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STUDIES ON THE MULTIFACETED INTERACTION OF ATOMS AND AN ELECTROMAGNETIC FIELD

by

Kari Härkönen

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From

Department of Physics and Astronomy
University of Turku
Finland

Supervised by

Kalle-Antti Suominen
Professor of Physics
Department of Physics and Astronomy
University of Turku
Finland

Jyrki Piilo
Docent of Theoretical Physics
Department of Physics and Astronomy
University of Turku
Finland

Reviewed by

Heinz-Peter Breuer
Professor of Theoretical Physics
Physikalisches Institut
Albert-Ludwigs-Universität Freiburg
Germany

Kurt Jacobs
Assistant Professor of Physics
Department of Physics
University of Massachusetts at Boston
USA

Opponent

Andreas Buchleitner
Professor of Theoretical Physics
Physikalisches Institut
Albert-Ludwigs-Universität Freiburg
Germany

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Abstract

In this Thesis the interaction of an electromagnetic field and matter is studied from various aspects in the general framework of cold atoms. Our subjects cover a wide spectrum of phenomena ranging from semiclassical few-level models to fully quantum mechanical interaction with structured reservoirs leading to non-Markovian open quantum system dynamics.

Within closed quantum systems, we propose a selective method to manipulate the motional state of atoms in a time-dependent double-well potential and interpret the method in terms of adiabatic processes. Also, we derive a simple wave-packet model, based on distributions of generalized eigenstates, explaining the finite visibility of interference in overlapping continuous-wave atom lasers.

In the context of open quantum systems, we develop an unraveling of non-Markovian dynamics in terms of piecewise deterministic quantum jump processes confined in the Hilbert space of the reduced system — the non-Markovian quantum jump method. As examples, we apply it for simple 2- and 3-level systems interacting with a structured reservoir. Also, in the context of ion-cavity QED we study the entanglement generation based on collective Dicke modes in experimentally realistic conditions including photonic losses and an atomic spontaneous decay.

List of articles

This thesis consists of an introductory review and the following six articles:

I K. Härkönen, O. Kärki, and K.-A. Suominen,
Tailoring of motional states in double-well potentials by time-dependent processes,
Phys. Rev. A **74**, 043404 (2006) [9 pages].

II J. Piilo, S. Maniscalco, K. Härkönen, and K.-A. Suominen,
Non-Markovian quantum jumps,
Phys. Rev. Lett. **100**, 180402 (2008) [4 pages].

III J. Piilo, K. Härkönen, S. Maniscalco, and K.-A. Suominen,
Open system dynamics with non-Markovian quantum jumps,
Phys. Rev. A **79**, 062112 (2009) [17 pages].

IV K. Härkönen, F. Plastina, and S. Maniscalco,
Dicke model and environment-induced entanglement in ion-cavity QED,
Phys. Rev. A **80**, 033841 (2009) [15 pages].

V K. Härkönen,
Jump probabilities in the non-Markovian quantum jump method,
J. Phys. A: Math. Theor. **43**, 065302 (2010) [10 pages].

VI K. Härkönen, O. Vainio, and K.-A. Suominen,
Wave-packet analysis of interference patterns in output coupled atoms,
Phys. Rev. A **81**, 043638 (2010) [7 pages].

Chapter 1

Introduction

The interaction of an electromagnetic (EM) field and matter is described by quantum mechanics in the most fundamental level as an exchange of a single excitation, a quantum, of energy between a field mode and a single atom. In the complete absence of the surrounding gas of particles, provided in a laboratory by an ultra high vacuum chamber, the only interface to a single atom or a cloud of atoms is through the EM field. Fortunately, such interface equips us with a collection of tools capable of trapping the atoms in a confined volume, manipulating their dynamical state, and finally measuring the state — everything ultimately delivered by the same interaction. For all these many different purposes, the interaction enters the dynamical description in a variety of forms.

The immense versatility and controllability of the lasers and magnetic fields has enabled trapping [65, 79], cooling [100] and dynamical control of the atoms [22]. Understanding how to control the dynamics enables us to study the fundamental structure of physics itself: high-precision measurements [23] allow us to test our definitions about the laws of nature. On the other hand, it is possible to fabricate physical setups which mimic the features of phenomena that are impossible to study directly [8], which broadens our knowledge even more.

An atom interacting with a (infinitely) large collection of EM modes is most naturally described as an open quantum system [14]. From the point of view of the atom, the modes constitute an environment in which the atom is submerged. As is known, when the coupling with the environment is weak, the open system is subject to irreversible processes, such as spontaneous relaxation, and the dynamics is well approximated by a Markov process [34]. With special mode structures the correlations between the open system and the environment are strong, which reflects into further

dynamics. The same applies when looking at very short time scales, when even the weak correlations have had no time to vanish. Therefore, there is a back-action in the dynamics and it can not be described by a Markov process anymore. An increasing interest towards phenomena of faster time scales and structured environments has revealed such non-Markovian dynamics in many fields of physics, such as quantum optics [34], solid state physics [57], quantum chemistry [90], quantum information processing [1], and even in biological systems [81, 96].

In quantum optics, the measurement of the state is ultimately always based on a scattering process, where a controlled input field interacts with the atom and the scattered output field is detected. In quantum mechanics the state is characterized by its statistical properties, which are determined by repeating the measurements many times for the same state. A master equation describes the dynamics of the state exactly in terms of such statistical averages, but it tells nothing about the single measurement events. The unraveling of the master equation in terms of stochastic processes aims at bringing back this information beyond the ensemble-averaged quantities [20].

Already the quantum characterization of radiation by Einstein in 1917 [29] was by its nature a stochastic quantum jump process. For long the dynamics of single quantum objects were thought to be only of an academic curiosity without practical relevance, since all the experiments were based on macroscopic samples, such as a gas of atoms. However, the experimental advances enabled a direct observation of discrete quantum jumps with single trapped ions in 1986 by many groups [6, 67, 85]; also the quantum jumps in electromagnetic modes have been verified recently in 2007 by Gleyzes *et al.* [45].

The construction of the Thesis is as follows. We start in Chapter 2 with a concise review about the interaction of the EM field and atoms. In Chapter 3 we present the general formalism of the open quantum systems enabling us to work with infinite collections of modes. Stochastic methods for unraveling the dynamics of open quantum systems are then discussed in Chapter 4. In Chapter 5 we review the most important dynamical characterizations used in the research papers constituting the Thesis and Chapter 6 introduces briefly the applied numerical methods. Finally, we summarize the results and conclude in Chapter 7.

Chapter 2

Interaction of atoms and an electromagnetic field

Maxwell's equations for electric and magnetic field vectors $\mathbf{E}$ and $\mathbf{B}$ in vacuum are

$$\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0}\rho, \qquad \text{Gauss's law} \tag{2.1}$$

$$\nabla \cdot \mathbf{B} = 0, \qquad \text{Gauss's law for magnetism} \tag{2.2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \qquad \text{Maxwell–Faraday equation} \tag{2.3}$$

$$\nabla \times \mathbf{B} = \mu_0\epsilon_0\frac{\partial \mathbf{E}}{\partial t} + \mu_0\mathbf{J}, \qquad \text{Maxwell–Ampère equation} \tag{2.4}$$

where ρ is the free charge density, $\mathbf{J}$ is the free current density vector, and ϵ_0 and μ_0 are the vacuum permittivity and permeability (see, e.g., Ref. [87]). Electric and magnetic fields are induced by local charges and currents. In free space where the charge and current densities vanish the field propagates radiatively at the speed of light $c = 1/\sqrt{\mu_0\epsilon_0}$.

An atom is a complex compound of a nucleus surrounded by a cloud of electrons. The internal dynamics is governed by the Coulomb interaction of the charged constituent particles. In quantum mechanics the structure is organized by solving the eigenstates of the Hamiltonian operator H_A describing the sources of energy within the atom. Depending on the level of precision needed, corresponding terms are added into the Hamiltonian and the structure gets correspondingly more detailed [10]. Same characterization in terms of eigenstates applies to external, phase-space, degrees of freedom.

Declaring such basis of eigenstates, the internal dynamics of the atom is then characterized by transitions between the basis states; this is an immense simplification as compared to solving the structural model of the atom. Transitions arise because any distortion, e.g., by presence of an EM field, changes the eigenstate structure corresponding to the total system. By symmetry and resonance arguments, the field allows transitions between selected eigenstates, while other connections are much weaker and can be neglected. Preparing the atom to a specific initial state allows us to describe the complex atomic dynamics by a selected set of electronic eigenstates, which are effectively intercoupled by the field (this is the case in papers **II**, **III**, and **IV**). Equally, the internal state may be left intact and the dynamics is purely in the motional state (paper **I**), or the internal and motional states may by intertwined (paper **VI**).

