A stochastic approach to open quantum systems

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Received 8 December 2011, in final form 20 April 2012
Published 20 June 2012
Online at stacks.iop.org/JPhysCM/24/273201

Abstract
Stochastic methods are ubiquitous to a variety of fields, ranging from physics to economics and mathematics. In many cases, in the investigation of natural processes, stochasticity arises every time one considers the dynamics of a system in contact with a somewhat bigger system, an environment with which it is considered in thermal equilibrium. Any small fluctuation of the environment has some random effect on the system. In physics, stochastic methods have been applied to the investigation of phase transitions, thermal and electrical noise, thermal relaxation, quantum information, Brownian motion and so on.

In this review, we will focus on the so-called stochastic Schrödinger equation. This is useful as a starting point to investigate the dynamics of open quantum systems capable of exchanging energy and momentum with an external environment. We discuss in some detail the general derivation of a stochastic Schrödinger equation and some of its recent applications to spin thermal transport, thermal relaxation, and Bose–Einstein condensation. We thoroughly discuss the advantages of this formalism with respect to the more common approach in terms of the reduced density matrix. The applications discussed here constitute only a few examples of a much wider range of applicability.

(Some figures may appear in colour only in the online journal)
1. Introduction

In the scientific investigation of a natural system, usually the first step of the modelling process is to consider the system as closed and isolated. The system then evolves following its natural laws. The direct observation of the system—our experience—helps us in identifying the natural laws that many systems obey. An abstraction process allows us to formulate a coherent set of principles we believe are valid for a wide class of physical systems and we therefore create a theory [1]. However, from the same experience we know that no system is isolated or closed. For as small a scale as we can think of, there is always some leakage or coupling, nor forgetting the observation process, which itself does not allow for a complete decoupling of the dynamics of the system from the external environment. One of the major challenges of theoretical physical modelling has been to investigate this coupling and its effects on the ‘natural’ system. This situation is even more striking for a quantum mechanical system. Here, the interaction of the quantum system with an external device can have dramatic effects that are neither adiabatic nor small. A textbook example is the measurement process: we might consider the coupling between the quantum mechanical system and the measurement tool to be as small as possible, but the effects on the dynamics can be large enough so as to completely change the state of the quantum system. This issue is so fundamental that it is in fact one of the distinguishing factors between classical and quantum mechanical theory.

If this is the situation, the investigation of real quantum systems might appear hopeless: the coupling with an external environment will destroy any information we have on the system itself, replacing it with some kind of forced dynamics. However, we have to realize that on many occasions the coupling between the system and—for example—a thermal bath has some random nature. From this point of view, it appears natural, in order to describe the dynamics of our quantum mechanical system coupled to an external environment, to use a stochastic approach that will give some ‘average behaviour’. An example from classical mechanics is Brownian motion, where a large particle in a liquid is hit multiple times by the smaller particles forming the liquid. For this reason, the large particle appears to be ‘suspended’ in the liquid. At first glance it seems to be stationary, but a closer look reveals that it is in constant random motion. The investigation of this motion led Langevin to search for an equation of motion for the large particles following the result obtained by Einstein [2]: Langevin modelled the force from the liquid particles as a small stochastic force with zero mean and with certain correlation properties, related to the temperature of the liquid [3]. The success of the theory essentially opened the field of stochastic equations. Another interesting aspect of the Langevin work must be pointed out. Normally, the force that determines the dynamics in the Newton equation depends solely on the position of all the particles forming the system. If this is the case, we usually say that the system is ‘closed’ and the dynamics is solely determined by the initial conditions. There is a general consensus that, enlarging the system under investigation, one in principle could ‘close’ the equation of motion and obtain a force that is only a function of the position of all the particles in the system and the environment. It is clear, however, that in many cases, this is not what we want to do. On the one hand, the number of degrees of freedom is so large as to make any attempt at solving the problem beyond hope, while on the other hand we deal with a large amount of information that is essentially useless for describing the dynamics we are interested in. Again we can revert to the classical Brownian motion for a simple example: to close the equation of motion we need to include the dynamics of all the particles in the liquid; certainly a large number of extra degrees of freedom. Langevin was able to ‘fold’ these extra degrees of freedom into the stochastic term in his effective equation of motion. Further developments have established a few ‘standard’ ways to perform this folding while nonetheless trying to maintain the important features of the liquid dynamics.

In describing the dynamics of a quantum mechanical system coupled to an external environment we will follow a similar approach. Our starting point will be the Schrödinger equation for the system and the environment. We will then operate with a selection of the relevant degrees of freedom—obviously a utterly arbitrary step, especially if the system and the environment are made of the same interacting particles—and integrate out those that are deemed irrelevant. In this way, we obtain an effective Schrödinger equation, which will be stochastic in nature, for the ‘state’ of the system. The theory we will be developing in this way is similar to the formalism for the density matrix. There one usually, starting from the von Neumann equation for the total density matrix, derives an equation of motion for a reduced density matrix, a master equation that contains the physical information of the subsystem of interest. We will show how it is possible to derive such an equation of motion for the reduced density matrix from the stochastic Schrödinger equation. For this reason, the latter has been seen as the unravelling of a master equation.

In this review we will concentrate on stochastic Schrödinger equations that simulate the average behaviour of a variety of condensed matter systems interacting with their environments. In doing so, we will build an ensemble of states and to obtain any physical quantity we will average over this ensemble. For this reason, we do not require that a single ‘state’ of the system describes a physical quantum trajectory: for example, the state might be not normalized at each instance of time, and moreover the time evolution might change the normalization. On the other hand, in the quantum theory of measurement, the case where the bath is under continuous observation with some type of measurement device has been investigated [4, 5]. This analysis leads to stochastic Schrödinger equations whose solutions are single system trajectories, so-called ‘true’ quantum trajectories [5]. The theory is of great importance for designing feedback control on open quantum systems [6], to exploit the localization property to reduce the number of basis states needed to represent the state vector [7], or to monitor the state of a Bose–Einstein condensate [8, 9]. However, whether the individual paths of the stochastic Schrödinger equation are
true or not does not affect the validity of the average results we are interested in. The interested reader could possibly start from [5] to explore the development of the continuous monitoring theory.

One of the questions we will try to address is what are the physical conditions for the establishment of a steady state, and if this steady state corresponds to any known thermal equilibrium between the system and the environment. We will focus on the case in which there is no particle exchange between the system and the environment, the latter then representing a thermal bath able to supply energy and momentum to the system. For this reason we will talk about thermal relaxation of the system towards some equilibrium. There are in the literature a few examples of equations of motion for the state of the system which are built to describe the relaxation of the system towards a steady state [10, 11]. While some of them have been widely used to investigate the relaxation towards a steady state, they are usually not derived but rather assumed due to some sought characteristics of the dynamics they impose. We refer the interested reader to the available literature [10, 4, 12] for a more complete review of those results.

This review aims at becoming a seed for a growing research field. It is organized as follows: in section 2 we will derive the stochastic Schrödinger and the master equation both in the Markovian and non-Markovian approximation. We will also discuss some of the issues in solving numerically the stochastic equation. This ingredient is fundamental if we want to discuss some applications to real systems. Section 3 will present some recent results on how to simplify the numerical investigation of many-body open quantum systems with techniques from density functional theory [13]. We will also discuss the possibility of closing the Kohn–Sham system, as suggested recently [14].

Section 4 deals with some examples of the application of the stochastic equation to real systems: we will discuss the cases of spin thermal transport, Bose–Einstein condensation, thermal relaxation and the effect of electron energy dissipation on ionic motion.

2. Open quantum systems

The theory of open quantum systems has a long history, dating back to the beginning of quantum theory. The inclusion of the coupling between a quantum system and an external environment reached a certain degree of maturity with the pioneering works of Vernon and Feynman [15] together with Caldeira and Legget [16]. The general idea is to derive an effective dynamics for the quantum system that takes into account the coupling with the environment without solving the equation of motion for the environment. The starting point was the von Neumann equation for the density matrix, since the latter can be easily connected to the thermodynamical properties of the system [17, 18]. Within the so-called master-equation formalism, an impressive number of results have been obtained, setting it to be the ‘de facto’ standard for the theory of open systems.

More or less in parallel, as happened in the classical theory with the Langevin and the Fokker–Planck equations, one can derive an effective dynamics for the ‘state’ of the quantum subsystem, the so-called stochastic Schrödinger equation (SSE). The theory began with an attempt to, mimicking the situation of the Langevin theory of Brownian motion, introduce a stochastic term to describe the relaxation dynamics of an open quantum system [11, 19–25]. It then found application in the theory of quantum optics, where the environment is the electromagnetic radiation [26]. The stochastic equation was meant to reproduce the dynamics derived from the density matrix after some average was taken. Recently, Gaspard and Nagaoka [27] formalized the theory, starting with the equation of motion for the environment, the system and their coupling. With some approximations, which are similar to those invoked for the derivation of the master equation, they arrived at a general expression for the stochastic Schrödinger equation [27]. The idea behind this approach is similar to the Gibbs’ ensemble theory [17, 18, 28]: we build many replicas of the same system, each identified by a certain realization of the dynamics of the environment—assumed in thermal equilibrium—and let them evolve independently. To obtain physical quantities from this amount of information we perform averages over the many realizations of the micro-state of the environment.

2.1. Stochastic Schrödinger equation

We begin by considering a subsystem described by the Hamiltonian $\hat{H}_S$ coupled to an external environment, given by $\hat{H}_B$, through an interaction potential $\lambda \hat{W}$, the Schrödinger equation for the closed system reads ($\hbar = 1$ hereafter in this review)

$$i \frac{d}{dt} \langle \Psi(t) \rangle = \left( \hat{H}_S + \hat{H}_B + \lambda \hat{W} \right) |\Psi(t)\rangle dt.$$  \hspace{1cm} (1)

We depict a possible situation in figure 1, where a system is coupled to three different baths. Each of the baths is characterized by its own thermodynamical micro-states, as we will discuss in the following.
This differential equation describes the exact dynamics of the closed system. However, the exact microscopic description of the dynamics of the macroscopic environment and its influence on the subsystem are in most cases not feasible. Consequently, this equation will serve as a starting point for the derivation of an equation of motion for the reduced wavefunction expressed in the Hilbert space of the subsystem. The following deduction is very much in the spirit of Gaspard and Nagao [27], who applied a so-called Feshbach projection-operator method [29, 30] to the Schrödinger equation (1) and derived a non-Markovian stochastic Schrödinger equation (NMSSE).

By considering a complete and orthonormal basis for the environment,

\[ \mathbb{1}_B = \sum_n |n\rangle \langle n|, \quad \hat{H}_B|n\rangle = \varepsilon_n|n\rangle, \]

the total wavefunction can be expanded in this basis as

\[ |\Psi(t)\rangle = \sum_n |\phi^n(t)\rangle \otimes |n\rangle. \]

Due to the normalization of the total wavefunction,

\[ 1 = \langle \Psi|\Psi\rangle = \sum_n \langle \phi^n|\phi^n\rangle, \]

the coefficient wavefunctions \(|\phi^n\rangle\) are not normalized and the square of their norm can be interpreted as the probability that the environment is in the state |n\rangle. As a consequence, the wavefunctions \(|\phi^n\rangle\) form a statistical ensemble which determines the total state of the combined system. In order to extract a typical representative of the ensemble, one defines the projection operators

\[ \hat{P} = \mathbb{1}_S \otimes |l\rangle \langle l|, \quad \hat{Q} = \mathbb{1}_S \otimes \sum_{m \neq l} |n\rangle \langle n|, \]

and thus can be used for the Feshbach projection-operator method. Conveniently, this method is performed in the interaction picture

\[ i d\hat{P}|\Psi_t(t)\rangle = \lambda \hat{W}(t)|\Psi_t(t)\rangle \; dt, \]

and the other is a differential equation for \(\hat{Q}|\Psi\rangle\) and describes the time evolution of all the other coefficient wavefunctions. Thus, by solving the second equation and inserting its solution into the first, one obtains a closed differential equation for \(\hat{P}|\Psi\rangle\). To follow this plan, we apply the projection operators (4) to the time-dependent Schrödinger equation (6), leading to

\[ i d\hat{P}|\Psi_t(t)\rangle = \lambda \hat{W}(t)\hat{P}|\Psi_t(t)\rangle \; dt + \lambda \hat{W}(t)\hat{Q}|\Psi_t(t)\rangle \; dt, \]

the second expression is an inhomogeneous linear differential equation for \(\hat{Q}|\Psi_t(t)\rangle\) and can be solved by the method of variation of constants

\[ \hat{Q}|\Psi_t(t)\rangle = \hat{U}(t)\hat{Q}|\Psi_t(0)\rangle \]

where \(\hat{U}(t)\) is the time-evolution operator of the corresponding homogeneous differential equation and thus obeys

\[ i d\hat{U}(t) = \lambda \hat{W}(t)\hat{U}(t) \; dt. \]

Inserting (10) into (8) leads to a closed differential equation for \(\hat{P}|\Psi_t\rangle\),

\[ i d\hat{P}|\Psi_t(t)\rangle = \lambda \hat{W}(t)\hat{P}|\Psi_t(t)\rangle \; dt + \lambda \hat{W}(t) \left( \hat{U}(t)\hat{Q}|\Psi_t(0)\rangle \right. \]

\[ - i\lambda \int d' \hat{U}(t - t') \hat{Q}\hat{W}(t')\hat{P}|\Psi_t(t')\rangle \; dt' \]

