = 0.5;
(*RHS of QME*)
rhs[r_?MatrixQ, j_, Nth_] := -I e1 (sz[j].r - r.sz[j]) -
  I l1 (sx[j].r - r.sx[j]) + (g/(4 j)) (Nth +
     1) (2 sm[j].r.sp[j] - (sp[j].sm[j].r +
       r.sp[j].sm[j])) + (g/(4 j)) Nth (2 sp[j].r.sm[
       j] - (sm[j].sp[j].r + r.sm[j].sp[j]))
(*Initial condition, Sx = j now*)
tempv[k_] := Table[Sqrt[Binomial[2 k, n - 1]], {n, 1, 2 k + 1}];
init[k_] := Outer[Times, tempv[k], tempv[k]]/Norm[tempv[k]]^2;
sol[j_, Nth_] :=
  NDSolve[{rho'[t] == rhs[rho[t], j, Nth], rho[0] == init[j]},
   rho, {t, 0, tmax}];
(*Plotting the exp. value of Jz when j=1, nth = 2*)
Plot[{Evaluate[Tr[rho[t].sz[1]] /. sol[1, 2]], {t, 0, tmax}]
```