In the following, we will see how the EM field is capable of producing all this variety of dynamical effects for the atom. We will look at the quantum theory of the EM radiation interacting with an atom, and as a limiting case the corresponding classical plane wave description. Furthermore, we will see how the field can be utilized for producing an external potential landscape for the motional dynamics.

2.1 Quantum theory

The quantized radiative EM field components are

$$\mathbf{E}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda} \hat{\mathbf{e}}_{\mathbf{k},\lambda}\, \mathcal{E}_{\mathbf{k}}\, a_{\mathbf{k},\lambda}\, e^{-i\nu_k t + i\mathbf{k}\cdot\mathbf{r}} + H.c., \tag{2.5}$$

$$\mathbf{B}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda} \frac{\mathbf{k}\times\hat{\mathbf{e}}_{\mathbf{k},\lambda}}{\nu_k}\, \mathcal{E}_{\mathbf{k}}\, a_{\mathbf{k},\lambda}\, e^{-i\nu_k t + i\mathbf{k}\cdot\mathbf{r}} + H.c., \tag{2.6}$$

where $\hat{\mathbf{e}}_{\mathbf{k},\lambda}$ are the two orthogonal complex field polarization vectors; λ is the polarization state; $\mathcal{E}_{\mathbf{k}} = \sqrt{\hbar\nu_k/2\epsilon_0 V}$, with the quantization (mode) volume V, is the field strength unit; $a_{\mathbf{k},\lambda}$ are the bosonic mode annihilation operators; and *H.c.* denotes a Hermitian conjugate. The self-energy of the field is then given by a Hamiltonian

$$H_F = \frac{1}{2}\int_V \mathrm{d}^3\mathbf{r}\left[\epsilon_0|\mathbf{E}(\mathbf{r},t)|^2 + \frac{1}{\mu_0}|\mathbf{B}(\mathbf{r},t)|^2\right] = \sum_{\mathbf{k},\lambda}\hbar\nu_k\left(a^\dagger_{\mathbf{k},\lambda}a_{\mathbf{k},\lambda} + \frac{1}{2}\right). \tag{2.7}$$

As a non-interacting boson, the field mode is analogous to a harmonic oscillator, and the free radiation field is diagonalized by Fock states $|\{n_{\mathbf{k},\lambda}\}\rangle = \bigotimes_{\mathbf{k},\lambda}|n_{\mathbf{k},\lambda}\rangle$.

The free atomic energy is likewise diagonalized as

$$H_A = \sum_i \hbar\omega_i |i\rangle\langle i|, \tag{2.8}$$

where i covers an appropriate set of quantum numbers relevant for the case. Starting with a definite atomic initial state, the dynamics will be essentially restricted to levels for which the (Bohr) transition frequencies $\omega_{ij} = \omega_i - \omega_j$ reside in the immediate vicinity of the field mode range. Reversely, only modes which are in the vicinity of the possible transition frequencies need to be considered. Therefore, the description of the dynamics is readily simplified by considering only such quasiresonant transitions.

The total Hilbert space of the atom-field system is $\mathcal{H}_T = \mathcal{H}_A \otimes \mathcal{H}_F$, such that the total Hamiltonian is $H_T = H_A \otimes I_F + I_A \otimes H_F + H_I$, where I_α is the identity operator and H_I contains the coupling between the atom and the field.

In the dipole approximation (wavelength of the radiation is assumed large as compared to atomic dimensions), the leading term in the atom-field coupling comes from the electric field $\mathbf{E}$ interacting with the atomic dipole moment $\mathbf{d}$ [10], such that the interaction Hamiltonian is

$$H_I \simeq -\mathbf{d} \cdot \mathbf{E}. \tag{2.9}$$

The dipole moment operates in the atomic space $\mathcal{H}_A$ and is expressed in terms of the eigenstates of H_A as $\mathbf{d} = \sum_{ij} \mathbf{d}_{ij} |i\rangle\langle j|$, where $\mathbf{d}_{ij} = \langle i|\mathbf{d}|j\rangle$ is the matrix element. Transitions $i \leftrightarrow j$ for which $\mathbf{d}_{ij} \neq 0$ are dipole allowed; others are forbidden in which case otherwise negligibly weak magnetic dipole and electric quadrupole transitions may contribute. Typically, the atomic states are parity eigenstates, which implies that $\mathbf{d}_{ii} = 0$ and that there is no permanent dipole moment.

2.1.1 Coupling of a single atom with a single mode

The quantum mechanical interaction between an EM field and an atom is described by an interchange of excitations between the atom and a field mode. The prototype model for such mechanism was provided in the 1960's by Jaynes and Cummings [52], who considered a single-mode field ($\nu_k = \omega_F$ and $\hat{\mathbf{e}}_{\mathbf{k},\lambda} = \hat{\mathbf{e}}_F$) interacting quasiresonantly with a two-level atom (Bohr frequency $\omega_A = \omega_a - \omega_b$). The Hamiltonian is in a generic form

$$H_{JC} = \hbar\omega_F \Big(a^\dagger a + \frac{1}{2}\Big) + \hbar\omega_A \sigma_+\sigma_- + \big(\hbar g a^\dagger \sigma_- + H.c.\big), \tag{2.10}$$

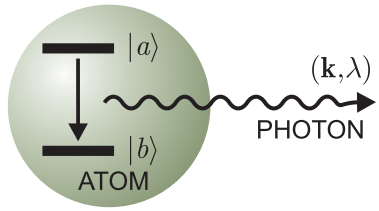

Figure 2.1: The interaction of an atom and an EM field is described as an exchange of an excitation: the atom relaxes from an excited state $|a\rangle$ to a ground state $|b\rangle$ and a photon in the mode $(\mathbf{k}, \lambda)$ is created. A reverse process annihilates the photon and excites the atom.

where a and $a^\dagger$ are the annihilation and the creation operators of the single quasiresonant EM mode and $\sigma_- = |b\rangle\langle a|$ and $\sigma_+ = \sigma_-^\dagger$ are the atomic lowering and raising operators for the relevant transition. The strength of the coupling is given by the coupling parameter $g = \mathbf{d}_{ba} \cdot \hat{\mathbf{e}}_F \mathcal{E}_\mathbf{k}/\hbar$. The coupling is written within the rotating wave approximation (RWA), or secular approximation, where energy-non-conserving terms are neglected [78, 87], see Fig. 2.1 for an illustration of the basic interaction process. The RWA is valid for $|g| \ll \omega_F, \omega_A$, i.e., weak coupling; otherwise the treatment must involve rediagonalization of the Hamiltonian in terms of dressed states.

2.1.2 Coupling of many atoms with a single mode

Interaction of N identical atoms with a classical EM field was studied by Dicke [25] in the 1950's. In terms of a quantized field, the straightforward generalization of the Jaynes–Cummings model (2.10) was provided by Tavis and Cummings [95] in the late 1960's as

$$H_{TC} = \hbar\omega_F\left(a^\dagger a + \frac{1}{2}\right) + \sum_{j=1}^{N} \hbar\omega_A \sigma_+^{(j)}\sigma_-^{(j)} + \sum_{j=1}^{N}\left(\hbar g^{(j)} a^\dagger \sigma_-^{(j)} + H.c.\right), \quad (2.11)$$

Under homogeneous conditions, where each atom couples to the field identically ($g^{(j)} = g$), the model can also be written in terms of collective spin operators $S_\alpha = \sum_{j=1}^{N} \sigma_\alpha^{(j)}$, with $\alpha = \pm, z$, fulfilling the same angular momentum commutation relations as the single-atom operators. Therefore, the collection of N atoms can be described collectively as a single spin object, a Dicke state. This is the origin of superradiance and subradiance [47, 49] discussed more in Sec. 5.5.