It is worth mentioning that until now no approximations have been made, so that (11) describes the exact time evolution of the \(l\)th coefficient of the total wavefunction. Hence, (11) can also be considered as a suitable starting point for a derivation of a stochastic Schrödinger equation beyond the weak coupling approximation. Unfortunately, this equation is as difficult to solve as the Schrödinger equation for the closed system (1) and thus we will consider a subsystem which is weakly coupled to the environment. To this end, we perform a perturbation expansion to second order in the coupling parameter \(\lambda\),

\[ i d\hat{P}|\Psi_t(t)\rangle = \lambda \hat{W}(t)\hat{P}|\Psi_t(t)\rangle \; dt + \lambda \hat{W}(t) \left( \hat{U}(t)\hat{Q}|\Psi_t(0)\rangle \right. \]

\[ - i\lambda^2 \hat{W}(t) \int_0^t d' \hat{U}(t - t') \hat{Q}\hat{W}(t')\hat{P}|\Psi_t(t')\rangle \; dt' + \mathcal{O}(\lambda^3), \]

where the time-evolution operator \(\hat{U}(t)\) has been expanded to second order in \(\lambda\). Until now the derivation was quite generic, no restriction on the form of the interaction potential \(\hat{W}\) or the Hamiltonians of the subsystem and environment has been imposed. In the following we assume the interaction potential to be of linear form, \(\hat{W} = \sum_v \hat{V}_v \otimes \hat{B}_v\), in the operators \(\hat{V}_v\) and \(\hat{B}_v\) of the subsystem and the environment, respectively. These operators can always be redefined as Hermitian operators [27], thus we use \(\hat{V}_v^\dagger = \hat{V}_v\) and \(\hat{B}_v^\dagger = \hat{B}_v\) in the following. If needed, this restriction can easily be lifted.
By multiplying (12) from the left with $|l\rangle$ and assuming that $|\langle l|\hat{B}_a(t)|l\rangle|$ vanishes, it simplifies to

$$i\,d|\phi(t)_l^l\rangle = |f(t)_l^l\rangle\,dt - i\lambda\sum_{a,\beta} \hat{V}_a(t)\int_0^t dt' \hat{V}_\beta(t')\times |\langle l|\hat{B}_a(t')\rangle|l\rangle |\phi(t')_l^l\rangle\,dt. \tag{13}$$

The forcing term

$$|f(t)_l^l\rangle = \lambda\sum_{a,\beta,\gamma\neq l} \hat{V}_a(t)\left|\langle l|\hat{B}_a(t)\rangle\right|n\rangle - i\lambda\int_0^t dt' \hat{V}_\beta(t')\left|\langle l|\hat{B}_a(t')\rangle\rangle\right|\phi(t')_l^l\rangle\right|\phi(l')_l^l\rangle\,dt. \tag{14}$$
describes the influence of all the other bath modes on the $l$th coefficient wavefunction and one sees that the initial conditions $|\phi^{\alpha}(0)\rangle$ enter here as an essential ingredient. By assuming that at $t = 0$ the subsystem is in a pure state and the bath is in thermal equilibrium, the total density operator can be written as

$$\hat{\rho}_T(0) = |\phi(0)\rangle \langle \phi(0)| \otimes \rho_B^{\text{eq}} = |\phi(0)\rangle \langle \phi(0)| \otimes \frac{e^{-\beta \hat{H}_B}}{Z_B}, \tag{15}$$

where $\beta'$ is the inverse of the temperature and $Z_B = \text{Tr}_B e^{-\beta \hat{H}_B}$. Nevertheless, we are interested in the initial wavefunction corresponding to this density operator. This can be established under the assumption that the initial condition for the total wavefunction is given by

$$|\Psi(0)\rangle = |\phi(0)\rangle \otimes \sum_n \sqrt{\frac{e^{-\beta\epsilon_n}}{Z_B}} e^{\epsilon_n} |n\rangle, \tag{16}$$

where $|\theta_n\rangle$ are independent random phases uniformly distributed over the interval $[0, 2\pi]$. Here, we want to point out the difference in the description of an open quantum system by wavefunction or master-equation methods: random phase factors have to be considered in the initial conditions. Due to this, the initial conditions can be written as

$$|\phi^{\alpha}(0)\rangle = \langle n|\Psi(0)|\rangle = |\phi(0)\rangle \sqrt{\frac{e^{-\beta\epsilon_n}}{Z_B}} e^{\epsilon_n} = |\phi^{\alpha}(0)\rangle \sqrt{\frac{e^{-\beta}\epsilon_n}}{Z_B} e^{\epsilon_n} \tag{17}$$

where we have used the fact that all coefficient wavefunctions at $t = 0$ are proportional to the same state $|\phi(0)\rangle$ of the subsystem and thus they can be expressed in terms of the $l$th. With the help of this, the forcing term (14) can be simplified further

$$|f(t)_l^l\rangle \approx \lambda\sum_{a,\beta,\gamma\neq l} \hat{V}_a(t)\left|\langle l|\hat{B}_a(t)\rangle\right|n\rangle - i\lambda\sum_{\beta} \int_0^t dt' \hat{V}_\beta(t')\left|\langle l|\hat{B}_a(t')\rangle\rangle\right|\phi(t')_l^l\rangle\right|\phi(l')_l^l\rangle\,dt. \tag{18}$$

Here, we have used that the expression in the square brackets gives the time evolution of the $l$th coefficient wavefunction in the interaction picture up to second order in $\lambda$ for (13). Also, we have included the stochastic noise in

$$\gamma_a^{\beta}(t) = \sum_{n\neq l} \langle\langle l|\hat{B}^l(t)|n\rangle\rangle e^{-\frac{\beta}{2}(\epsilon_n-\epsilon_l)} e^{i(\theta_n-\theta_l)}. \tag{19}$$

Additionally, one assumes that the expectation value of an operator from the bath for a typical eigenstate $|l\rangle$ is approximately equivalent to a thermal average of the temperature of the bath,

$$\langle\langle l|\hat{B}^l(t)|l\rangle\rangle \approx \text{Tr}_B[\rho_B^{\text{eq}} \hat{B}_a(t') \hat{B}_a(t')] \equiv C_{l,\beta}(t-t'). \tag{20}$$

For a more complete analysis on the validity of this assumption, see [31–36]. In this expression we have defined the bath correlation function $C_{l,\beta}$, which describes the influence of the bath on the system by tracing out the bath degrees of freedom in the dynamics.

In addition, if the bath is large enough, $\gamma_{\alpha}(t)$ consists of a sum of many complex oscillating terms, which leads to random Gaussian behaviour according to the central limit theorem. Hence, the noise is characterized by its mean value and its variance,

$$\gamma_{\alpha}(0) = 0, \quad \gamma_{\alpha}(t)\gamma_{\beta}'(t) = C_{\alpha,\beta}(t-t'), \tag{22}$$

where the relations $\epsilon_l(\theta_n+\theta_m) = 0, \epsilon_l(\theta_n-\theta_m) = \delta_{nm}$ and $\langle\langle l|\hat{B}^l(t)|l\rangle\rangle = 0$ have been used. We want to point out that the noise and the bath correlation function are not independent, more precisely, the covariance function of the noise is given by the bath correlation function. Collecting all the information, transforming back into the partial Schrödinger picture of the system and setting $\tau = t-t'$, (13) can be written as

$$i\,d|\phi(t)\rangle = \hat{H}_S|\phi(t)\rangle\,dt + \lambda\sum_{\alpha,\beta} \gamma_{\alpha}(t)\hat{V}_a|\phi(t)\rangle\,dt - i\lambda\sum_{\alpha,\beta} \int_0^t dt' e^{-i\beta\tau} \hat{V}_\beta \times C_{\alpha,\beta}(t-t')|\phi(t-t')\rangle\,dt. \tag{23}$$
Here we have suppressed the index \( l \), since we assume this wavefunction is a ‘typical representative’ of the dynamics of the system. This again corresponds to the Gibbs ensemble theory: with probability close to 1, we are sure that picking at random one of the coefficient wavefunction, it will evolve according to (23). In this equation the change of the wavefunction at time \( t \) depends not only on the current state \(|\phi(t)\rangle\) but also on an integral over the whole history of the state in the interval \([0, t]\). This behaviour is called non-Markovian and thus (23) is denominated NMSSE.

In (23) the coupling of the bath to the subsystem is described in an approximate manner and enters in the NMSSE through the bath correlation function \( C_{\alpha,\beta}(t) \) and the stochastic noise \( \gamma_{\alpha}(t) \) with the properties (22). Thus, all the information about the time evolution of the bath and its coupling to the subsystem is included in the bath correlation function. In most quantum optics cases the dependence on the past of the wavefunction can be neglected. This is due to the fact that the bath correlation function decays rapidly to zero on a timescale during which the system wavefunction does not vary significantly. For convenience, one neglects the non-Markovian behaviour by approximating the time dependence of the bath correlation function by a \( \delta \)-function, \( C_{\alpha,\beta}(t - t') \approx D_{\alpha,\beta}\delta(t - t') \), known under the name of a \( \delta \)-correlated bath approximation. As a result, the NMSSE reduces to

\[
\begin{align*}
    \text{i} \, d|\phi(t)\rangle & = \left[ \hat{H}_S + \lambda \sum_{\alpha} \gamma_{\alpha}(t) \hat{V}_{\alpha} 
    \right. \\
    & \left. - \frac{i\lambda^2}{2} \sum_{\alpha,\beta} \hat{V}_{\alpha} \hat{V}_{\beta} D_{\alpha,\beta} \right]|\phi(t)\rangle \, dt, 
\end{align*}
\]  

(24)

where \( \gamma_{\alpha}(t) \) are white-noise processes with \( \langle \gamma_{\alpha}(t) \rangle = 0 \) and \( \langle \gamma_{\alpha}(t)\gamma_{\beta}(t') \rangle = D_{\alpha,\beta}\delta(t - t') \). With the help of a unitary transformation \( U_{\gamma,\delta} \), which diagonalizes \( D_{\alpha,\beta} \) with corresponding eigenvalues \( d_{\alpha} \), (24) can be written in an Itô differential form

\[
\text{d}|\phi(t)\rangle = \left[ -\text{i}\hat{H}_S - \frac{1}{2} \sum_{\alpha} \hat{S}_{\alpha} \hat{S}_{\alpha} \right] dt \\
+ \sum_{\alpha} \hat{S}_{\alpha} \text{d}W_{\alpha}|\phi(t)\rangle, 
\]  

(25)

where the new set of bath operators is given by \( \hat{S}_{\alpha} = \lambda \sqrt{d_{\alpha}} \sum_{\beta} U_{\alpha,\beta} \hat{V}_{\beta} \). Furthermore, the stochastic processes are included in \( \text{d}W_{\alpha} = -\text{i}/\sqrt{d_{\alpha}} \sum_{\gamma} U_{\gamma,\alpha} \gamma_{\gamma} dt \) and one can show that these satisfy the properties

\[
\begin{align*}
    \text{d}W_{\alpha} = 0, \\
    \text{d}W_{\alpha} \text{d}W_{\beta} = \delta_{\alpha,\beta} dt. 
\end{align*}
\]  

(26)

We will call (25) the Markovian stochastic Schrödinger equation (MSSE) and we want to point out that this equation does not follow standard rules of calculus. The state \(|\phi(t)\rangle\) is a stochastic function and its time derivation is not defined at any instant of time. In addition, the differential noise \( \text{d}W \) scales on average as \( \sqrt{dt} \) and thus can be interpreted as a differential increment of an underlying Wiener process. As a result, this differential equation is not tractable with standard calculus and the rules have to be modified according to the Itô calculus. Since this will bring us too far from the scope of this review, here we will state only the important results of the Itô calculus needed in the following sections. For a more complete treatment of the Itô formalism one can consult the vast literature on the subject, of which we here just point out a few standards \([37, 38]\). An important result from this calculus is the Itô chain rule \([4, 39]\),

\[
\text{d} \langle \phi \rangle \langle \psi \rangle = (\text{d}\langle \phi \rangle)\langle \psi \rangle + \langle \phi \rangle (\text{d}\langle \psi \rangle) + (\text{d}\langle \phi \rangle)(\text{d}\langle \psi \rangle), 
\]  

(27)

where \( \phi \) and \( \psi \) are two states evolving according to the MSSE (25). In addition, the rules for the Itô differentials

\[
\begin{align*}
    \text{d}W_{\alpha} \text{d}W_{\beta} = \delta_{\alpha,\beta} dt, \\
    \text{d}W_{\alpha} \text{d}t = 0, \\
    \text{d}W_{\alpha} = 0, \\
    \frac{\text{d}W_{\alpha}}{dt} = \delta_{\alpha,\beta} dt, \\
\end{align*}
\]  

(28)

should be kept in mind. In the following section we will apply these Itô rules in order to derive the master equation that corresponds to the MSSE. In the case of the NMSSE, where one is confronted with non-white noises, Itô calculus cannot be applied and one has to find another approach to derive the corresponding master equation.

2.2. Density matrix formalism

In section 2.1 we have discussed the dynamics of a quantum mechanical system coupled to an external environment from the point of view of what we have identified as the ‘state’ of the system, \(|\phi\rangle\). However, for historical and practical reasons this is not the standard starting point. It has been easier, as we will discuss in a moment, to start from the dynamics of the reduced density matrix or statistical operator of the system, defined as

\[
\hat{\rho} = \langle \phi | \langle \phi \rangle = (\text{d}\langle \phi \rangle)(\langle \phi \rangle + (\text{d}\langle \phi \rangle)(\text{d}\langle \phi \rangle)). 
\]  

(29)

To obtain the equation of motion for the density matrix that corresponds to the MSSE (25), we can start from (29) and calculate the differential

\[
\text{d}\hat{\rho} = \text{d}\langle \phi \rangle \langle \phi \rangle = (\text{d}\langle \phi \rangle)(\langle \phi \rangle + (\text{d}\langle \phi \rangle)(\text{d}\langle \phi \rangle)). 
\]  

(30)

Unlike in normal calculus, one also has to keep the term \( \text{d}\langle \phi \rangle \text{d}\langle \phi \rangle \), as it contributes on average to first order in \( dt \). In the Markovian case, where one has to deal with white-noise processes, we can apply the Itô rules (27) and (28), which lead us to

\[
\begin{align*}
    \text{d}\hat{\rho} & = \left[ -\text{i}\hat{H}_S \, dt + \sum_{\alpha} \left[ -\frac{1}{2} \hat{S}_{\alpha} \hat{S}_{\alpha} \, dt + \hat{S}_{\alpha} \, \text{d}W_{\alpha} \right] \right] \hat{\rho} \\
    & + \left[ \hat{H}_S \, dt + \sum_{\beta} \left[ -\frac{1}{2} \hat{S}_{\beta} \hat{S}_{\beta} \, dt + \hat{S}_{\beta} \, \text{d}W_{\beta} \right] \right] \hat{\rho} \\
    & + \sum_{\alpha,\beta} \hat{S}_{\alpha} \, \text{d}W_{\alpha} \hat{S}_{\beta} \, \text{d}W_{\beta} + \mathcal{O}(dt^2) \\
    & = -\text{i} \left[ \hat{H}_S, \hat{\rho} \right] \, dt - \frac{1}{2} \sum_{\alpha} \left[ \hat{S}_{\alpha} \hat{S}_{\alpha} \hat{\rho} + \hat{\rho} \hat{S}_{\alpha} \hat{S}_{\alpha} \right] \\
    & - \hat{2} \hat{S}_{\alpha} \hat{\rho} \hat{S}_{\alpha}^{\dagger} \, dt + \mathcal{O}(dt^2). 
\end{align*}
\]  

(31)
This well-known Lindblad master equation is the most general type of a Markovian master equation, which is known to preserve not only the norm but also positivity and hermiticity [40]. This means that the MSSE (25) describes on average an open system dynamics which coincide with the Lindblad dynamics. Here, we have assumed that the Hamiltonian of the system is non-stochastic. However, if the Hamiltonian is stochastic, one has to deal with an ensemble of Hamiltonians and the corresponding equation of motion will most likely differ from the Lindblad master equation. We will discuss this issue in depth in section 2.5, where a gas of interacting bosons will be considered.

As mentioned before, Itô stochastic calculus is only applicable for white-noise processes. However, in the NMSSE (23) one encounters coloured noise which is not δ-correlated. A stochastic calculus for coloured noise has not been so extensively investigated as the Itô calculus. Hence, one has to find an alternative procedure for deriving an equation of motion for the density operator that corresponds to the NMSSE. To this end, a comparable master equation for the NMSSE up to fourth order in λ can be derived by performing a perturbative expansion in λ to arrive at [27]

$$\frac{d \hat{\rho}(t)}{dt} = -i \left[ \hat{H}_S, \hat{\rho}(t) \right] + \lambda^2 \int_0^t d\tau \sum_{\alpha,\beta} C_{\alpha,\beta}(\tau) \hat{V}_{\alpha} \hat{\rho}(t) e^{-i\hat{H}_S \tau} \hat{V}_{\beta} e^{i\hat{H}_S \tau} + \cdots \tag{32}$$

In the following, we will call this equation the non-Markovian master equation, as it corresponds to the NMSSE. Also here, we have assumed that the Hamiltonian is non-stochastic. In the limit $t \to \infty$ in the history term, the non-Markovian master equation simplifies to

$$\frac{d \hat{\rho}(t)}{dt} = -i \left[ \hat{H}_S, \hat{\rho}(t) \right] + \sum_{\alpha} \left( \hat{K}_\alpha \hat{\rho}(t) \hat{V}_\alpha + \hat{V}_\alpha \hat{\rho}(t) \hat{K}_\alpha^\dagger \right) - \hat{V}_\alpha \hat{K}_\alpha \hat{\rho}(t) - \hat{\rho}(t) \hat{K}_\alpha^\dagger \hat{V}_\alpha \hat{K}_\alpha^\dagger, \tag{33}$$

where

$$\hat{K}_\alpha = \lambda \sum_\beta \int_0^\infty d\tau \ C_{\alpha,\beta}(\tau) \ e^{-i\hat{H}_S \tau} \hat{V}_\beta \ e^{i\hat{H}_S \tau}. \tag{34}$$

This time-local evolution is the well-known Redfield master equation [41] and has been widely applied to systems where the dynamics of the environment is much faster than the system dynamics. This equation in general provides information on the long-time relaxation dynamics of the density matrix. In conclusion, we have seen that the MSSE describes on average a dynamics that corresponds to the one obtained from a Lindblad master equation and the NMSSE corresponds to the master equation (32), if the Hamiltonian is not stochastic. Hence, the SSEs can also be seen as an unravelling of the corresponding master equation, i.e., a quick and dirty way to obtain the solution of a master equation; especially when the system size grows one expects a better scaling behaviour of the SSEs.

2.3. Equation of motion for observables

Given the equation of motion for the density matrix and the SSE, either in the non-Markovian or in the Markovian approximation, the next step is to derive a general equation of motion for the expectation value of any observable. By definition, given a physical observable $P$, described by the operator $\hat{P}$, its expectation value is given by

$$\langle \hat{P} \rangle = \frac{\langle \phi(t) \mid \hat{P} \mid \phi(t) \rangle}{\langle \phi(t) \mid \phi(t) \rangle} = \text{Tr}_S(\hat{\rho}(t) \hat{P}) \equiv \langle P \rangle$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_1^N \langle \phi_i(t) \mid \hat{P} \mid \phi_i(t) \rangle \tag{35}$$

where, again, the $\langle \cdots \rangle$ represents the standard quantum mechanical average and $\overline{\cdots}$ the average over the noise as we have introduced them in section 2.1. To understand this last process, we can think of (35) as having built a certain number of replicas of the system, labelled by the index $i, \phi_i(t)$, see figure 2. Each replica evolves according to the SSE with a given realization of the noise. Averaging over the noise therefore corresponds to summing up all the weighted contributions to the given observable coming from each replica.

It should be evident from (35) why the density matrix has received such an amount of attention: if one were able to solve...
the equation of motion for the density with the proper initial conditions, the expectation value of any observable would come essentially at no extra cost. From (29), it is clear that the process of averaging over the many realizations of the stochastic behaviour that is driving the dynamics of $|\Psi\rangle$ is a crucial part in the definition of the density matrix. It is this average that builds up the correlation between the different trajectories of the stochastic dynamics. The same average step makes the SSE difficult to handle; even if one were able to write down an explicit solution to the SSE, the physical quantities will appear only after the average over many realizations of the noise is taken. For the density matrix, this step is embedded in the definition, and is thus carried out before the dynamics is solved, obtaining therefore an equation for the averaged quantities.

We want to derive an equation of motion for $\hat{P}$. To this end, we consider the case of the Lindblad equation or the MSSE (25). The generalization to the non-Markovian model is lengthy, involving the expansion of the equation of motion in terms of the coupling parameter $\lambda$ [27].

Considering the case of a single Wiener process, $dW$, we have, by using Itô calculus,

$$d\langle \hat{P} \rangle = (d\langle \phi \rangle \hat{P} \langle \phi \rangle + \langle \phi \rangle d\langle \hat{P} \rangle \langle \phi \rangle + (d\langle \phi \rangle \hat{P} \langle \phi \rangle) dW + (d\langle \phi \rangle \hat{P} \langle \phi \rangle) (dW)^2) + O(dW^2).$$

The equation of motion for the ensemble-averaged expectation value is obtained immediately from (36),

$$\partial_t \langle \hat{P} \rangle = -i [\hat{P}, \hat{H}] - \frac{1}{2} \left( \langle \hat{S}^\dagger \hat{S} \hat{P} \rangle + \langle \hat{P} \hat{S}^\dagger \hat{S} \rangle - 2\langle \hat{S}^\dagger \hat{S} \hat{P} \rangle \right) + \frac{1}{2} \left( \langle \hat{P} \hat{S}^\dagger \hat{S} \rangle - 2\langle \hat{S}^\dagger \hat{S} \hat{P} \rangle \right).$$

One could arrive at the same equation by using the master equation for the density matrix. It is immediately seen that the coupling to an external environment modifies the dynamics of the observable if $\hat{P}$ and $\hat{S}$ do not commute, i.e., $[\hat{P}, \hat{S}] \neq 0$. The second term on the right-hand side of (38) describes the dynamics of the expectation value in the presence of the expansion of the relaxation induced by the environment. A steady state for any observable will be reach when a competition between the two terms is established so as to make the right-hand side of (38) vanishing.

Of importance for the investigation of the dynamics of open quantum systems, is the time evolution of the single-particle density, i.e., the expectation value of the single-particle density operator. In standard quantum mechanics, i.e., for closed systems, the equation of motion for the single-particle density is the continuity equation, which essentially embodies the important principle of particle conservation. Namely, if $n(r, t)$ is the single-particle density and $\dot{r}(r, t)$ the single-particle current density, we have

$$\partial_t n(r, t) = -\nabla \cdot \dot{r}(r, t).$$

When the system is open, the equation of motion for the single-particle density appears more complex. We have from (38) that

$$\partial_t n(r, t) = -\nabla \cdot \dot{r}(r, t) - \frac{1}{2} \left( \langle \hat{S}^\dagger \hat{S} \hat{n} \rangle + \langle \hat{n} \hat{S}^\dagger \hat{S} \rangle - 2\langle \hat{S}^\dagger \hat{S} \hat{n} \rangle \right).$$

It may appear that this equation breaks the important physical principle of particle conservation, since the second term in (40) can hardly be recognized as a divergence of any current. Improbable as it might seem, Gebauer and Car [42] were able to show that, at least in the Markov approximation, the right-hand side of (40) can be written as the divergence of a new current density, $\dot{r}_C$, where $\dot{r}_C$ describes the transfer of momentum between the system and the environment.

As it will be important when we will discuss in the following section the development of a density functional approach to open quantum systems, let us discuss something that might appear as a trivial point. From a mathematical point of view, the continuity equation, given the initial condition and the current density $\dot{r}(r, t)$, uniquely determines the particle density everywhere and at any time. This is because a simple integration of (39) gives

$$n(r, t) = n(r, t = 0) - \int_0^t d\tau \cdot \nabla \cdot \dot{r}(r, \tau).$$

The opposite is not true. Given $n(r, t)$ and the initial conditions, the current density $\dot{r}(r, t)$ is not uniquely determined. Indeed, given $\dot{r}(r, t)$ and $\dot{r}(r, t) + \nabla \times \hat{v}(r, t)$, where $\hat{v}(r, t)$ is an arbitrary vector in space and time, these two currents solve the continuity equation with the same density $n(r, t)$. For this reason, one usually says that the particle density only determines the longitudinal current density, while the transverse part is left unknown. Indeed, only the longitudinal current is responsible for the transfer of particles across any given surface.

The situation appears more complex if one starts with the continuity equation for open systems. Even if one were to consider the total current $\dot{r}_C + \dot{r}_C$, the density is not uniquely determined. This is because the current $\dot{r}_C$ is determined by the density and the current density itselfselves, therefore making (40) a nonlinear equation whose solution appears non-trivial. The situation has not been clarified, and in the following we will assume that, similarly to what happens with the continuity equation, (40) uniquely determines the single-particle density.

With logical steps similar to those which led us to the equation of motion for the single-particle density [43], we can derive the equation of motion for the ensemble-averaged current density for a system of interacting identical particles of mass $m$, in the presence of an external vector potential $A_{\text{ext}}$.

$$\partial_t \dot{r}(r, t) = n(r, t) - \dot{r}(r, t) \times \frac{1}{m} \nabla \times A_{\text{ext}}(r, t) + \frac{\langle \hat{F}(r, t) \rangle}{m} + \frac{\langle \dot{\hat{G}}(r, t) \rangle}{m},$$

where we have defined

$$\dot{\hat{G}}(r, t) = \frac{\hat{S}^\dagger \dot{r}(r, t) \hat{S}}{2} - \frac{1}{2} \frac{\hat{r}(r, t) \hat{S}^\dagger \hat{S}}{2} - \frac{1}{2} \frac{\hat{S}^\dagger \hat{S} \hat{r}(r, t)}{2}. $$

\[ \text{Equation (43)} \]
\[ \dot{\mathbf{F}}(r, t) = -m \sum_{i \neq j} \delta(r - \hat{r}_i) \nabla U_{\text{int}}(\hat{r}_i - \hat{r}_j) + m \nabla \cdot \mathbf{\dot{r}}(r, t) \]

with the stress tensor \( \mathbf{\dot{r}}(r, t) \) given by

\[ \mathbf{\dot{r}}(r, t) = -\frac{1}{2} \sum_{i,j,k} \{ \dot{\hat{r}}_i, [\dot{\hat{r}}_j, \mathbf{\mathbf{\dot{r}}}(r - \hat{r}_k)] \}. \]

In these equations \( \nabla_j \) contains the derivatives with respect to the coordinates of the \( j \)th particle, i.e., in 3D, \( \nabla_j = (\partial_x, \partial_y, \partial_z) \), and the current operator is defined as

\[ \mathbf{j}(r, t) = \frac{1}{2} \sum_i \{ \delta(r - \hat{r}_i), \dot{\hat{r}}_i \} \]

with

\[ \dot{\hat{r}}_i = \frac{\dot{\hat{p}}_i + eA_{\text{ext}}(\hat{r}_i, t)}{m}, \]

the velocity operator of particle \( i \), and the symbol \( [\hat{A}, \hat{B}] \equiv (\hat{A}\hat{B} + \hat{B}\hat{A}) \) is the anti-commutator of any two operators \( \hat{A} \) and \( \hat{B} \).