2.1.3 Coupling of a single atom with many modes

A collection of modes interacting with an atom is described by a Hamiltonian

$$H = \sum_{\mathbf{k},\lambda} \hbar\nu_{\mathbf{k}} \left(a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + \frac{1}{2} \right) + \hbar\omega_A \sigma_+\sigma_- + \sum_{\mathbf{k},\lambda} (\hbar g_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k},\lambda} \sigma_- + H.c.). \quad (2.12)$$

In the limit of large mode volume, $V \to \infty$, the modes form a continuum. This kind of coupling is treated by the Weisskopf–Wigner theory [99] which explains the phenomenon of spontaneous emission of radiation [29] by coupling to the surrounding vacuum. Passing to the continuum of modes goes by substitution

$$\sum_{\mathbf{k},\lambda} \longrightarrow 2V \int \frac{\mathrm{d}^3k}{(2\pi)^3} = \frac{1}{4\pi} \int \mathrm{d}\Omega \int_0^\infty \mathrm{d}\nu_k \, D(\nu_k), \quad (2.13)$$

where $D(\nu_k)$ is the density of modes at frequency ν_k. Looking at the evolution of an initial state $|\psi(0)\rangle = \big[c_a(0)|a\rangle + c_b(0)|b\rangle\big] \otimes |0\rangle$ (field vacuum $|0\rangle = \bigotimes_{\mathbf{k},\lambda} |0_{\mathbf{k},\lambda}\rangle$) into state $|\psi(t)\rangle = c_a(t)|a;0\rangle + c_b(t)|b;0\rangle + \sum_{\mathbf{k},\lambda} c_{b\mathbf{k}\lambda}(t)|b;\mathbf{k},\lambda\rangle$ (single-excitation state $|\mathbf{k},\lambda\rangle = a^\dagger_{\mathbf{k},\lambda}|0\rangle$), and applying Fermi's golden rule, i.e., assuming that only modes in the immediate vicinity of the transition frequency $\nu_k \simeq \omega_A$ contribute, the excited state amplitude evolves as $\partial_t c_a(t) = -\Gamma(\omega_A) c_a(t)/2$, such that

$$\Gamma(\omega_A) = 2\pi \langle |g_{\mathbf{k},\lambda}|^2_{\nu_k=\omega_A} \rangle_\Omega D(\omega_A), \quad (2.14)$$

where the average is taken over the angular distribution Ω. Therefore, the population of the excited state decays exponentially as $|c_a(t)|^2 = e^{-\Gamma(\omega_A)t} |c_a(0)|^2$. In the homogeneous free space, the density of modes is $D(\nu) = V\nu^2/\pi^2c^3$, which implies that the occupation of the excited atomic state will decay spontaneously at rate

$$\Gamma_{\text{free}}(\omega_A) = \frac{1}{4\pi\epsilon_0} \frac{4\omega_A^3 |d_{ba}|^2}{3\hbar c^3}. \quad (2.15)$$

With structured mode densities $D(\nu)$, e.g., in the case of a cavity resonator, the decay rate is modified accordingly. This is the origin of the Purcell effect [49, 77], where the spontaneous decay of an atom is enhanced or suppressed with respect to the free space value Γ_{free}, according to availability of modes at the Bohr frequency ω_A.

2.2 Semiclassical theory

Coherent states $|\alpha\rangle = e^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle$, introduced by Glauber [44] and Sudarshan [94] in the 1960's, are the eigenstates of the field annihilation operator a with an eigenvalue $\alpha \in \mathbb{C}$, and hence unaffected by the operation of a on it. The average of the electric field operator with a coherent state in a single mode $(\mathbf{k}, \lambda)$ is

$$\langle \mathbf{E}(\mathbf{r}, t)\rangle_\alpha = \hat{\mathbf{e}}_{\mathbf{k},\lambda}\mathcal{E}_{\mathbf{k}}\alpha e^{-i\nu_k t + i\mathbf{k}\cdot\mathbf{r}} + c.c. \tag{2.16}$$

This corresponds to a classical plane wave and output from a laser operating far above its threshold [78]. Since the mode population is $n = \langle a^\dagger_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda}\rangle = |\alpha|^2$, the field amplitude scales as $\sqrt{n}$. With strong coherent fields, i.e., $n \gg 1$, the state of the field is not modified by the presence of the atom, and its dynamics is hence decoupled from the atomic one. Therefore, in such circumstances the interaction Hamiltonian is

$$H_I = \hbar g a^\dagger \sigma_- + H.c. \simeq \hbar\Omega\sigma_- + H.c., \tag{2.17}$$

with $\Omega = g\sqrt{n}$, and the state of the field remains constant during the evolution. Consequently, the field can be described by a classical oscillator $\mathbf{E}(\mathbf{r}, t) = \hat{\mathbf{e}}_F\mathcal{E}e^{-i\nu t + i\mathbf{k}\cdot\mathbf{r}} + c.c.$, which is driving a quantum mechanically described atom via electric dipole moment $\mathbf{d}$. This is the semiclassical theory of atom-field interaction.

2.2.1 Optical traps

In a weak coupling limit, the population transfer from a lower atomic state $|b\rangle$ to an upper one $|a\rangle$ is negligible, especially so if the Bohr and mode frequencies are detuned, $\delta = \omega_F - \omega_A \neq 0$, from each other [87]. Hence, the excited state can be removed from the equation of motion altogether. However, the mere presence of the excited state affects the dynamics of the lower state. With $|\Omega| \ll |\delta|$, the coupling induces an energy shift, an AC Stark shift, which is given by an adiabatic elimination procedure as well as equal second order perturbation theory considerations [73]. This can be viewed as an interaction between induced dipole moment $\langle \mathbf{d}\rangle = \alpha\mathbf{E}$, where α is the polarizability of the atom, with the electric field. The shift is then

$$\Delta E(\mathbf{r}) = -\frac{1}{2}\alpha\langle \mathbf{E}^2(\mathbf{r}, t)\rangle_t, \tag{2.18}$$

where the time-averaged field amplitude $\langle \mathbf{E}^2(\mathbf{r}, t)\rangle_t = 2|\mathcal{E}(\mathbf{r})|^2$, and $\alpha(\delta) = -|\mathbf{d}_{ba}\cdot\hat{\mathbf{e}}_F|^2/\hbar\delta$, giving a shift $\Delta E(\mathbf{r}) = \hbar\Omega^2(\mathbf{r})/\delta$; the spatial dependency

comes from the transverse beam profile. Moreover, including the finite lifetime of the excited atomic state (cf. Sec. 2.1.3) heuristically as an additional imaginary contribution to the energy, $\hbar\omega_a \mapsto \hbar\omega_a - i\hbar\Gamma_a/2$, the polarizability becomes a complex quantity. Correspondingly, the energy shift is now given by $\Delta E(\mathbf{r}) = V(\mathbf{r}) - i\hbar\Gamma_b(\mathbf{r})/2$, where the real part is

$$V(\mathbf{r}) = \hbar \frac{\delta^2}{\delta^2 + (\Gamma_a/2)^2} \frac{\Omega^2(\mathbf{r})}{\delta} \tag{2.19}$$

and the effective decay rate of the ground state is

$$\Gamma_b(\mathbf{r}) = \frac{\delta^2}{\delta^2 + (\Gamma_a/2)^2} \frac{\Omega^2(\mathbf{r})}{\delta^2} \Gamma_a. \tag{2.20}$$

The spatial dependence of the induced energy shift $\Delta E(\mathbf{r})$ corresponds to an effective force $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ acting on the atom. Since $\mathrm{sign}[\alpha(\delta)] = -\mathrm{sign}(\delta)$, the direction of the induced electric dipole as compared to the electric field depends on the detuning. Hence, if the driving is below resonance, i.e., $\delta < 0$, the field maximum corresponds to the energy shift minimum, and vice versa. This has been utilized by experiments with cold atoms [73] in order to create a trapping potential for the gaseous atoms inside a vacuum of matter. A single laser beam creates a simple attractive or repulsive potential (depending on the sign of the detuning δ) in its transverse profile, while with opposing beams a periodic standing wave emerges in the longitudinal direction forming a sequence of potential minima and maxima, i.e., an optical lattice (see Refs. [8, 53] for a review).

2.2.2 Magnetic traps

In the radiation field, the coupling of the magnetic field to an atom is weak as compared to the electric dipole coupling. However, in the non-radiative case, e.g., a classical field $\mathbf{B}(\mathbf{r}, t)$ induced by a current $\mathbf{J}$ according to Ampère's law (2.4), the influence of the magnetic field may be significant. The magnetic field couples with the intrinsic dipole moment of the atom $\boldsymbol{\mu} = -\mu_0(g_S\mathbf{S} + g_L\mathbf{L} + g_I\mathbf{I})/\hbar$, where $\mu_0 = |e|\hbar/2m_e$ is the Bohr magneton and g_α are the Landé g-factors for electronic spin (S), orbital (L), and nuclear spin (I) angular momentum [10]. The interaction Hamiltonian is

$$H_I = -\boldsymbol{\mu} \cdot \mathbf{B}. \tag{2.21}$$

With low magnetic fields, when the resulting energy shift is small compared to the hyperfine splitting, the eigenstates of the total angular momentum

$\mathbf{F} = \mathbf{I}+\mathbf{L}+\mathbf{S}$, $|F, M_F\rangle$, diagonalize the Hamiltonian describing the internal degrees of freedom by a good approximation, and the term corresponds to a linear Zeeman splitting $U(\mathbf{B}) = U(F) + \mu_0 g_F \mathbf{F} \cdot \mathbf{B}$. An inhomogeneous magnetic field amplitude $\mathbf{B}(\mathbf{r})$ forms therefore a spatial potential, which is dependent on the internal state of the atom. According to Maxwell's equations it is possible to create only a field minimum in the charge- and current-free space. Correspondingly, atoms in the low-field-seeking Zeeman sublevels M_F, for which the interaction energy decreases towards the lower field strength, can be trapped in the magnetic field minimum [73].