The first two terms on the right-hand side of (42) describe the effect of the applied electromagnetic field on the dynamics of the many-particle system; the third is due to particle–particle interactions while the last term is the ‘force’ density exerted by the bath on the system. This last term is responsible for the momentum transfer between the quantum mechanical system and the environment. It should be pointed out that the first three terms on the right-hand side of (42) are present also in the standard equation of motion for the single-particle current density [43]. Equation (42) can be seen as the equation for the ‘forces’ acting on a single particle.

### 2.4. Solving the stochastic Schrödinger equation

For a single realization of the noise, the numerical solution of the SSE is similar to the integration of the Schrödinger equation [44, 45], and one can use some of the standard techniques for the numerical integration of partial differential equations [46]. However, the noise effectivelly reduces the stability and efficiency of the numerical algorithms [44]. For this reason, higher-order techniques, such as the standard fourth-order Runge–Kutta, do not offer the usual improvement as in the integration of the standard dynamical equations. Indeed, the usual parameter used to identify this efficiency is the scaling of the numerical error, \( \epsilon \), in terms of the time step of the numerical integration, \( \Delta t \). Typically, we have a power-law scaling, i.e.,

\[ \epsilon \propto \Delta t^\nu. \]

For example, for ordinary differential equations, the second-order Runge–Kutta has \( \nu = 2 \), while the fourth-order Runge–Kutta has \( \nu = 4 \). For Markovian systems, it is found quite surprisingly that for any standard technique, e.g. the second- and fourth-order Runge–Kutta methods, we have the same \( \nu \) [47]. Indeed, it has been shown that, in general, any method which involves only Wiener processes will have the same scaling [47] as the simpler Euler or Heun scheme (second-order Runge–Kutta). Higher-order schemes which improve the scaling with the integration time step can be found, and have been proposed—see for example [44, 48] and references therein—which involve the evaluation of a class of stochastic processes, beyond the simple Wiener processes, in building the numerical approximation to the exact solution of the SSE. These terms appear in the Taylor-like expansion of the solution to high orders [44, 48]. On the other hand, to the best of our knowledge, for NMSSE there are no clear results and a complete analysis of the error scaling is missing. The reader should also be warned of some attempts at building higher-order schemes to the solution of MSSE, such as in [49], starting from the standard Runge–Kutta schemes. These are based on the assumption \( \Delta W \Delta W = \Delta t \), which is however valid only when the average over many realizations of the noise is performed. Although it seems these schemes improve the convergence, their validity is doubtful [50] and most likely restricted to a small class of equations.

In this review, we will not discuss in detail any algorithm for the numerical solution of the SSE. A nice step-by-step tutorial on the solution of stochastic differential equations can be found in [45], while more advanced techniques can be found in [44, 50]. Here, we would like just to add that we can find a nonlinear SSE which preserves, at each time step, the norm of the wavefunction and which reproduces the same physical quantities as the linear SSE [51]. It is our experience that using this nonlinear SSE usually improves the stability of the integration algorithm.

When dealing with the NMSSE, we face the problem of simulating the correlated coloured noise \( \gamma(t) \) in (22). Many solutions to this problem have been proposed: they do differ on the amount of information we need at our disposal about the function \( C_{\alpha, \beta}(t) \). For example, for simple correlation functions the algorithm proposed in [52] is probably the most efficient, but it does require the knowledge of a first-order differential equation, whose \( C_{\alpha, \beta}(t) \) is a solution. This works well for \( C_{\alpha, \beta}(t) \propto e^{-|t|} \) [52]. For more complex cases, this approach cannot be used, and we can revert to the solution proposed by Rice [53], and recently revisited [54]. This algorithm might not be the most efficient [55, 56], but is based on the sole knowledge of the Fourier transform of \( C_{\alpha, \beta}(t) \), the power spectrum, practically the minimal amount of information we need. Moreover, this Fourier transform can be known analytically for some models: this is due to the fact that we might have access to, or we can approximate it to a certain degree, the power spectrum of the bath. A variant of this algorithm has been recently proposed in [57] for the case in which we know the function \( C_{\alpha, \beta}(t) \) at each instance of time, and we do not want to store the full Fourier transform for computational purposes. However, this algorithm does have a large numerical overhead, which makes its application to the SSE too expensive [58].

### 2.5. Difference between the stochastic Schrödinger equation and the master equation

We want to discuss the equivalence between the master equation for the reduced density matrix and the SSE. In
particular, we want to show one case of general interest in which the two formalisms give different results. We argue that this originates from the different ways in which they deal with interaction.

Let us consider the Hamiltonian of a one-dimensional boson system (in second quantization) which, when the bath is not present, reads

\[
\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} = \int dx \psi^\dagger(x) \left( -\frac{1}{2m} \frac{d^2}{dx^2} + V_{\text{ext}}(x) \right) \psi(x) + \int dx dx' \psi^\dagger(x) \psi^\dagger(x') U_{\text{int}}(x-x') \psi(x') \psi(x),
\]

(49)

where \( \psi(x) \) destroys a boson at position \( x \), \( V_{\text{ext}}(x) \) is a confining potential, and \( U_{\text{int}}(x-x') \) is the boson–boson interaction potential. We consider here the case of a diluted gas of alkali atoms, since this is a system of great interest [59–61]. For these gases the interaction potential can be substituted with the contact potential, i.e.,

\[
U_{\text{int}}(x-x') = g_0(N-1)\delta(x-x') = \frac{\tilde{g}}{2} \delta(x-x'),
\]

(50)

where \( g_0 = 4\pi h^2 \alpha / m \) is determined by the scattering length \( \alpha \) of the boson–boson collision in the dilute gas and \( N \) is the total number of bosons in the trap, so that \( ||\psi|| = 1 \) [61].

In what corresponds to a Hartree approximation for the boson wavefunction, we can go from the equation of motion for the annihilation operators to the equation of motion for single-particle wavefunction \( \Psi(x,t) \), when the external bath is not coupled to the boson gas,

\[
\frac{d}{dt} \Psi(x,t) = \left[ -\frac{1}{2m} \frac{d^2}{dx^2} + V_{\text{ext}}(x) \right] \Psi(x,t) + \tilde{g} n(x,t) \Psi(x,t),
\]

(51)

where \( n(x,t) = ||\Psi(x,t)||^2 \) is the single-particle density of the boson gas [62, 63]. Equation (51) (and its generalization to two and three dimensions) correctly describes the physical properties and especially the dynamics of a Bose–Einstein condensate [59–61]. That is, \( \Psi(x,t) \) describes the dynamics of the ground state of the system, when the temperature of the gas is well below the critical temperature for the Bose–Einstein condensation [18, 17, 61].

A harmonic confinement is routinely generated in the magneto-optical traps used in the realization of the condensation in alkali gases [59–61], so we choose

\[
V_{\text{ext}}(x) = \frac{1}{4} m \omega_0^2 x^2.
\]

(52)

When the boson system is coupled to the external environment, we assume that the Hamiltonian is not affected by this coupling, i.e., we neglect the Lamb shift, and the system evolves according to the MSSE

\[
d\Psi(x,t) = -i \left( -\frac{1}{2m} \frac{d^2}{dx^2} + \frac{1}{4} m \omega_0^2 x^2 + \tilde{g} n(x,t) \right) \Psi(x,t)
\]

\[
+ \tilde{g} \int dx' \hat{\Psi}(x,t) \hat{\Psi}(x',t) dt + \hat{\Psi}(x,t) dW',
\]

(53)

where we have assumed that the coupling with the environment is given by a single operator \( \hat{S} \). Here, \( dW \) is a standard Wiener process with properties (28).

For convenience, we restate this equation in terms of the physical quantities \( \omega_0, x_0 = 1/\sqrt{\omega} \), and \( g = \tilde{g} / x_0 \) to arrive at

\[
d\Psi(x,t) = -i \omega_0 \left( -\frac{x^2}{2m} \frac{d^2}{dx^2} + \frac{x^2}{2\omega_0^2} + \frac{g}{\omega_0} n(x,t)x_0 \right) \Psi(x,t)
\]

\[
\times dt + \frac{i}{2} \hat{S} \hat{\Psi}(x,t) dt + \hat{\Psi}(x,t) dW.
\]

(54)

We begin by considering the case of non-interacting bosons, i.e., we set \( g = 0 \). In this case, the Hamiltonian admits a natural complete basis, the set of Hermite–Gauss wavefunctions

\[
\varphi_j(x) = \frac{1}{\sqrt{\sqrt{\pi} \omega_j 2^{j!}}} H_j(x/x_0) e^{-x^2/2\omega_j^2},
\]

(55)

where \( H_j(x/x_0) \) are the standard Hermite polynomials [64]. If we expand the wavefunction \( \Psi(x,t) = \sum \varphi_j(t) \varphi_j(x) \), and make use of the orthonormality properties of the Hermite–Gauss wavefunctions, we obtain the (stochastic) dynamical equation for the coefficients \( a_j \),

\[
da_j = \sum_j \left( H_j^0 a_j + \frac{1}{2} \left( \hat{\mathcal{S}}^i \hat{\mathcal{S}}^j \right)_{ij} \right) dt + \int_j S_{ij} dW
\]

(56)

where \( H_j^0 = (j+1/2) \omega_j \delta_{ij} \).

Together with (56) we can study the dynamics of the density matrix via the quantum master equation (31), which in the same representation as (56) reads

\[
\partial_t \rho_{ij} = -i \sum_k \left( H_{ik} \rho_{kj} - \rho_{ik} H_j^0 \right)
\]

\[
+ \sum_{k,k'} \left( \hat{S}_{ik} \rho_{kj} \hat{S}_{k'i}^* - \frac{1}{2} \hat{S}_{ik}^* \hat{S}_{k'i} \rho_{ij} - \frac{1}{2} \rho_{ik} \hat{S}_{k'i} \hat{S}_{k'j} \right),
\]

(57)

The connection between (56) and (57) is established by the identity \( \rho_{ij} = a_i^* a_j \), which is valid for any pair of indices \( i \) and \( j \). It was shown [65] that when the interaction is set to vanish, the two formalisms yield the same result in the limit of a large number of realizations.

When one turns on the particle–particle interaction \( U_{\text{int}} \), this corresponds to adding to the free Hamiltonian an interaction part, \( \hat{H}_{\text{int}} \), which in the basis representation of the Gauss–Hermit polynomials reads

\[
\hat{H}_{i,j} = \sum_{k,q} F_{i,j,k,q} a_k^* a_q,
\]

(58)

where \( F_{i,j,k,q} \) is the fourth-rank tensor defined as

\[
F_{i,j,k,q} = \frac{g}{\pi \omega_0} 2^{-(q+j+k+q)/2} \sqrt{i i' j k' k' !} q !
\]

\[
\times \int_{-\infty}^{\infty} dx \hat{H}_i(x) \hat{H}_j(x) \hat{H}_k(x) \hat{H}_q(x) e^{-x^2}.
\]

(59)

A long but straightforward calculation, worked out in full detail in [66], brings us to an expression for \( F_{i,j,k,q} \) in terms
of Euler gamma functions and a hypergeometric function [66, 64]. It can be shown that the hypergeometric function reduces to the summation of a few—at most min(i, j)—terms [65]. In the case of the density matrix approach the interaction Hamiltonian is immediately written as

$$H_{i,j}^{\text{int}} = \sum_{k,q} F_{i,j,k,q} \rho_{k,q}. \quad (60)$$

In solving the dynamics of the system described either by the SSE (54) or the master equation (57) when the interaction is present, we have assumed that at any instant of time the bath operator brings the system towards the instantaneous ground state of the total interacting Hamiltonian $H^{(0)}_j + H^{\text{int}}_{i,j}$. Formally, in the basis set that diagonalizes the total Hamiltonian, this corresponds to choosing

$$S_{i,j} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (61)$$

for the bath operator. In addition, the interaction potential (and hence the total Hamiltonian), being defined in terms of the instantaneous density, is stochastic; namely it is different for each element of the ensemble. While we take this into account explicitly in the SSE (54), in the master equation (57) we must consider the interaction Hamiltonian averaged over all realizations.

In figure 3 we plot the occupation probability $p_j(t)$ of the state $j$ for the first three energy levels of the free Hamiltonian $(p_j(t) = |\psi_j(t)|^2)$ from the SSE or $p_j(t) = \rho_{j,j}(t)$ from the density matrix). We have assumed an interaction strength $g/\omega_0 = 5$, considered the first 20 energy levels, used a time step $\omega_0 \Delta t = 60/2^{17}$ and we have performed 100 independent runs of the SSE. The initial condition is such that all the energy levels are occupied with the same probability. From the figure it is evident that the system reaches, in the long time, the same steady state, but it is also clear that the state calculated with the SSE relaxes slower to this steady state than the state obtained from the density matrix equation. This is a spurious effect in the density matrix dynamics, where the average density defines the interaction potential without accounting for the fluctuations of the state, and hence of the stochastic Hamiltonian.

We have also tested that the steady state reached during the dynamics is consistent with the eigenstates of the Gross–Pitaevskii equation [61, 67]. In particular, the ground state of the interacting system, when the interaction is strong, can be obtained by neglecting the kinetic contribution to the Hamiltonian. In this case, a good approximation to the ground state density reads [61]

$$|\Psi_0(x)|^2 = \frac{\mu - 1/2m\omega_0^2 x^2}{\omega_0} \theta \left( \mu - 1/2m\omega_0^2 x^2 \right)$$

$$+ \text{terms proportional to } \frac{1}{g^2}, \quad (62)$$

where $\mu$ is the chemical potential, i.e., in this case the energy of the ground state, and $\theta(x) = 0$ if $x < 0$ and $\theta(x) = 1$ if $x \geq 0$.

In the inset of figure 3 we plot the density obtained at $\omega_0 \Delta t = 60$ from the SSE (black, dashed line) and the density obtained from the approximation (62) (orange, solid line). Notice that the value of the parameters $g$ and $\mu$ have been obtained from the best fit with the numerics: indeed one can show that the approximation (62) is exact in the limit of very large interaction [67, 61], which is not reached in our calculations.

We have therefore shown that the master equation and the SSE, for a system where the Hamiltonian is stochastic, i.e., it does contain terms that depend on the wavefunction, could lead to different results. This is expected, since in the master equation we replace the effective stochastic term with an ‘average’ contribution, without having any control on it. For example, in the case discussed the approximation corresponds to replacing terms such as $\bar{n}(x,t)\bar{n}(x',t)$ with $\bar{n}(x,t) \times \bar{n}(x',t)$. In the SSE, this approximation is not performed, since the average over the stochastic noise is done after the full evolution is calculated.

3. Stochastic density functional theory

As we will see for example in section 4.1, one severe limitation of the applicability of the theory is the presence of interaction between the particles of the system. This is nothing new, since similar problems arise also in the case of closed systems where the presence of interaction makes obtaining the exact solution of the dynamics of the system an almost impractical task. However, in the theory of many-particle systems, whenever we are interested only in certain quantities, it has been found that the complexity of the problem can be greatly reduced, to the level of making it treatable with numerical techniques. These results go under the name of density functional theory (DFT) [68, 69, 13]. Nowadays, there are different flavours of what one can call density functional theories, and the interested reader can find better introductions to that field, for example in [13]. For
our purposes, it is sufficient to say that, if we focus on the
dynamics of one observable, let us say the single-particle
density, then we can obtain this dynamics by investigating
a system of non-interacting particles, called the Kohn–Sham
(KS) system in the presence of a certain external potential [70,
71]. This potential is built to give exactly the dynamics of the
single-particle density of the real system [13]. However, it is
important to stress that any other quantity calculated within
the KS system and which cannot be expressed in terms of the
single-particle density alone, cannot, in general, be trusted.

For the sake of this review, of even more interest is the
case in which the current density is the quantity we would
like to obtain. For this case, it has been shown that one can
build a system of non-interacting quasi particles that, in
the presence of an appropriate vector potential, is able to mimic
the dynamics of the current density of the real system [72,
73]. Again, one must add the usual caveat that, in principle,
only the current density and all the physical quantity that can
extracted from it with simple operations (such as for example
the single-particle density) have a physical meaning. All the
others bear little resemblance to the same quantity of the real
system, although, in some cases one can realize that some
physical information can still be extracted from the dynamics
of the Kohn–Sham system [74].

The advantage of this formulation is many-fold and so
far reaching that Kohn was awarded the Nobel Prize in
Chemistry for the initial formulation of the theory, which dealt
with the properties of the ground state. Indeed, it essentially
paves the way to the numerical investigation of complex
many-body systems. It would be of great interest if one were
able to bring together the formulation of the open quantum
systems we have discussed so far and the KS theory of
many-body systems. This result has been achieved recently
by various groups [75, 76, 65, 14] with different formulations
of the theory. Also, in this case, the parallel between the
density matrix formalism and the SSE appears evident and
not surprisingly in certain cases one can reproduce the result
of one formalism in the other. However, as we will point out
more clearly in the following, a KS formulation in terms of the
density matrix of open quantum systems appears flawed [65],
since at the very basic level the KS Hamiltonian does contain
nonlinear terms of the state of the system, thus making the
derivation of a closed equation of motion for the density
matrix problematic, as we have discussed in section 2.

3.1. Stochastic time-dependent (current-)density functional theory

Let us begin by revising, without proof, the theorems of
time-dependent density functional theory. We consider N
non-relativistic particles of charge e, mutually interacting
via the Coulomb interaction, in a time-dependent external
potential, either a vector or scalar potential. We consider the
general Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \left[ \frac{\hat{p}_i + e \vec{A}_{\text{ext}}(\vec{r}_i, t)}{2m} \right]^2 + V_{\text{ext}}(\vec{r}_i, t)$$

$$+ \sum_{i<j}^{N} U(\vec{r}_i - \vec{r}_j), \quad (63)$$

where $\vec{A}_{\text{ext}}(r, t)$ is the external vector potential, $V_{\text{ext}}(r, t)$ the
external scalar potential, and $U(r)$ is the particle–particle
interaction potential. The many-body system evolves according
to the time-dependent Schrödinger equation,

$$\frac{d\Psi(t)}{dt} = \hat{H}\Psi(t). \quad (64)$$

When there is only a scalar potential $V_{\text{ext}}$, we have the
following theorems of time-dependent density functional
theory (TDDFT) [70–72, 77, 13]:

**Theorem 1 (Runge–Gross [70]).** We consider $N$ non-
relativistic electrons, mutually interacting via the Coulomb
repulsion, in a time-dependent external potential. Two single-
particle densities $n(r, t)$ and $n'(r, t)$ evolving from a common
initial state $|\Psi(t = 0)\rangle$ under the influence of two potentials
$V_{\text{ext}}(r, t)$ and $V'_{\text{ext}}(r, t)$ (both Taylor expandable about the
initial time $0$) eventually differ if the potentials differ by more
than a purely time-dependent $\left(r - \text{independent}\right)$ function:
$V_{\text{ext}}(r, t) - V'_{\text{ext}}(r, t) \neq c(t)$. Under these conditions, there is a
one-to-one mapping between densities and potentials, which
implies that the potential is a functional of the density.

The theorem is similar to the one that Hohenberg and
Kohn [68] proved in 1964 and that allowed, a year later, Kohn
and Sham [69] to formulate the DFT. The key point being
that one can obtain physical information about a many-body
system by investigating the behaviour of a simpler system
where particle–particle interaction is turned off.

The initial formulation of the Runge–Gross theorem was
not satisfactory since it was based on the existence of some
action that in the dynamical case did not respect causality [71].
Some years later, van Leeuwen was able to extend the theorem
and prove that there is no need to define an action from where
the equation of motion can be derived. Recently, Vignale has
shown that the initial formulation can be made consistent by
considering carefully the boundary and initial conditions for
the dynamics [73].

**Theorem 2 (van Leeuwen [71]).** Let $\hat{H}(t)$ and $\hat{H}'(t)$ be
two Hamiltonians of the form (63) containing not only two
different time-dependent local potentials $V_{\text{ext}}(r, t)$ and $V'_{\text{ext}}(r, t)$ but also two different particle–particle interactions $U$ and $U'$. Let $n(r, t)$ be the density that evolves from the initial state $|\Psi(t = 0)\rangle$ under the Hamiltonian $\hat{H}(t)$, and let $|\Psi'(t = 0)\rangle$ be another initial state with the same density and the
same value of the density gradient. Then the time-dependent
density $n(r, t)$ uniquely determines, up to a time-dependent
constant, the potential $V'_{\text{ext}}(r, t)$ that yields $n(r, t)$ starting
from $|\Psi'(t = 0)\rangle$ and evolving under $\hat{H}'$. It can be easily seen that the van Leeuwen’s theorem includes
the Runge–Gross results as a simple corollary, by considering
two systems evolving with the same interaction and with two
external local potentials.

The case for which a vector potential is present has been
investigated first by Ghosh and Dhara [78], and later Vignale
proposed a theorem along the proof of van Leeuwen. Here, for
simplicity, we report only the second theorem, again the result
by Ghosh and Dhara follows as a simple corollary. Vignale’s theorem for time-dependent current-density functional theory (TCDFT) states:

**Theorem 3** (Vignale [72]). Consider a many-particle system described by the time-dependent Hamiltonian

\[
\hat{H}(t) = \sum_i \left[ \frac{1}{2m} \left( \hat{p}_i + \hat{A}_{\text{ext}}(\vec{r}_i, t) \right)^2 + V_{\text{ext}}(\vec{r}_i, t) \right] + \sum_{i<j} U(\vec{r}_i - \vec{r}_j),
\]

where \( V_{\text{ext}}(r, t) \) and \( \hat{A}_{\text{ext}}(r, t) \) are given external scalar and vector potentials, which are analytic functions of time in a neighbourhood of \( t = 0 \), and \( U(r, t) \) is a translationally invariant two-particle interaction. Let \( n(r, t) \) and \( j(r, t) \) be the particle density and current density that evolve under \( \hat{H} \) from a given initial state \( |\Psi(0)\rangle \). Then, under reasonable assumptions, the same density and current density can be obtained from another many-particle system, with Hamiltonian

\[
\hat{H}'(t) = \sum_i \left[ \frac{1}{2m} \left( \hat{p}_i + \hat{A}'(\vec{r}_i, t) \right)^2 + V'(\vec{r}_i, t) \right] + \sum_{i<j} U'(\vec{r}_i - \vec{r}_j),
\]

starting from an initial state \( |\Psi(0)\rangle \) which yields the same density and current density as \( |\Psi(0)\rangle \) at time \( t = 0 \). The potentials \( V'(r, t) \) and \( \hat{A}'(r, t) \) are uniquely determined by \( V_{\text{ext}}(r, t) \) and \( \hat{A}_{\text{ext}}(r, t) \) and bath operators \( |\hat{S}_a\rangle \), \( \langle \hat{S}_a | \), up to gauge transformations of the form

\[
V'(r, t) \rightarrow V'(r, t) - \frac{\partial \Lambda(r, t)}{\partial t},
\]

\[
\hat{A}'(r, t) \rightarrow \hat{A}'(r, t) + \nabla \Lambda(r, t),
\]

where \( \Lambda \) is an arbitrary regular function of \( r \) and \( t \), which satisfies the initial condition \( \Lambda(t = 0) = 0 \).

TDDFT and TCDFT have been quite successful in describing the dynamics of closed quantum systems, especially whenever one needed to calculate the response of the system to an external perturbation [13]. These theories allow one to go beyond the actual state-of-the-art in many fields, e.g., in electron transport in nanoscale devices, where it does predict novel and interesting results [79]. The secret of this success is in the fact that the theory allows the treatment of complex systems with relative ease, since only the dynamics of a closed non-interacting many-body system is computed.

It appears therefore natural to try to generalize the theorem of TDDFT and TCDFT to the case of open quantum systems. This generalization has been achieved by using both the reduced density matrix and the SSE formalisms [75, 76, 65]. Let us assume that the quantum mechanical system described by the Hamiltonian (63) is coupled, via given many-body operators, to one or many external baths that can exchange energy and momentum with the system. If we assume that the dynamics of each bath is described by a series of independent memory-less processes, the dynamics of the system is governed by the stochastic Schrödinger equation in the Markov approximation,

\[
d|\Psi(t)\rangle = -i\hat{H}|\Psi(t)\rangle \, dt - \frac{i}{2} \sum_a \hat{S}_a^\dagger \hat{S}_a |\Psi(t)\rangle \, dt + \sum_a dW_a(t) \hat{S}_a |\Psi(t)\rangle,
\]

where \( \{\hat{S}_a\} \) describe the coupling of the system with the environment. In (68), we could have time-dependent Hamiltonian and bath operators. This would not change the following discussion.

As discussed in section 2.3, here assume that the knowledge of the current density is sufficient to obtain the single-particle density, and moreover this solution is unique, i.e., it depends solely on the single-particle current density and the initial conditions. If this is not the case, the proof of the following theorem, as we report it, does not hold and we have to revert to a more cumbersome yet similar proof where we need to assume that the ensemble-averaged single-particle density is differentiable to all orders in time.

We have the following result [76]:

**Theorem 4.** Consider a many-particle system described by the dynamics in (68) with the many-body Hamiltonian given by (63). Let \( n(r, t) \) and \( j(r, t) \) be the ensemble-averaged single-particle density and current density, respectively, with dynamics determined by the external vector potential \( \hat{A}_{\text{ext}}(r, t) \) and bath operators \( |\hat{S}_a\rangle \). Under reasonable physical assumptions, given an initial condition \( |\Psi(0)\rangle \) and the bath operators \( |\hat{S}_a\rangle \), another potential \( \hat{A}'(r, t) \) which gives the same ensemble-averaged current density must necessarily coincide, up to a gauge transformation, with \( \hat{A}_{\text{ext}}(r, t) \).

A theorem of similar content for the one-to-one correspondence between the single-particle density and the scalar potential has been discussed in [75]. The starting point of those authors was the equation of motion for the density matrix of the system, described in the Markov approximation. In [14, 80], the theorem by Burke et al [75] and the previous one have been extended to the non-Markovian dynamics. The proofs of these theorems follow essentially the same logical steps as the ones we will present in the following.

**Proof.** We follow a line of reasoning common to the proofs of the van Leeuwen and Vignale theorems [71, 72]. Recently, a more elegant proof of the Runge–Gross and van Leeuwen theorems has been proposed [77], but the application of this method to the equation of motion for the current density does not appear clear. Let us continue by assuming that the current density \( j(r, t) \) is obtained from another many-particle system with Hamiltonian

\[
\hat{H}'(t) = \sum_i \left[ \hat{p}_i + e\hat{A}'(\vec{r}_i, t) \right]^2 \frac{1}{2m} + \frac{1}{2} \sum_{i\neq j} U'(\vec{r}_i - \vec{r}_j),
\]

evolving from an initial state \( |\Psi(0)\rangle \) and following the stochastic Schrödinger equation (68) with the same bath operators \( \hat{S}_a \). By assumption, \( |\Psi'(0)\rangle \) gives—in the primed
system—the same initial current and particle densities as in the unprimed system. The equation of motion for the ensemble-averaged current density is (42).