Chapter 3

Open quantum system

As discussed briefly in Sec. 2.1.3, in a large space the EM modes cover the spectrum densely. Therefore, it is no longer possible to single out an individual mode driving the interaction and neglect the neighboring modes altogether. Mathematically, a conceptually valid Hamiltonian for the total system can be written down and the corresponding unitary evolution is therefore formally soluble. However, in practice the calculations become unfeasible. The same limitation is encountered in classical statistical mechanics, when a system evolves in an irreversible way when coupled to a thermodynamical reservoir [49]. Moreover, one may not even be interested in the exact dynamics of the total system, but desires information only about a selected part of it. The quantum optical examples described in Chapter 2 are an example of such scenario. Indeed, any realistic physical system is inevitably subject to interactions with the surrounding EM modes, and a complete isolation from the outside world is always a mere approximation.

The theory of open quantum systems [14] provides the machinery for characterizing the dynamics of the relevant degrees of freedom, while the existence of the rest enters the description in an effective way. The total (T) Hilbert space is divided correspondingly into system (S) and environment (E) parts as $\mathcal{H}_T = \mathcal{H}_S \otimes \mathcal{H}_E$, and the microscopical Hamiltonian for the total system, if such is known, is accordingly of form $H_T = H_S \otimes I_E + I_S \otimes H_E + H_I$. Formally, the reduced state evolution in $\mathcal{S}(\mathcal{H}_S)$ (space of density operators of $\mathcal{H}_S$) is then given by $\rho_S(t_0) \mapsto \rho_S(t) \equiv \mathrm{tr}_E[\rho_T(t)] = \mathrm{tr}_E[U(t,t_0)\rho_T(t_0)U^\dagger(t,t_0)] \equiv \Phi(t,t_0)\rho_S(t_0)$, where $\Phi(t,t_0)$ is a dynamical map, which reflects the unitary evolution of the total system as restricted in the reduced space, reached by a partial trace over the environment degrees of freedom. In general, the dynamics is non-unitary in the reduced state

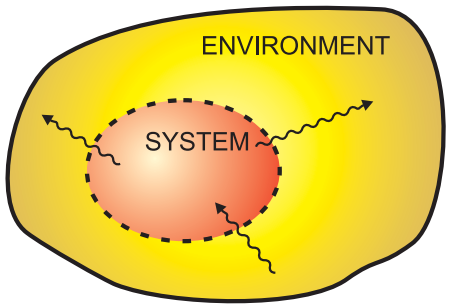

Figure 3.1: An open quantum system is a limited part of a larger entity. Interaction with the environmental degrees of freedom results in exchange of energy and information, which reflects into non-coherent dynamics of the reduced state.

space, and the state has to be characterized by a density operator, whose equation of motion is a called a master equation.

3.1 Projection operator techniques

Exact master equations for the dynamics of an open quantum system $\rho_S(t)$ based on the microscopical model of the total system are provided systematically by projection operator techniques. There are essentially two different approaches: (i) a method developed by Nakajima [68] and Zwanzig [105] in the late 1950's, which produces an integro-differential master equation, and (ii) the corresponding method by Shibata [21, 91] from the late 1970's forming a time-convolutionless (TCL) master equation.

3.1.1 Nakajima–Zwanzig approach

For future perturbative purposes, let us denote the interaction Hamiltonian by αH_I, where α is a unitless scaling factor. In the interaction picture the total closed system evolves as

$$\frac{\partial}{\partial t}\rho(t) = -\frac{i}{\hbar}\alpha[H_I(t), \rho(t)] \equiv \alpha\mathcal{L}(t)\rho(t), \tag{3.1}$$

where $\mathcal{L}(t)$ is the Liouville superoperator. Introducing a projection $\mathcal{P} : \rho(t) \mapsto \mathrm{tr}_E[\rho(t)] \otimes \rho_E = \rho_S(t) \otimes \rho_E$, with a stationary environment state $\rho_E \in \mathcal{S}(\mathcal{H}_E)$, and a complementary projection $\mathcal{Q} = I - \mathcal{P}$, an exact equation

of motion for $\mathcal{P}\rho(t)$ is given by

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \alpha\mathcal{P}\mathcal{L}(t)\mathcal{G}(t,t_0)\mathcal{Q}\rho(t_0) + \alpha\mathcal{P}\mathcal{L}(t)\mathcal{P}\rho(t) + \alpha^2\int_{t_0}^{t}\mathrm{d}s\,\mathcal{P}\mathcal{L}(t)\mathcal{G}(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}\rho(s), \tag{3.2}$$

where the propagator is $\mathcal{G}(t,t_0) = \mathcal{T}_{\leftarrow}\exp\left[\alpha\int_{t_0}^{t}\mathrm{d}s\,\mathcal{Q}\mathcal{L}(s)\right]$, with a time-ordering operator $\mathcal{T}_{\leftarrow}$. Especially, the above Nakajima–Zwanzig master equation is valid with any initial total state $\rho(t_0)$ and any coupling strength characterized by α. However, solving such an integro-differential equation is in general difficult.

With factorizing initial state $\rho(t_0) = \rho_S(t_0)\otimes\rho_E$ and under a technical assumption of vanishing odd moments of $H_I(t)$, the equation simplifies into

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \int_{t_0}^{t}\mathrm{d}s\,\mathcal{K}(t,s)\mathcal{P}\rho(s), \tag{3.3}$$

where the memory kernel $\mathcal{K}(t,s) = \alpha^2\mathcal{P}\mathcal{L}(t)\mathcal{G}(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}$ connects the whole past evolution $\mathcal{P}\rho(t_0) \to \mathcal{P}\rho(t)$ to the momentary evolution $(\partial/\partial t)\mathcal{P}\rho(t)$.

3.1.2 Time-convolutionless approach

To overcome the practical difficulty of solving an integro-differential equation, the exact Nakajima–Zwanzig master equation (3.2) can be cast into a TCL form by introducing a backward propagator $G(t,t_0) = \mathcal{T}_{\rightarrow}\exp\left[-\alpha\int_{t_0}^{t}\mathrm{d}s\,\mathcal{L}(s)\right]$, such that $\rho(s) = G(t,s)\rho(t)$. Therefore, one arrives at another exact master equation

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t) + I(t)\mathcal{Q}\rho(t_0), \tag{3.4}$$

where the TCL generator is $\mathcal{K}(t) = \alpha\mathcal{P}\mathcal{L}(t)[1-\Sigma(t)]^{-1}\mathcal{P}$ and the inhomogeneity term $I(t) = \alpha\mathcal{P}\mathcal{L}(t)[1-\Sigma(t)]^{-1}\mathcal{G}(t,t_0)\mathcal{Q}$, with $\Sigma(t) = \alpha\int_{t_0}^{t}\mathrm{d}s\,\mathcal{G}(t,s)\mathcal{Q}\mathcal{L}(s)\mathcal{P}G(t,s)$. Correspondingly, the TCL master equation is now local in time, i.e., it depends explicitly only on $\rho(t)$ in contrast to the Nakajima–Zwanzig form (3.2), where the past evolution enters through the time convolution.