Equations similar to (45)–(47) are written for the system with the vector potential \( \vec{A}(r, t) \). Similar force terms \( \mathcal{F}' \) and \( \mathcal{G}' \) appear in these equations. \( \mathcal{F}' \) and \( \mathcal{G}' \) differ from the forces in the unprimed system, since the initial state, the external vector potentials, and the velocity \( \dot{v} \) are different. By assumption, the ensemble-averaged current and particle densities are the same, therefore

\[
\frac{\partial j_l(r, t)}{\partial t} = \frac{n(r, t)}{mF_l(r, t)} - \frac{j(r, t)}{m} \times [\nabla \times \vec{A}(r, t)] + \mathcal{F}'(r, t) + \vec{G}'(r, t). \tag{70}
\]

Taking the difference of (42) and (70) we arrive at

\[
n(r, t)\delta A_l(r, t) = \frac{j(r, t)}{m} \times [\nabla \times \vec{A}(r, t)] + \Delta Q(r, t), \tag{71}
\]

where \( \Delta \vec{A}(r, t) \equiv \vec{A}'(r, t) - \vec{A}_{\text{ext}}(r, t) \) and \( \Delta Q(r, t) \equiv \mathcal{Q}'(r, t) - \mathcal{Q}(r, t) \), with \( \mathcal{Q}(r, t) = (\mathcal{F}(r, t) + m\vec{G}(r, t)) \) and \( \mathcal{Q}'(r, t) \) the same quantity but in the primed system.

We next prove that (71) admits only one solution, i.e., \( \Delta \vec{A}(r, t) \) is completely determined by the averaged dynamics of the current and particle densities, once the coupling with the environment via \( \delta \vec{S}_g \), is assigned. To this end we expand (71) in series about \( t = 0 \) and obtain an equation for the \( l \)th derivative of the vector potential \( \Delta \vec{A}(r, t) \). We thus arrive at the equation

\[
\frac{n_0(t)}{t} + 1 \Delta \vec{A}_{l+1}(r) = -\sum_{k=0}^{l-1} (k+1)n_{l-k}(r) \Delta \vec{A}_{k+1}(r)
+ \Delta Q(r)
+ \sum_{k=0}^{l} \frac{j \dot{n}_{l-k}(r)}{t} \times [\nabla \times \Delta \vec{A}_k(r)]. \tag{72}
\]

where, given an arbitrary function of time \( f(r, t) \), we have defined the series expansion

\[
f_l(r) = \frac{1}{l!} \left. \frac{\partial^l f(r, t)}{\partial t^l} \right|_{t=0}. \tag{73}
\]

To prove that the right-hand side of (72) does not contain any term \( \Delta \vec{A}_{l+1}(r) \) we use the fact that the dynamics of any ensemble-averaged operator is given by (38). Indeed, this implies that the \( l \)th time derivative of any operator can be expressed in terms of its derivatives of order \( k < l \), time derivatives of the Hamiltonian of order \( k < l \), and powers of the operators \( \hat{S}_u \) and \( \hat{S}_g \). The time derivatives of the Hamiltonian do contain time derivatives of the vector potential \( \vec{A}(r, t) \), but always of order \( k < l \). Then on the right-hand side of (72) no time derivative of order \( l + 1 \) appears. Equation (72) can be thus viewed as a recursive relation for the time derivatives of the vector potential \( \Delta \vec{A}(r, t) \). To complete the recursion procedure we only need to assign the initial value \( \Delta \vec{A}_0(r) = \vec{A}'(r, t = 0) - \vec{A}_{\text{ext}}(r, t = 0) \).

Since in the unprimed and primed systems the densities and current densities are, by hypothesis, equal, the initial condition is simply given by \( \bar{n}(r, t = 0) \Delta \vec{A}_0(r) = \langle \Psi(0)|\hat{j}_p(r, t = 0)|\Psi(0) \rangle - \langle \Psi'(0)|\hat{j}_p(r, t = 0)|\Psi'(0) \rangle \), where \( \hat{j}_p(r) = (1/2m) \sum_{i} [\dot{p}_i, \delta(r - r_i)] \) is the paramagnetic current-density operator.

The same considerations as in [72] about the finiteness of the convergence radius of the time series (72) apply to our case as well. We rule out the case of a vanishing convergence radius by observing that it seems implausible that the smooth (in the ensemble-averaged sense) dynamics induced by (68) can introduce a dramatic explosion of the initial derivatives of \( \Delta \vec{A}(r, t) \). If this holds, the expansion procedure (72) can be iterated from the convergence radius time onward. We have then proved that (72) completely determines the vector potential \( \Delta \vec{A}(r, t) \) but thus, since \( \vec{A}_{\text{ext}}(r, t) \) is assumed known, it determines \( \vec{A}'(r, t) \) uniquely, up to a gauge transformation.

To finalize our proof, we consider the case in which \( U = \hat{U}' \) and \( |\Psi(0) \rangle = |\Psi'(0) \rangle \). If this holds, \( \Delta \vec{A}_0(r) \equiv 0 \). Then the recursion relation admits the unique solution \( \Delta \vec{A}_l(r) \equiv 0 \) for any \( l \), and at any instant of time \( t \) we have \( \vec{A}(r, t) = \vec{A}'(r, t) \) (still up to a gauge transformation). \( \square \)

The theorem states that the one-to-one correspondence is between the averaged current density and the vector potential applied to the system. In view of this, the KS vector potential is therefore a functional of the averaged current density, i.e., \( \vec{A}_{\text{KS}}(r) = \vec{A}'(r, t) \), \( |\Psi(0) \rangle = |\Psi'(0) \rangle \). Obviously, as in the case of any DFT theory, nobody knows the form of this functional, therefore the quality of the results we will obtain from our stochastic approach depends on the quality of the approximations we are able to make for this functional. At the moment, this is an open area of research. The hope is obviously that standard approximations that have proven very useful in the past, such as for example the adiabatic-local-density approximation [13, 43] and its refinements, will provide a solid foundation to explore the reach of this approach.

By looking at the statements of the theorems, we notice that they all establish a one-to-one correspondence between two quantities that have the same ‘spatial dimension’. With that we mean that the correspondence is either between a scalar (the single-particle density) and another scalar (the potential) or between a vector (the single-particle current density) and another vector (the vector potential). It is then easy to prove that if one tries to establish a correspondence between the current density and the scalar potential, then it is going to fail [74]. From a mathematical point of view this appears quite easy to understand: in creating a connection between two different spaces (the one of the densities and the one of the potentials, for example) one has to be sure that the dimensions of these spaces are the same. For this reason, one should be able to accept that, if the continuity equation is not valid (see discussion in section 2.3), then the only physical information we can extract by using the TDCTDFT theorem is the current density. For this reason, for example, the results of [14] appear to be lacking a solid foundation.
3.2. Closing the system

The proof we have presented for the theorem 4 leaves open a very fascinating possibility. What happens if we do assume that the bath operators $\hat{S}_\alpha$ are not the same in the two systems? Interestingly, it can be seen that the proof remains the same, i.e., one arrives at the conclusion that whenever the interaction potentials, initial conditions, and now the bath operators are the same then the vector potential is uniquely identified [14]. A similar result holds for the scalar potential [80]. One therefore arrives at the amazing conclusion that, if one is interested in the dynamics of selected observables then we can close the system, i.e., we set $\hat{S}_\alpha \equiv 0$ in the KS system, and still get the exact result. The KS system becomes then a closed and isolated system, exactly identical to the ones we already know in standard quantum mechanics. We therefore do not need to study the evolution of the system under a random influence of the environment. Although this possibility opens up a new way to look at the dynamics of open quantum systems, care needs to be applied in understanding its range of applicability. Indeed, one can easily see that the KS scalar or vector potentials needed to reproduce the exact dynamics are a functional of the coupling with the external environment. A priori, very little is known on the way this coupling enters into the KS potentials, and it is very likely that any local approximation, so successful in DFT, will fail miserably. Moreover, the KS potential in this way loses completely its generality, since it will be strongly affected by the system under investigation. It is clear, however, that further investigation along these very interesting and potentially promising lines is needed.

4. Applications of the stochastic Schrödinger equation

In this section, we will discuss some applications of the stochastic Schrödinger equation to investigate the dynamics of interesting systems. Our excursion must be limited, due to the variety of approaches that have characterized this field. Our point of view will be starting from systems that evolve according to a SSE as we have discussed in section 2.1. This cuts out a certain number of interesting, phenomenological, results that do not fit easily in this approach. In selecting the material for this review, we have indeed preferred to maintain a certain degree of consistency, rather than present a scattered amount of results. The interested reader can look into a series of beautifully written books where these topics are covered in more detail [4, 39, 10, 12].

In selecting the topics, we have also maintained a focus on solid-state physics to match the audience of this journal: we will discuss spin thermal transport, the onset of Bose–Einstein condensation in alkali gases, and the general problem of relaxation in the presence of a thermal bath at given temperature. This list cannot be exhaustive of the field, but, we believe, it gives a flavour of the directions of research one could tackle within this working framework.

Figure 4. A chain of spins is connected to two energy reservoirs having different temperatures via the spins at the beginning and end of the chain. The reservoirs transfer or absorb energy from the chain. The spins are interacting with a nearest neighbour interaction of parameter $Q$. A position-independent magnetic field $\vec{h} = \omega/2\hat{z}$ is present.

4.1. Spin thermal transport

A neat application of a SSE is the investigation of the thermal transport in one-dimensional spin chains. The simplest system we can think of is a chain of $N$ spin 1/2 atoms kept at fixed positions. A nearest neighbourhood interaction is present, and we can consider also the presence of a magnetic field. The two ends of the chain are connected to two thermal reservoirs at different temperatures: those two spins fluctuate due to the stochastic interaction with the reservoir, energy is transferred or absorbed from the neighbouring sites, and the whole chain reaches a steady state in the long-time regime. A simple schematic of the system can be seen in figure 4. The Hamiltonian for this system, when the coupling is not present, is written as

$$\hat{H} = -Q \sum_{n=0}^{N-2} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} + \sum_{n=0}^{N-1} \frac{\omega}{2} \sigma^z_n. \quad (74)$$

where $\vec{\sigma}_n = (\sigma^x_n, \sigma^y_n, \sigma^z_n)$, $\sigma^i_n$ is the spin operator of the site $n$ along the direction $i = \{x, y, z\}$, and $Q$ is the interaction constant we have assumed constant through all the sites. We have embedded the system into a uniform magnetic field, which we assume oriented along the $\hat{z}$ axis and of strength $\omega/2$. For a $N$ site chain we have that

$$\sigma^i_n = \mathbb{1} \otimes \mathbb{1} \otimes \hat{z}^i \otimes \mathbb{1} \otimes \mathbb{1}, \quad (75)$$

where $\mathbb{1}$ is the identity in the $2 \times 2$ space and $\hat{z}^i$ is the $i$th $2 \times 2$ Pauli matrix. It is then clear that each operator $\sigma^i_n$ is a sparse matrix of dimension $2^N \times 2^N$.

An effective way to define the effect of the thermal reservoirs is the following. At each instance of time, the direction of the first and last spin are randomized: the new spin directions are chosen according to a Boltzmann statistical weight which depends on the ‘local temperature’ of the last and first spins, i.e., to the temperature of the reservoir they are attached to [81]. An equivalent way is to solve the dynamics via either a Lindblad equation or, more conveniently, via
an appropriate SSE [81, 82]. The Lindblad equation for the system is written as
\[
\frac{d}{dt} \hat{\rho}(t) = -i[\hat{H}, \hat{\rho}(t)] + D_L \hat{\rho}(t) + D_R \hat{\rho}(t) \tag{76}
\]
where
\[
D_L \hat{\rho}(t) = 2 \sum_{k,l=1}^2 \gamma_{k,l}(T_L) \left( F_k \hat{\rho}(t) F_l^\dagger - \frac{1}{2} F_k \hat{\rho}(t) F_l^\dagger F_l + \frac{1}{2} F_l \hat{\rho}(t) F_k^\dagger F_l \right), \tag{77}
\]
\[
D_R \hat{\rho}(t) = 2 \sum_{k,l=1} \gamma_{k,l}(T_R) \left( G_k \hat{\rho}(t) G_l^\dagger - \frac{1}{2} G_k \hat{\rho}(t) G_l^\dagger G_l + \frac{1}{2} G_l \hat{\rho}(t) G_k^\dagger G_k \right). \tag{78}
\]
In (78), the operators \( F \) and \( G \) are the raising and lowering operators for the first and last spin, respectively, i.e.,
\[
F_1 = \sigma_0^+, \quad F_2 = \sigma_0^-,
\]
\[
G_1 = \sigma_{N-1}^+, \quad G_2 = \sigma_{N-1}^-,
\tag{79}
\]
which are built starting from the raising and lowering spin \( 1/2 \times 2 \times 2 \) operators in a similar fashion as in (75)
\[
\hat{\sigma}^+ = \hat{\sigma}^x + i \hat{\sigma}^y, \quad \hat{\sigma}^- = \hat{\sigma}^x - i \hat{\sigma}^y. \tag{80}
\]
The coupling matrix \( \gamma \) is given by [82]
\[
\gamma(\omega) = \lambda I(\omega) \left( \frac{f(\beta, \omega)}{f(\beta, \omega)^2 + f(\beta, \omega)} \sqrt{f(\beta, \omega)^2 + f(\beta, \omega)} + \frac{1}{f(\beta, \omega)} \right), \tag{81}
\]
where \( f(\beta, \omega) = [\exp(\beta \omega) - 1]^{-1} \) is the Bose–Einstein distribution function at temperature \( \beta = 1/k_B T \). \( I(\omega) \) is the bath spectral function, and \( \lambda \) is the coupling strength, all evaluated at the energy of the magnetic field, \( \omega \). Once the matrix \( \gamma \) is diagonalized with \( \alpha_1 = 0 \) and \( \alpha_2 \) as the eigenvalues, one can rewrite the Lindblad equation in the equivalent form
\[
\frac{d}{dt} \hat{\rho}(t) = -i \left[ \hat{H}, \hat{\rho}(t) \right] + \alpha_2(T_L)
\times \left( L^L \hat{\rho}(t) L^L - \frac{1}{2} L^L \hat{L}^L \hat{\rho}(t) - \frac{1}{2} \hat{\rho}(t) L^L \hat{L}^L \right) + \alpha_2(T_R)
\times \left( L^R \hat{\rho}(t) L^R - \frac{1}{2} L^R \hat{L}^R \hat{\rho}(t) - \frac{1}{2} \hat{\rho}(t) L^R \hat{L}^R \right), \tag{82}
\]
where the operators \( L^L \) and \( L^R \) are linear combination of the operators \( F \) and \( G \). Being in the diagonal Lindblad form, we know that we can easily rewrite the dynamics induced by this master equation into an equation for a stochastic wavefunction \( \Psi(t) \) [81]. For this problem, going from the master equation to the SSE offers a great numerical advantage. The dimension of each of the matrices entering the Lindblad equation is indeed \( 2^N \times 2^N \), which even for a short chain of 10 spins, means more than \( 10^6 \) elements. Although many of those matrices will be sparse, the same is not true for the density matrix itself, therefore one cannot rely on using any efficient numerical tool for sparse matrices. In contrast, for the SSE the wavefunction is a vector of \( 2^N \) elements and, since all the spin operators are sparse matrices, one can reduce the amount of memory and operations by orders of magnitude, thus making a larger number of spins in the chain affordable. Even in this case, the number of elements in the chain has to be restricted to about 20. Two ways out are possible. On the one hand, a reformulation of the problem in terms of Majorana fermions [83] seems to allow longer chains, up to 100 elements, to be tackled at least to investigate the steady-state regime. On the other hand, one could reformulate the problem in terms of spin-density waves [43]: by reducing the Hilbert space to the low-energy waves, one could effectively reduce the dimensionality of the problem.

In figure 5, the magnetic energy of a given site, \( H_n \), over a long-time single realization of the stochastic noise. The parameters \( \beta_L = 0.41, \beta_R = 1.39, Q = \lambda = 0.01, \) and \( \omega = 1 \) have been chosen. For the realization, a final time \( t_{fin} = 10^5 \) in units of \( \omega^{-1} \) has been used. Reproduced with permission from [81].

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In figure 6 the behaviour of the thermal conductivity of the spin chain as a function of the length of the chain is reported. Interestingly, the thermal conductivity starts to grow for larger system sizes, suggesting that a ballistic thermal transport regime might be reached for this chain.
one is interested in the conditions for thermal relaxation and the SSE, this begs the question of whether the NMSSE is still an equilibrium process. In order to describe realistic open systems, we would like to discuss. The generalization to an operator, as this case contains all the essential characteristics.

Here, we consider the environment as described by one operator, as this case contains all the essential characteristics we would like to discuss. The generalization to an environment described by many operators requires some additional care. If the same temperature is uniform, we do expect the system to reach a thermal equilibrium at the given temperature. If the temperature is not uniform, we should not expect any thermal relaxation: the system is continuously driven out-of-equilibrium by the temperature gradients between the different parts of the environment. One can see that the coupling of the system with the environment enters the equation of motion only through two quantities, namely the bath correlation function $C(\tau)$, which is connected with the noise, and the system’s coupling operator $\hat{V}$. Whether the system is driven towards thermal equilibrium by the coupling to the heat bath can thus only depend on these two quantities. However, one naturally expects that the operator $\hat{V}$ from the reduced Hilbert space of the system does not contain information about the environment, such as for example its temperature. Hence, thermal relaxation processes have to be highly dependent on the structure of the bath correlation function $C(\tau)$ as it is the only quantity that describes the coupling from the side of the environment.

As we have seen before, the SSE describes an ensemble of wavefunctions evolving under the influence of different stochastic processes. Consequently, only on average will one be able to state whether thermal equilibrium is reached and thus we will use the master equation (32) derived in section 2.2 for the discussion of thermal relaxation processes. First of all, we are interested in whether or not thermal equilibrium is reached, and thus it is sufficient to investigate this with the help of the Redfield master equation (33) in the limit $t \to \infty$. One expects, indeed, the master equation (32), which corresponds to the NMSSE, and Redfield equation (33) to have the same steady states. In order that the thermal equilibrium state of the system is a stationary state of the NMSSE, the following equation has to be satisfied

$$\lim_{t \to \infty} \frac{d\hat{\rho}_S^{\text{eq}}(t)}{dt} = 0.$$  (87)

This requirement and the fact that the equilibrium density operator commutes with the system Hamiltonian lead to a condition for the NMSSE to ensure thermal relaxation,

$$0 = \lim_{t \to \infty} \frac{d\hat{\rho}_S^{\text{eq}}}{dt} = \hat{K} \hat{\rho}_S^{\text{eq}} \hat{V} + \hat{V} \hat{\rho}_S^{\text{eq}} \hat{K}^\dagger - \hat{\rho}_S \hat{K}^{\text{eq}} \hat{V} + O(\lambda^4),$$  (88)

where

$$\hat{K} = \lambda^2 \int_0^{\infty} d\tau C(\tau) e^{-i\hat{H}_S \tau} \hat{V} e^{i\hat{H}_S \tau}.$$  (89)

From this one can obtain the conditions for stochastic relaxation processes. To this end, we will change to the energy basis of the system,

$$\hat{H}_S |n\rangle = \epsilon_n |n\rangle, \quad \hat{V} = \sum_{n,m} v_{nm} |n\rangle \langle m|,$$  (90)

in which (88) can be written as

$$\lim_{t \to \infty} \frac{d\hat{\rho}_S^{\text{eq}}}{dt} = \lambda^2 \sum_{n,m,l} \langle l| v_{nm} v_{ml} \times \int_0^{\infty} d\tau \left\{ C(\tau) e^{-i(\epsilon_n - \epsilon_m)\tau} e^{-\beta \epsilon_m} + C^*(\tau) e^{-i(\epsilon_n - \epsilon_m)\tau} e^{-\beta \epsilon_m} - C(\tau) e^{-i(\epsilon_n - \epsilon_m)\tau} e^{-\beta \epsilon_m} - C^*(\tau) e^{i(\epsilon_n - \epsilon_m)\tau} e^{-\beta \epsilon_m} \right\} + O(\lambda^4).$$  (91)
As discussed before we are interested in system-independent conditions under which the right-hand side of (91) vanishes. Hence, these have to be connected with the bath correlation function,

$$C(\tau) = \text{Tr}_B[\hat{\rho}_B^{\text{eq}} \hat{B}(\tau) \hat{B}(0)],$$

(92)

and by using the fact that $\hat{B}$ is a Hermitian operator, one can conclude that

$$C^*(\tau) = C(-\tau).$$

(93)

As a result of this, the ‘half Fourier transform’ in (91) can be written as

$$\int_0^\infty d\tau \ C(\tau) e^{-i\omega \tau} = \frac{1}{2} \int_{-\infty}^\infty d\tau C(\tau) e^{-i\omega \tau} + \frac{i}{2\pi} \int_0^\infty d\tau \left\{ C(\tau) e^{-i\omega \tau} - C^*(\tau) e^{i\omega \tau} \right\} = \frac{1}{2} \hat{C}(\omega) + iD(\omega),$$

(94)

where $D(\omega)$ is the imaginary part of this half Fourier transform and, as a consequence, the Fourier transform of the bath correlation function, $\hat{C}(\omega)$, is a real-valued function. Furthermore, if the half Fourier transform (94) is analytic in the upper complex half plane of $\omega$ and vanishes faster than $|\omega|^{-1}$ as $\omega$ goes to infinity, one can apply the Kramers–Kronig relation,

$$D(\omega) = \frac{1}{2\pi} \int_{-\infty}^\infty \frac{d\omega'}{\omega - \omega'} \hat{C}(\omega').$$

(95)

Here, $P \int$ denotes the Cauchy principal value of the integral.

In the same spirit the half Fourier transform of the conjugate bath correlation function can be written as

$$\int_0^\infty d\tau \ C^*(\tau) e^{-i\omega \tau} = \hat{C}(\omega) + \frac{1}{2\pi} \int_{-\infty}^\infty \frac{d\omega'}{\omega' - \omega} \hat{C}(\omega') = \frac{1}{2} \hat{C}(\omega) + iF(\omega).$$

(96)

Inserting equations (96) and (94) into (91) leads to

$$\lim_{t \to \infty} \frac{d\hat{\rho}^{\text{eq}}}{dt} = \sum_{n,m,l} |n\rangle \langle l| v_{nmvl} \left\{ (\frac{1}{2} \hat{C}(\omega_{nm}) + iF(\omega_{nm})) e^{-\beta \epsilon_{nm}} + (\frac{1}{2} \hat{C}(\omega_{ml}) + iF(\omega_{ml})) e^{-\beta \epsilon_{ml}} - (\frac{1}{2} \hat{C}(\omega_{mn}) + iF(\omega_{mn})) e^{-\beta \epsilon_{mn}} - (\frac{1}{2} \hat{C}(\omega_{nl}) + iF(\omega_{nl})) e^{-\beta \epsilon_{nl}} + O(\lambda^4) \right\},$$

(97)

where $\omega_{ij} = \epsilon_i - \epsilon_j$. We want to point out that in order to satisfy the requirement of thermal relaxation, the right-hand side of this equation has to vanish. In addition, the Fourier transform of the bath correlation function can be interpreted as the power spectrum of the noise, and hence describes the probabilities for energy transitions in the system. By assuming that this power spectrum satisfies a so-called detailed-balance relation,

$$\hat{C}(-\omega) = e^{\beta \omega} \hat{C}(\omega),$$

(98)

(97) simplifies to

$$\lim_{t \to \infty} \frac{d\hat{\rho}^{\text{eq}}}{dt} = \sum_{n,m,l} |n\rangle \langle l| v_{nmvl} \left\{ D(\omega_{nm}) e^{-\beta \epsilon_{mn}} + F(\omega_{ml}) e^{-\beta \epsilon_{ml}} + D(\omega_{mn}) e^{-\beta \epsilon_{mn}} - F(\omega_{nm}) e^{-\beta \epsilon_{nm}} \right\} + O(\lambda^4).$$

(99)

The detailed-balance relation (98) ensures that the energy transitions in the system are balanced according to Boltzmann statistics. Furthermore, we want to point out that (99) has only imaginary components and by inserting the explicit integrals into (99) we arrive at

$$\lim_{t \to \infty} \frac{d\hat{\rho}^{\text{eq}}}{dt} = \sum_{n,m,l} |n\rangle \langle l| v_{nmvl} \left\{ \hat{C}(\omega_{nm}) (1 - e^{-\beta (\epsilon_n - \epsilon_m - \omega)}) e^{-\beta \epsilon_{mn}} + \hat{C}(\omega_{ml}) (1 - e^{-\beta (\epsilon_m - \epsilon_l - \omega)}) e^{-\beta \epsilon_{ml}} - \hat{C}(\omega_{mn}) (1 - e^{-\beta (\epsilon_n - \epsilon_m + \omega)}) e^{-\beta \epsilon_{mn}} + O(\lambda^4) \right\}.$$$$\int_0^\infty d\tau C(\tau) e^{-i\omega \tau} = D(\omega) \approx 0,$$

(100)

In this expression there is no longer any need to write the principal value since the integral is no longer singular. It can be shown that the diagonal components of (100) cancel each other, i.e.,

$$\langle l | \frac{d\hat{\rho}^{\text{eq}}}{dt} | l \rangle = 0.$$$$\int_0^\infty d\tau C(\tau) e^{-i\omega \tau} = D(\omega) \approx 0,$$

(101)

This can be done by changing $\omega_{nm}$ to $-\omega_{nm}$, changing the integration variable in the second integral of (100) from $a$ to $-a$, and applying the detailed-balance relation (98) again.

As a result, one can conclude that the NMSSE (23) has a stationary solution which coincides with the thermal-equilibrium state up to first order in $\lambda$. Furthermore, if the detailed-balance relation is satisfied, the corresponding master equation (33) drives the system towards a stationary state that coincides in the diagonal elements in the energy basis with the thermal-equilibrium state up to fourth order. Additionally, neglecting either the off-diagonal components of the density matrix in the long-time behaviour or the imaginary contribution of the half Fourier transform,

$$\int_0^\infty d\tau C(\tau) e^{-i\omega \tau} = D(\omega) \approx 0,$$

(102)

the system will be driven towards equilibrium if the equation is considered up to fourth order. It can be argued that this imaginary part can be included in the system Hamiltonian [12], leading to the so-called Lamb shift. This means that the equilibrium density operator will not commute with this effective Hamiltonian. Nevertheless, this energy shift will not introduce dissipative dynamics in the system [85].
In conclusion, the bath correlation function should satisfy the detailed-balance relation in order to describe thermal relaxation behaviour. Hence, by the Markovian approximation, \( C_{a,b}(\tau) \approx D_{a,b}(\tau) \), one neglects this property of the bath correlation function. Therefore, the description of thermal relaxation processes with the help of the MSSE seems to be questionable.