Obviously, the evaluation is still in general difficult, but a systematic expansion of the generator in terms of the coupling parameter α as $\mathcal{K}(t) =$

$\sum_n \alpha^n \mathcal{K}_n(t)$ is possible, see Ref. [14] for details. In the second order, the TCL generator is

$$\mathcal{K}_2(t) = \int_{t_0}^{t} \mathrm{d}s\, \mathcal{P}\mathcal{L}(t)\mathcal{L}(s)\mathcal{P}, \tag{3.5}$$

which upon insertion of the Liouvillian (3.1) and tracing over the environment degrees of freedom gives

$$\frac{\partial}{\partial t}\rho_S(t) = -\alpha^2 \int_{t_0}^{t} \mathrm{d}s\, \mathrm{tr}_E\Big\{\big[H_I(t), [H_I(s), \rho_S(t)\otimes\rho_E]\big]\Big\}. \tag{3.6}$$

3.1.3 Lindblad structure

Curiously, it can be shown [12, 14, 46] that in any order the structure of the TCL master equation is

$$\begin{aligned}\frac{\partial}{\partial t}\rho_S(t) = &-\frac{i}{\hbar}[H(t), \rho_S(t)] \\ &+ \sum_k \Delta_k(t)\Big[C_k(t)\rho_S(t)C_k^\dagger(t) - \frac{1}{2}\big\{C_k^\dagger(t)C_k(t), \rho_S(t)\big\}\Big],\end{aligned} \tag{3.7}$$

where $H(t)$ is the renormalized system Hamiltonian consisting of the original $H_S(t)$ and the Hermitian contribution due to the presence of the environment, $C_k(t)$ are the Lindblad (jump) operators for channel k, and $\Delta_k(t) \in \mathbb{R}$ are the corresponding decay rates. The Lindblad operators arise because of the interaction with the environment degrees of freedom, and they produce non-unitary dynamics in contrast with the commutator part, which corresponds to the Liouville–von Neumann equation, cf. Eq. (3.1), for closed quantum systems.

This general structure is particularly interesting. Its time-independent version with $\Delta_k > 0$ has been studied in the mid-1970's by Gorini *et al.* [46] and Lindblad [61], who proved that a bounded generator of any semigroup of completely positive trace-preserving dynamical maps, i.e., $\Phi(t+s) = \Phi(t)\Phi(s)$, can be cast into such form, the Lindblad form, with countable number of operators C_k and vice versa. By this analogy, the time-dependent generalization expressed in Eq. (3.7) is said to have a Lindblad structure, though it is not guaranteed that the corresponding dynamical maps generated by it would have the above-mentioned general mathematical properties.

3.2 Approximations

3.2.1 Born approximation

Born approximation relies on a weak coupling between the system and the environmental degrees of freedom. In terms of the Nakajima–Zwanzig approach, it corresponds to restricting to the lowest non-trivial order of the coupling parameter α, i.e., setting $\mathcal{G}(t,s) \simeq 1$, which gives

$$\frac{\partial}{\partial t}\rho_S(t) = -\alpha^2 \int_{t_0}^{t} \mathrm{d}s\, \mathrm{tr}_E\Big\{\big[H_I(t),[H_I(s),\rho_S(s)\otimes\rho_E]\big]\Big\}. \qquad (3.8)$$

The corresponding TCL master equation (3.6) expanded in the same order of α differs only by being local in time.

3.2.2 Markov approximation

A Markov approximation is a further assumption that the system does not have time to evolve significantly during the interval in which the memory kernel $\mathcal{K}(t,s)$ contributes in the time convolution (3.3). Consequently, in the Born approximation (3.8), $\rho(s)$ may be replaced by $\rho(t)$ making it identical to the TCL equation (3.6), and the integration over time can be likewise extended to infinity. This approximation corresponds to a coarse-graining of the time evolution: it neglects any correlations appearing between the system and the environment by supposing them to disappear at a rate much faster than the system evolution time scale.

3.3 Quantum optical master equation

3.3.1 Spontaneous decay into vacuum

In Sec. 2.1.3 the coupling of an atom and an infinite reservoir of environment modes was examined in the weak coupling limit by Weisskopf–Wigner approach, which revealed an irreversible decay of the excited state population. Let us now revisit the situation in a more general context using the projection operator techniques. In the interaction picture and within RWA, the interaction Hamiltonian is of form $H_I(t) = \sigma_+(t)\otimes B(t) + \sigma_-(t)\otimes B^\dagger(t)$, where $B(t) = \sum_{\mathbf{k},\lambda} g_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} e^{-i\nu_k t}$, with $g_{\mathbf{k},\lambda} = \mathbf{d}_{ba}\cdot\hat{\mathbf{e}}_{\mathbf{k},\lambda}\mathcal{E}_k/\hbar$. In the Born approximation, the resulting second order master equation has a Lindblad

structure

$$\frac{\partial}{\partial t}\rho_S(t) = -iS(t)\big[\sigma_+\sigma_-, \rho_S(t)\big] + \gamma(t)\Big[\sigma_-\rho_S(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S(t)\}\Big], \tag{3.9}$$

where the time-dependent frequency shift $S(t)$ and the decay rate $\gamma(t)$ are given by

$$S(t) = \int_0^t \mathrm{d}s \int_0^\infty \mathrm{d}\omega\, J(\omega) \sin\big[(\omega_A - \omega)(t-s)\big], \tag{3.10}$$

$$\gamma(t) = 2\int_0^t \mathrm{d}s \int_0^\infty \mathrm{d}\omega\, J(\omega) \cos\big[(\omega_A - \omega)(t-s)\big]. \tag{3.11}$$

These factors are expressed in terms of a spectral density $J(\omega) = \langle |g_{\mathbf{k},\lambda}|^2_{\nu_k=\omega}\rangle_\Omega D(\omega)$, where $D(\omega)$ is the density of modes. The spectral properties depend on the physical setup, and reflect directly into the dynamics of the reduced state through the time-dependent decay rates and shifts. Long-time limit gives the corresponding Born–Markov solution, where the decay rate $\gamma = \lim_{t\to\infty}\gamma(t) = 2\pi J(\omega_A) \geq 0$ coincides with the golden rule result (2.14), though the short time behavior may involve periods where $\gamma(t)$ is even negative.

3.3.2 Born–Markov master equation in thermal bath

In the Born–Markov and RWA schemes, the quantum optical master equation for an atom interacting with a thermal reservoir, or a bath, of EM modes at temperature T is

$$\frac{\partial}{\partial t}\rho_S(t) = -\frac{i}{\hbar}[H_{LS}, \rho_S(t)] + \mathcal{D}[\rho_S(t)]. \tag{3.12}$$

In the thermal equilibrium state $\rho_E = e^{-H_E/k_BT}/\mathrm{tr}[e^{-H_E/k_BT}]$, where k_B is the Boltzmann constant, the mode occupation numbers $N(\nu_k) = 1/(e^{\hbar\nu_k/k_BT} - 1)$ are in accordance with the Bose–Einstein distribution. Above, the Hermitian $H_{LS} = \sum_\omega \hbar S(\omega)\mathbf{A}^\dagger_\omega \cdot \mathbf{A}_\omega$ is the environment-induced rescaling of the energies by the Lamb shift (induced by vacuum fluctuations, i.e., the finite $T \to 0$ limit) and the Stark shift (induced by the radiation field), with a rate factor

$$S(\omega) = \frac{1}{4\pi\epsilon_0}\frac{2}{3\pi\hbar c^3}\mathrm{P}\int_0^\infty \mathrm{d}\nu_k\, \nu_k^3 \left[\frac{1+N(\nu_k)}{\omega - \nu_k} + \frac{N(\nu_k)}{\omega + \nu_k}\right]. \tag{3.13}$$

Altogether, the master equation is in Lindblad form, and the non-unitary part is

$$\mathcal{D}[\rho_S] = \sum_{\omega>0} \frac{1}{4\pi\epsilon_0}\frac{4\omega^3}{3\hbar c^3}[1+N(\omega)]\Big(\mathbf{A}_\omega \rho_S \mathbf{A}_\omega^\dagger - \frac{1}{2}\big\{\mathbf{A}_\omega^\dagger \mathbf{A}_\omega, \rho_S\big\}\Big) + \sum_{\omega>0} \frac{1}{4\pi\epsilon_0}\frac{4\omega^3}{3\hbar c^3} N(\omega)\Big(\mathbf{A}_\omega^\dagger \rho_S \mathbf{A}_\omega - \frac{1}{2}\big\{\mathbf{A}_\omega \mathbf{A}_\omega^\dagger, \rho_S\big\}\Big). \tag{3.14}$$

The atomic operator $\mathbf{A}_\omega = \sum_{a,b:\omega_a-\omega_b=\omega} \mathbf{d}_{ba}|b\rangle\langle a|$ operates simultaneously on every pair of states separated by the same energy $\hbar\omega$. From the point of view of measurement theory, this corresponds to detecting a photon at frequency ω without knowledge about which transition emitted it. In the limit of $T \to 0$ and a two-level atom, the non-unitary part simplifies into

$$\mathcal{D}[\rho_S(t)] = \Gamma(\omega_A)\Big(\sigma_-\rho_S\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S\}\Big), \tag{3.15}$$

where the decay rate $\Gamma(\omega_A)$ is exactly the same as given by the free-space Weisskopf–Wigner theory in Sec. 2.1.3.