As an example to demonstrate the previous considerations about thermal relaxation processes we will discuss a simple model. Namely, a tight-binding model with three sites,

\[
\hat{H}_S = -\Gamma(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_3 + \hat{c}_3^\dagger \hat{c}_2),
\]

(103)

where the operators \( \hat{c}_i^\dagger \) create an electron at the \( i \)th tight-binding position and \( \Gamma \) is the hopping integral. We will couple this electronic system to the electromagnetic field inside a cavity. For this model one can derive the power spectrum in the dipole approximation (\( c = 1 \)),

\[
\hat{C}_{\text{cavity}}(\omega) = \frac{|\alpha|^3}{\pi \Omega_\omega} [f(\beta, |\alpha|) + \theta(\omega)] \quad \text{if} \quad |\alpha| < \omega_c,
\]

(104)

where \( f(\beta, \omega) = 1/(\exp(\beta \omega) - 1) \), \( \theta(\omega) \) is the Heaviside function, \( \omega_c \) is a cutoff frequency (determined by the dimensions of the system to satisfy the dipole approximation) and \( \Omega \) is the volume of the cavity. For \( |\alpha| > \omega_c \) this function vanishes. We want to point out that this power spectrum contains naturally the detailed-balance relation and hence the model is suitable to describe thermal relaxation processes.

In addition, one can derive the system’s coupling operator for the considered model as

\[
\hat{V} = -q \sum_{l,p} \overrightarrow{u} \cdot \langle \overrightarrow{r}|p\rangle \hat{c}_l^\dagger \hat{c}_p,
\]

(105)

where \( q \) is the electron charge and the operator \( \hat{c}_l^\dagger \) creates an electron in the \( l \)th energy eigenstate of the system. Here, we have assumed for simplicity that each mode of the cavity has the same polarization direction \( \overrightarrow{u} \), parallel to the chain of the three tight-binding sites. We want to point out that the form of this operator should be immaterial for the establishment of a thermal equilibrium, since this is only determined by the power spectrum (104). Moreover, if the same operator is used in a Markov approximation, a steady state is established that is not the equilibrium configuration.

In figure 7 we report the probability of occupying the three eigenstates of the Hamiltonian (103) as a function of time, obtained from the numerical solution of (32). The system is driven towards thermal equilibrium, represented by the three final points in the figure, in the long-time regime.

Figure 7. The probability of occupying the three eigenstates of the Hamiltonian (103) as a function of time, obtained from the non-Markovian master equation.

4.3. Ionic motion

An interesting extension of the result of the preceding section 3 on DFT has been proposed recently by Appel and Di Ventra [86]. They used the electrons present in a certain molecule as the ‘link’ between the ions and the external environment, therefore investigating how some vibrational modes, excited at the initial time and coupled to the electron motion, can be effectively dissipated [86]. The starting point is a theory similar to the one we have discussed in section 3, where one considers the total current and charge densities, namely, including in those expressions also the ionic contribution. In a system of electrons and ions, where the former are connected to external baths, one proves that the total electrical current density is in a one-to-one correspondence with the external vector potential, thus establishing a stochastic TDDFT scheme for the system under investigation. This clearly allows for energy dissipation from the ionic degrees of freedom via the electrons. In figure 8, the dynamics of the ionic positions of a neon molecule is shown [87]. In the left pane, the electrons are disconnected from the environment, and the system undergoes a periodic motion determined by the initial conditions. In the right pane, the electrons are connected with an external bath that continuously extracts energy from them: the ions relax to the equilibrium configuration of the neon dimer, with the electrons in the ground state. It is clear that this is a simple example of what is an interesting and promising technique.
to investigate the correlated dynamics of electrons and ions coupled to an external environment. For example, this dissipative dynamics could possibly explain the appearance of broadening on the electron and phonon spectrum.

4.4. Bose–Einstein condensation

As a last example of application of the stochastic Schrödinger equation we consider again the Bose–Einstein condensation [17, 15] of alkali gases [61]. In this case, we depart from the SSE we have discussed in previous sections, and introduce the case of particle exchange between the system and its environment. This allows us to investigate the dynamics of the condensate formation and predict the condensation temperature. To do so, we will need to introduce a stochastic term that is not ‘multiplicative’, i.e., it does not multiply the wavefunction as happens in 2.1, but ‘additive’ as we will discuss in a moment.

In the experimental realization of the condensate, the gas is trapped in a confining harmonic potential generated by a magnetic field obtained by focusing two laser fields [59, 60]. In these systems the final temperature is about a few hundreds of nanokelvin. To reach this fantastic result, a novel technique was developed—the evaporative cooling of the gas. At temperatures above the condensation temperature, the gas follows a Boltzmann statistics. The evaporative cooling selectively removes from the gas the particles with the highest kinetic energy. This is possible since the highest kinetic energy states are those which have a finite probability density at the border of the magnetic trap. Therefore, another laser focused around the boundaries of the magneto-optical trap can cause those bosons to be released from the trap. The gas, where the tail of the Boltzmann distribution has been cut, relaxes via boson–boson collisions to a new distribution with lower temperature, since the total kinetic energy is lower than before. By selectively removing the hottest atoms, the temperature of the alkali gas can be reduced below the condensation temperature and one can observe a condensation both in momentum and position space [61, 59, 60].

As we have briefly discussed in section 2.5, the Gross–Pitaevskii (GP) equation is the standard theoretical tool to describe the physics of the condensate system [61]. The equation has proven successful in describing both the dynamics and static properties of the condensate. Due to its simplicity and striking successes, many people have tried to generalize the GP equation to study the dynamics of the condensate formation. In this system, the ground state and the excited states are separated well in energy—this separation is dictated by the confining potential—and one could regard the excited states as a reservoir of particles and energy for the condensate. With an expansion on the particle–particle interaction, by using the Keldysh formalism Stoof [88] arrived at the following stochastic GP equation

\[ i\partial_t \Phi(r, t) = \left[ -\frac{\nabla^2}{2m} + V_{\text{ext}}(r) - \mu - iR(r, t) + g|\Phi(r, t)|^2 \right] \times \Phi(r, t) + \eta(r, t). \] (106)

Here, \( \Phi(r, t) \) describes the condensate phase, \( V_{\text{ext}} \) is the confining potential, \( \mu \) is the chemical potential, and \( g \) the interaction constant. Finally, \( R(r, t) \) and \( \eta(r, t) \) are the terms coming from the coupling of the condensate to the non-condensate atoms which form the ‘environment’ for the condensate. Notice that \( \eta(r, t) \) does not multiply the wavefunction \( \Phi(r, t) \), but is added to the equation of motion. For this reason, \( \eta \) is an additive noise for our problem. This is necessary in order for (106) to allow particle exchange with the environment, i.e., the norm of the function \( \Phi(r, t) \) can vary with time. Clearly, the term \( R(r, t) \) represents a dissipative contribution denoting the coupling between the condensate and the non-condensate phase, while \( \eta(r, t) \) accounts for the incoherent collisions within the gas, analogously to the description of the Brownian motion. Interestingly, one can arrive at a similar equation using a completely different technique. This technique, developed in parallel and independently from the one we present here, looks promising in building a theory to investigate the dynamical formation of the Bose–Einstein condensate in alkali gases [89–91]. Its first application to the investigation of vortex formation close to the transition temperature has provided results in good quantitative agreement with the experiments [92]. Here, however, we do not feel it necessary to give the details of this theory, of which the interested reader can find a clear exposition in [89].

The noise \( \eta \) is characterized by a Gaussian correlation function

\[ \eta^*(r', t') \eta(r, t) = \frac{i}{2} \Sigma^2(r, t) \delta(t - t') \delta(r - r'). \] (107)
where \( \Sigma^k(r, t) \) is the Keldysh self-energy of the gas of alkali atoms [88, 93, 94]. As one could expect, there is an equivalent form of the dissipation–relaxation relation which connects the dissipation term \( R \) to the noise \( \eta \):

\[
iR(r, \epsilon) = -\frac{\Sigma^k(r, \epsilon)}{2(1 + f(\beta, \epsilon))}, \tag{108}\]

where \( R(r, \epsilon) \) and \( \Sigma^k(r, \epsilon) \) are the Fourier transform of \( R(r, t) \) and \( \Sigma^k(r, t) \), respectively, and \( f(\beta, \epsilon) \) is the Bose–Einstein distribution at temperature \( T \).

The dynamics of the condensate formation can be obtained numerically in one dimension. In 2D and 3D, although in principle the equations are still valid, their numerical integration is more difficult. Besides the obvious numerical overhead associated with dimensionality, this is due to the more complex spectrum of the system. Although strictly speaking in one dimension the Bose–Einstein condensation for an ideal gas does not exist [17, 18], in practice one considers the formation of a so-called quasi-condensate which corresponds to a macroscopic occupation of the ground state of the confining potential. To obtain an effective equation of motion, one splits the wavefunction into a radial and transverse component. Then the radial component is assumed to be Gaussian and integrated out. The process gives rise to an effective one-dimensional interaction constant, \( g_{1d} \). This approximation works in an excellent way for cigar-shaped potentials [61], where the confinement along the radial component is stronger than along the transverse direction. In figure 9, we report the dynamics of formation of the quasi-condensate at different times. At the end of the process, a quasi-condensate of 20000 particles is formed at a temperature of about 100 nK. A key quantity to establish the presence of a phase transition is the so-called first-order correlation function, defined as

\[
g^{(1)}(-z/2, z/2; t) = \frac{\Phi^*(z/2, t)\Phi(-z/2, t)}{|\Phi^*(z/2, t)|^2 |\Phi(-z/2, t)|^2}. \tag{109}\]

This quantity can be measured experimentally [95–97], thus providing a test for the theory. In figure 9, distances are scaled to the quasi-condensate dimension at equilibrium. The effective radius \( R_{TF}(T) \) varies with temperature, starting from the Thomas–Fermi expression at zero temperature \( R_{TF}(0) = \frac{\sqrt{2\mu}/m\omega^2}{\omega \sqrt{\pi}} \) if \( \omega \) is the frequency of the confining harmonic potential in the \( z \) direction, and \( \mu \) is the chemical potential, i.e., the energy of the condensate. For the discussion on how to calculate \( R_{TF} \) at finite temperature see [94] and references therein.

The results of figure 9 can be compared with the experimental results obtained since 1995, the year of the first experimental observations of the Bose–Einstein condensate in ultra-cold alkali atomic gases [59, 60]. The theoretical modelling is able to describe the quasi-condensate formation with a thorough investigation of the dynamics. It is also important that the theory contains essentially no fitting parameters, since all of them can be quantitatively determined from the knowledge of the experimental setup.

Bose–Einstein condensation in alkali gases has proven to be an important tool for a deeper understanding of quantum mechanical phenomena. In particular, the relative ease in manipulating it and its relative stability have allowed a series of interesting experiments on quantum measurement theory to be carried out. Indeed, the condensate can allow for either invasive or non-destructive probing of certain physical quantities. In this respect, it has been recently possible to develop a stochastic theory to describe the case in which the condensate is interacting with a laser field which is under
continuous measurement. As is the case with the theory of continuous quantum measurement in other systems, this theory does not fall into the form of the SSE we have extensively presented in this review. The interested reader could start from [8, 9].

5. Summary

The stochastic Schrödinger equation is a ubiquitous tool that can be used to describe the dynamics of an open quantum system, namely a system in interaction with an external environment. The accurate use of this tool requires a deep understanding of the physical approximations used to derive, from the Schrödinger equation of the total system, an effective equation of motion for the subsystem of interest. In this review we have mainly focused on only one class of SSE, those that have a quite specific form and structure, derived from a few assumptions on the dynamics of the environment and on the coupling between the system and its environment. To give to the reader a feeling of how wide is the range of applicability of these concepts, we have briefly discussed in section 4.4 a SSE with a different form, in particular with an additive noise, in contrast to the multiplicative noise we have discussed in the rest of this review. Other stochastic equations have been suggested in the past [10] to describe an effective dynamics of the system, without a clear step-by-step derivation of the equation of motion. We have not considered that class here. The reason for that is simple: each of these models requires a proper introduction, justification, and derivation, while we are more interested in presenting a unified, although restricted, point of view. The interested reader can start from [10] and explore the vast literature presented there. To make a connection with the knowledge of the reader, we have clearly established the link between the SSE and a master equation for the reduced density matrix. From this point of view, one can see the SSE as being a ‘Langevin’ type of equation and the master equation as its ‘Fokker–Planck’ counterpart. We have shown however, that the two theories can lead to significantly different results for physical quantities.

We have applied the SSE to different systems, from spin thermal transport, to Bose–Einstein condensation to thermal equilibrium in electronic systems. The list of examples could go further but we would find ourselves repeating the same, useful concepts.

Finally, we have discussed an interesting new topic in SSE, i.e., the inclusion of particle–particle interactions and its application to describe the dynamics of electronic devices. We have shown, in parallel with the DFT theory, how one can build an effective description of an open system that in the future should allow us to construct an ab initio modelling of electronic thermal transport, without relying too much on any assumption about the properties of the steady state.

The field is still in its infancy. For example, a clear connection between the NMSSE and its master-equation counterpart is missing: the actual derivation by Gaspard and Nagaoka [27] is incomplete and leaves many questions open; first of all the non-uniqueness of the derived equation. A deeper understanding of the condition for the establishment of a steady state or ‘thermal equilibrium’ is also missing. The ‘detailed balance’ is indeed not enough to ensure the system is driven towards a ‘thermal equilibrium’, at least in the form known from standard statistical mechanics. Also, a thorough exploration of the effect of particle–particle interaction, even at the basic level of mean-field theories, is lacking. We therefore foresee an interesting future for these techniques.

Acknowledgments

RB and RDA acknowledge financial support from MICINN (FIS2010-21282-C02-01 and PIB2010US-00652), the Grupos Consolidados UPV/EHU del Gobierno Vasco (IT-319-07) and ACI-Promociona (ACI2009-1036). RB acknowledges financial support from IKERBASQUE, Basque Foundation for Science. RDA acknowledges the financial support of the MICINN CONSOLIDER-INGENIO 2010 ‘NanoTherm’ (CSD2010-00044) and is grateful for the hospitality at the Physics Department of King’s College London.

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