3.4 Structured reservoirs

As noticed in Sec. 3.3, the influence of the environment is defined by the spectral density $J(\omega)$ and the state of the environment ρ_E. In flat structures, such as the free space, the Born–Markov scheme works well, and even the dynamics in short time scales, which is neglected in the Markov approximation, is by its character similar to the exact solution. However, elaborate structures may enhance the system-environment correlations such that the Born and the Markov approximations deviate significantly from the exact solution. Examples of such cases are provided by lossy cavity resonators [37, 49], which correspond to a Lorentzian spectral density peaked at the resonance frequency and broadened because of the losses, and photonic band gap materials [54, 103], which possess a characteristic feature of a complete absence of certain ranges of modes. With more involved structures, even the systematic TCL expansion of the dynamics may fail in any order, and alternative derivation methods have to be used [13]. The ability to control and modify the structure and the state of the environment gives an opportunity to influence the character of the system evolution. This approach is called reservoir engineering [59, 97].

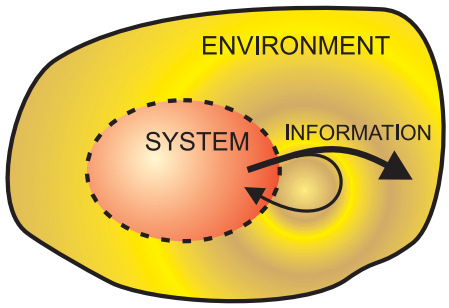

Figure 3.2: In the information-theoretical approach to non-Markovianity, the strong correlations between the system and the environment create a feedback of information, which the system has leaked to the environment earlier. This back-flow generates non-Markovian reduced system dynamics. The correlations may be enhanced by structured environments.

3.5 Markovian and non-Markovian dynamics

Non-Markovian dynamics is described as being dependent on its own past. Recently, there have been proposals for quantifying this memory property rigorously in the context of open quantum systems [16, 62, 82, 101]. Breuer *et al.* [16, 58] define non-Markovianity in terms of a flow of information from the environment back to the system (Fig. 3.2). This flow is detected by looking at the evolution of the trace distance of two different initial states under the influence of the dynamical map Φ: any increase in the distance $D[\rho_1(t), \rho_2(t)] = \frac{1}{2}\mathrm{tr}|\rho_1(t) - \rho_2(t)|$, where $\rho_i(t) = \Phi(t, t_0)\rho_i(t_0)$ and $|A| = \sqrt{A^\dagger A}$, indicates non-Markovianity. The increase means that the distinguishability of the states increases in this period, i.e., information which had leaked into correlations between the system and the environment returns back to the system. It should be emphasized that this definition does not depend on any specific mathematical formulation of the dynamical map Φ, especially no assumptions about the underlying generator and master equation are made.

This definition of non-Markovianity is related to the divisibility property of the completely positive trace-preserving (CPT) dynamical map, such that the non-Markovian maps $\Phi(t, t_0)$ can not be divided arbitrarily into products of consecutive CPT maps $\Phi(t, t_0) \neq \Phi(t, t_1)\Phi(t_1, t_0)$, with $t \geq t_1 \geq t_0$, in the spirit of a semigroup. If and only if such division is, however, always possible, the generator of the map can be cast into a

(time-dependent) Lindblad structure (3.7) with positive decay rates [58, 82]. Therefore, a (time-dependent) Lindblad structure with positive decay rates generates (time-dependent) Markovian dynamics. In conclusion, the appearance of negative decay rates seems to be closely connected with the notion of non-Markovianity [58], but they alone are not a sufficient requirement [64].

Lu *et al.* [62] have proposed a similar information-theoretical definition by dividing the total flow of (quantum Fisher) information into additive sub-flows corresponding to channels, such that any back-flow component indicates non-Markovianity. On the other hand, Rivas *et al.* [82] equate divisibility and Markovianity and, finally, Wolf *et al.* [101] approach the issue by snapshots of evolution at a given moment of time. The definitions are obviously not fully compatible with each other (see Ref. [58] for comparison).

Chapter 4

Stochastic methods for open quantum systems

Determining the evolution of a density operator from a given master equation analytically is in general beyond possibilities, even after various approximation schemes. Therefore, generic numerical methods are required. In the early 1990's powerful stochastic methods to solve Markovian open quantum system dynamics, described by a general master equation having a Lindblad structure

$$\frac{\partial}{\partial t}\rho_S = -\frac{i}{\hbar}[H(t),\rho_S] + \sum_k \Delta_k(t)\Big[C_k(t)\rho_S C_k^\dagger(t) - \frac{1}{2}\big\{C_k^\dagger(t)C_k(t),\rho_S\big\}\Big] \quad (4.1)$$

with positive decay rates, were introduced by Dalibard *et al.* [24, 66], Dum *et al.* [27, 28], Carmichael [19], and Gisin *et al.* [41, 42, 43]. The breakthrough was to unravel the evolution of the density operator in terms of an ensemble of single realizations (i.e., trajectories [19]) of an underlying stochastic process for pure states. Accordingly, all the physical quantities are determined as an ensemble average. The celebrated feature of this approach is that with pure states the dimensionality of the single problem is $D = \dim(\mathcal{H}_S)$, while with a corresponding density operator the dimension scales as D^2. The computational cost is thereby overwhelmingly reduced as D gets large, which is the case, e.g., in laser cooling studies [66].

4.1 Unraveling of the evolution

A projective Hilbert space $\mathcal{P}(\mathcal{H})$ is a space of rays, such that each point $|\psi\rangle \in \mathcal{P}(\mathcal{H})$ corresponds to an equivalence class $[\psi] = \big\{|\phi\rangle \in \mathcal{H}\big||\phi\rangle =$

$e^{i\theta}|\psi\rangle, \theta \in \mathbb{R}\}$ in $\mathcal{H}$; in the following we use symbol $\sim$ for this equivalence. Accordingly, any density operator $\rho(t) \in \mathcal{S}(\mathcal{H})$ can be expressed as $\rho(t) = \int \mathrm{d}\psi\, P[\psi,t]|\psi\rangle\langle\psi|$, where $P[\psi,t]$ is a probability distribution functional in $\mathcal{P}(\mathcal{H})$ and $\mathrm{d}\psi = \mathrm{D}\psi\mathrm{D}\psi^*$ is a volume element in a $\mathcal{H}$ [14]. Therefore, the dynamics of $\rho(t)$ is completely characterized by the dynamics of a distribution $P[\psi,t]$, though $P[\psi,t]$ is not uniquely defined for a given $\rho(t)$.

The purpose of the stochastic methods is to exchange the original problem of solving $\rho(t)$ by a computationally simpler problem of evolving a probability distribution functional $P[\psi,t]$. Moreover, the evolution of $P[\psi,t]$ may be expressed as a stochastic process for pure states $|\psi\rangle$, such that an ensemble of single realizations $\{|\psi_i(t)\rangle\}_{i=1}^N$ estimates the distribution by $P[\psi,t] \simeq N^{-1}\sum_i \delta[\psi - \psi_i(t)] = N^{-1}\sum_\alpha N_\alpha(t)\delta[\psi - \phi_\alpha(t)]$, where $\delta[\psi]$ is a functional δ-distribution and $N_\alpha(t)$ is the cardinality of the set $\big\{|\psi_i(t)\rangle\big||\psi_i(t)\rangle \sim |\phi_\alpha(t)\rangle\big\}$, i.e., number of ensemble members belonging to the same ray. Due to this random sampling, such approaches are called Monte Carlo methods. Unfolding the procedure, the evolution of the density operator is approximated by

$$\rho(t) \simeq \frac{1}{N}\sum_\alpha N_\alpha(t)|\phi_\alpha(t)\rangle\langle\phi_\alpha(t)|, \tag{4.2}$$

and the set $\{|\phi_\alpha(t)\rangle\}_{\alpha=1}^{N_{\mathrm{eff}}}$ is called an effective ensemble and $\{N_\alpha(t)\}$, with $\sum_\alpha N_\alpha(t) = N$, are their occupation numbers.

4.2 Markovian methods

There are roughly two categories of unravelings of the master equation as stochastic Schrödinger equations (SSE) [75]: (i) piecewise deterministic processes (PDP) employing quantum jumps at random times [19, 24, 27, 28, 66] and (ii) corresponding diffusive approximation as Itô stochastic equation for a Wiener process generating continuous but nowhere differentiable trajectories [41, 42, 43]. The difference of these quantum jump and quantum state diffusion (QSD) descriptions, correspondingly, is illustrated in Fig. 4.1

The applicability of the quantum-jump unravelings in Refs. [19, 24, 27, 28, 66] is limited to a Lindblad structure with positive decay rates, i.e., Markovian case, since the involved quantum jump probabilities are directly proportional to the decay rates. Likewise, the QSD method in Refs. [41, 42, 43] applies in the same domain.

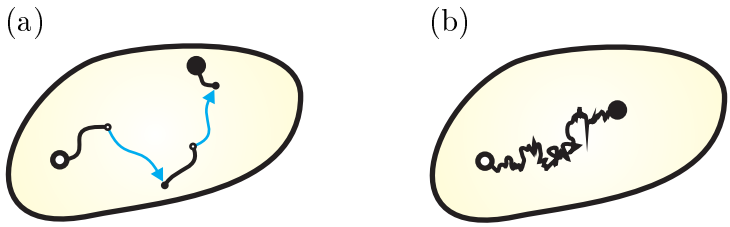

Figure 4.1: Schematic example trajectories in $\mathcal{H}$ generated by a stochastic Schrödinger equation: an initial state $|\psi(t_0)\rangle$ (open circle) evolves in time (along the black line) into a final state $|\psi(t)\rangle$ (close circle). (a) Piecewise deterministic processes generate smooth paths interrupted by quantum jumps (arrows) at random times transforming the state discontinuously. (b) Diffusive processes generate continuous but nowhere differentiable paths.

4.2.1 Piecewise deterministic processes

Starting from the general time-local master equation (4.1) with positive rates, the corresponding SSE in PDP form is, omitting the time arguments,

$$|\mathrm{d}\psi\rangle = -\frac{i}{\hbar}G[\psi]\mathrm{d}t + \sum_k \left(\frac{C_k|\psi\rangle}{\|C_k\psi\|} - |\psi\rangle\right)\mathrm{d}N_k, \tag{4.3}$$

where the non-linear deterministic drift is

$$G[\psi] = \left[H - \frac{i\hbar}{2}\sum_k \Delta_k\Big(C_k^\dagger C_k - \langle C_k^\dagger C_k\rangle_\psi\Big)\right]|\psi\rangle, \tag{4.4}$$

and the infinitesimal (time-inhomogeneous) Poisson increments have properties

$$\mathrm{d}N_k\,\mathrm{d}N_l = \delta_{kl}\,\mathrm{d}N_k, \qquad E[\mathrm{d}N_k] = \Delta_k\|C_k\psi\|^2\mathrm{d}t. \tag{4.5}$$

Above, the average $\langle A\rangle_\psi = \langle\psi|A|\psi\rangle$ and E denotes the expectation value for the random process.

The Monte Carlo wave function (MCWF) method by Dalibard *et al.* [24, 66] solves such SSE by a simple algorithm. A single realization is generated iteratively over a time interval $[0, T]$ by small time steps. The evolution over a single time step δt, $|\psi(t)\rangle \mapsto |\psi(t+\delta t)\rangle$, is done by randomly selecting between a quantum jump by a Lindblad operator C_k or a deterministic

evolution by a non-unitary propagator $U \simeq 1 - i\delta t\, H_{\text{eff}}/\hbar$, where the non-Hermitian Hamiltonian is

$$H_{\text{eff}} = H - \frac{i\hbar}{2}\sum_k \Delta_k C_k^\dagger C_k. \tag{4.6}$$

Using the notation of the effective ensemble, the state $|\psi(t)\rangle \sim |\phi_\alpha(t)\rangle$ for some α. For this generic state the jump probabilities for channels k are given by

$$P_\alpha^k = \delta t\, \Delta_k \langle\phi_\alpha|C_k^\dagger C_k|\phi_\alpha\rangle, \tag{4.7}$$

and the probability for the deterministic evolution is $\tilde{P}_\alpha = 1 - \sum_k P_\alpha^k$. The exclusive choice between a quantum jump or the deterministic evolution is done randomly (e.g., by a linear search [40] where a single uniformly distributed random number $\eta \in [0,1]$ is compared to the cumulative sum of the event probabilities $\{p_i\}_{i=1}^n$ such that the selected event is $I(\eta) = \min\{m \le n | \eta < \sum_{i=1}^m p_i\}$) and the state evolves to $|\psi(t+\delta t)\rangle = |\psi'\rangle/\|\psi'\|$, where the unnormalized state is

$$|\psi'\rangle = \begin{cases} C_k|\psi(t)\rangle, & \text{with probability } P_\alpha^k, \\ U|\psi(t)\rangle, & \text{with probability } \tilde{P}_\alpha. \end{cases} \tag{4.8}$$

Therefore, a quantum jump corresponds to mapping

$$|\phi_\alpha(t)\rangle \sim |\psi(t)\rangle \mapsto |\psi(t+\delta t)\rangle \sim \frac{C_k|\phi_\alpha(t)\rangle}{\|C_k\phi_\alpha(t)\|} \sim |\phi_\beta(t+\delta t)\rangle, \tag{4.9}$$

while deterministic evolution gives

$$|\phi_\alpha(t)\rangle \sim |\psi(t)\rangle \mapsto |\psi(t+\delta t)\rangle \sim \frac{U|\phi_\alpha(t)\rangle}{\|U\phi_\alpha(t)\|} \equiv |\phi_\alpha(t+\delta t)\rangle. \tag{4.10}$$

4.2.2 Quantum state diffusion

The standard form diffusion SSE [41, 42, 43] is

$$|\mathrm{d}\psi\rangle = -\frac{i}{\hbar}G[\psi]\mathrm{d}t + \sum_k \sqrt{\Delta_k}\big(C_k - \langle C_k\rangle_\psi\big)|\psi\rangle \mathrm{d}\xi_k \tag{4.11}$$

where

$$G[\psi] = \left[H - \frac{i\hbar}{2}\sum_k \Delta_k\Big(C_k^\dagger C_k - 2\langle C_k^\dagger\rangle_\psi C_k + \langle C_k^\dagger\rangle_\psi\langle C_k\rangle_\psi\Big)\right]|\psi\rangle \tag{4.12}$$

and $\mathrm{d}\xi_k$ are infinitesimal complex Wiener increments with properties

$$E[\mathrm{d}\xi_k] = E[\mathrm{d}\xi_k\,\mathrm{d}\xi_l] = 0, \qquad E[\mathrm{d}\xi_k^*\,\mathrm{d}\xi_l] = \delta_{kl}\,\mathrm{d}t. \tag{4.13}$$

There are several methods to solve such a SSE, see e.g. Ref. [14].

4.3 Non-Markovian quantum jumps

The MCWF method terminates as soon as any decay rate $\Delta_k(t)$ becomes negative, since the corresponding jump probability (4.7) is directly proportional to it. This problem is circumvented in the non-Markovian quantum jump (NMQJ) method, developed in paper **II**, by introducing a new jump process, a reverse jump, acting when the decay rate is negative. In contrast to the positive rate case, where the quantum jump transforms the state as $|\phi_\alpha\rangle \mapsto C_k|\phi_\alpha\rangle/\|C_k\phi_\alpha\| \sim |\phi_\beta\rangle$, the reverse jump acts by its name in the reverse direction:

$$\frac{C_k|\phi_\beta(t)\rangle}{\|C_k\phi_\beta(t)\|} \sim |\phi_\alpha(t)\rangle \sim |\psi(t)\rangle \mapsto |\psi(t+\delta t)\rangle \sim |\phi_\beta(t+\delta t)\rangle. \tag{4.14}$$

In this case there can be several different target states β per a single channel k fulfilling the condition $|\phi_\alpha\rangle \sim C_k|\phi_\beta\rangle/\|C_k\phi_\beta\|$ (as a technicality, the difference in the time argument for the state β in the above equation can be neglected as a second-order effect). The reverse jump probability is

$$P^k_{\alpha\to\beta} = \frac{N_\beta}{N_\alpha}\delta t\,|\Delta_k|\langle\phi_\beta|C_k^\dagger C_k|\phi_\beta\rangle. \tag{4.15}$$

The deterministic evolution remains intact; the channels with a negative decay rate tend to increase the norm under the action of the non-unitary propagator U instead of decreasing it as in the positive case.

4.3.1 Algorithm

Since in the NMQJ method the single realizations are interdependent, the notion of an ensemble does not have the same relevance as in the original formulation of the MCWF method [24, 66]: the evolution is most naturally done completely in terms of the effective ensemble members $|\phi_\alpha\rangle$ and their occupation numbers N_α. Simulating the dynamics with a pure initial condition $\rho(0) = |\psi_0\rangle\langle\psi_0|$, the effective ensemble consists of a single state $|\phi_0(0)\rangle = |\psi_0\rangle$, the occupation number of which is $N_0(0) = N$. The evolution of the effectively N single trajectories over a time interval $t \in [0, T]$ is then generated by repeating the following iterative NMQJ algorithm for a time step δt:

1. Repeat for each effective ensemble state α:

(a) For each channel k_+ with a positive decay rate $\Delta_{k_+} > 0$: evaluate the jump probability for a jump to an (unambiguous) target state β : $|\phi_\beta\rangle \sim C_{k_+}|\phi_\alpha\rangle/\|C_{k_+}\phi_\alpha\|$ as $P^{k_+}_{\alpha\to\beta} = \delta t\, \Delta_{k_+} \langle\phi_\alpha|C^\dagger_{k_+} C_{k_+}|\phi_\alpha\rangle$. Notice that the target state may not exist in the effective ensemble yet.

(b) For each channel k_- with a negative decay rate $\Delta_{k_-} < 0$: evaluate the jump probabilities for each (possibly many) target state β : $C_{k_-}|\phi_\beta\rangle/\|C_{k_-}\phi_\beta\| \sim |\phi_\alpha\rangle$ as $P^{k_-}_{\alpha\to\beta} = (N_\beta/N_\alpha)\delta t\, |\Delta_{k_-}| \langle\phi_\beta|C^\dagger_{k_-} C_{k_-}|\phi_\beta\rangle$. Notice that only target states already present in the ensemble need to be considered, since $P^{k_-}_{\alpha\to\beta} \propto N_\beta$.

(c) Repeat N_α times an exclusive random choice of a channel and a target state according to the above jump probabilities $\{P^{k_+}_{\alpha\to\beta}\}$, $\{P^{k_-}_{\alpha\to\beta}\}$ and a complementary no-jump option with probability $\tilde{P}_\alpha = 1 - \sum_{k_+} P^{k_+}_{\alpha\to\beta} - \sum_{k_-}\sum_\beta P^{k_-}_{\alpha\to\beta}$.

2. Create the possible new effective ensemble states due to positive-rate jumps and update the occupation numbers $\{N_\alpha(t)\} \mapsto \{N_\alpha(t+\delta t)\}$ according to the selections in step 1.(c).

3. Evolve the states deterministically over the time step $|\phi_\alpha(t)\rangle \mapsto |\phi_\alpha(t+\delta t)\rangle$.

Naturally, the above algorithm is also an optimization for the MCWF methods, in which case the step 1.(b) is simply skipped since the rates are always positive.

4.4 Interpretation

The NMQJ method sheds light into the unintuitive fact that a time-local master equation can produce non-Markovian dynamics in the first place. The ensemble unraveling shows that the memory associated with non-Markovianity is carried by the other ensemble members, and it is available during the negative decay rates through interdependent trajectories. Hence, decoherence can be reversed into recoherence and the ensemble is able to recreate quantum superpositions.

The NMQJ method is confined in the original Hilbert space of the open quantum system described by the master equation. As is clear by the structure of the method [cf. Eq. (4.2)], it always generates a positive density

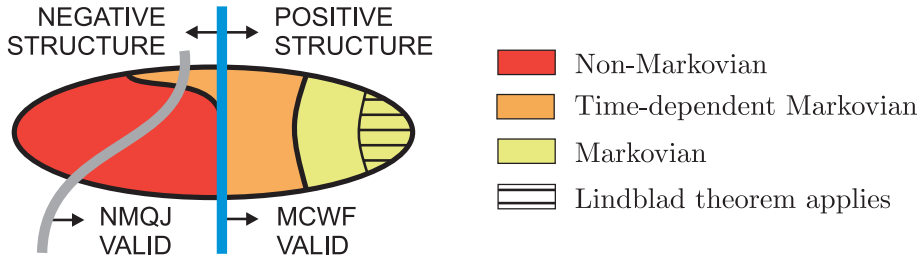

Figure 4.2: Schematic domains of validity for the NMQJ and the MCWF methods as compared to the type of Lindblad structure of the master equation. The MCWF method is valid with any positive structure, while the NMQJ method extends into the negative regime (an exact border is not known). As compared to the classification into non-Markovian, time-dependent Markovian, and Markovian processes (see Sec. 3.5), we see that the NMQJ method is always needed for non-Markovian dynamics, but on the other hand there are also Markovian processes [64] beyond both domains. In the other extreme, time-independent positive structure with bounded operators is where the Lindblad theorem applies.

operator. This feature is of interest, since a non-Markovian master equation with a Lindblad structure is not guaranteed to conserve positivity; a violation of positivity indicates a failure of the underlying approximation scheme. The non-Markovian PDP-type SSE corresponding to the NMQJ method was formulated by Breuer *et al.* [15], pointing out that the violation of positivity always leads to the termination of the NMQJ algorithm as the reverse jump probability (4.15) diverges. This happens when the occupation number of a source state for a reversed jump goes to zero. However, the reverse statement is not true, and there is a not-well-defined class of valid master equations with a negative Lindblad structure which can not be simulated by the NMQJ method, since the probabilities diverge. In Fig. 4.2 we sketch the domains of validity in terms of the master equation structure.

4.5 Alternative methods for non-Markovian dynamics

There is a class of methods, which describe the non-Markovian dynamics in the reduced space as a partial solution of a different, Markovian, dynamics

in a larger space. Hence, an extended but structurally simplified problem can be solved, and the reduced state dynamics can be deduced.

In 1994 Imamoğlu [51] presented an effective description for a reservoir causing non-Markovian dynamics. Approximating the spectral density by a finite superposition of positive Lorentzian distributions, the reservoir is replaced by auxiliary modes, which are coherently coupled to the reduced system and which are furthermore coupled to a modified environment, such that the dynamics of the extended open system is Markovian. The solution for the original problem is then reached by tracing out the extra degrees of freedom.

Garraway introduced in 1996 the pseudomode method [36, 37, 38], which generalizes the above description: the auxiliary modes are identified as poles of the spectral density. In situations where the spectral density is a meromorphic function the pseudomode method produces an exact reduced state dynamics.

Doubled Hilbert space method by Breuer *et al.* in 1999 [11] is a jump-type unraveling of the non-Markovian master equation in an extended Hilbert space, such that the ensemble consists of states $|\theta_i\rangle = (|\phi_i\rangle, |\psi_i\rangle) \in \mathcal{H} \oplus \mathcal{H}$ undergoing a modified piecewise deterministic quantum jump evolution. The solution for the original problem is given as $\rho \simeq N^{-1} \sum_i |\phi_i\rangle\langle\psi_i|$.

Triple Hilbert space method by Breuer in 2004 [12] introduces auxiliary degrees of freedom and a triple amount of modified decay channels in order to embed the non-Markovian dynamics in $\mathcal{H}$ into Markovian dynamics in $\mathcal{H} \otimes \mathbb{C}^3 \cong \mathcal{H} \oplus \mathcal{H} \oplus \mathcal{H}$. The master equation in the extended space has the Lindblad structure with positive rates, and the corresponding density operator $W(t)$ may be solved by standard Markovian methods. As compared to the pseudomode method, the whole dynamics is reformulated, such that the solution for the original problem is given by the normalized coherences of the extended solution: $\rho(t) = \mathcal{N}\langle 1|W(t)|2\rangle$.

The non-Markovian QSD method introduced by Diósi *et al.* in 1998 [26, 93] reformulates the diffusive SSE (4.11) in terms of colored noise corresponding to the environment correlation function; in Markovian case these correlations are neglected and the noise is white. The method assumes that the environment consists of harmonic oscillators, such as EM modes in the quantum optical applications.

Yet another approach as hidden variable interpretations is provided by Gambetta *et al.* for diffusive [32] and jump-like [33] non-Markovian processes. They consider the problem from the point of view of a measurement scheme, which is driving the dynamics.

Chapter 5

Characterization of the dynamics

All the studies in the papers constituting this Thesis are based on the common playground of atom-field interaction. The studied dynamical features are however diverse and the most important characterizations are introduced here.

5.1 Adiabatic evolution

In the context of non-stationary circumstances due to time-dependent processes involved in the dynamics, the eigenstate structure is likewise time dependent. Therefore, a time-dependent Schrödinger equation $-i\hbar\partial_t\psi(t) = H(t)\psi(t)$ does not have general stationary solutions which would be valid at all times. The adiabatic theorem in quantum mechanics states that if the rate of change in H is slow, the system remains in a momentary stationary state of $H(t)$ at all times. The theorem was discussed in 1928 by Born and Fock [9] in the case of a discrete eigenvalue spectrum and later in 1950 by Kato [55] in more general terms allowing continuous degenerate spectra.

More quantitatively, given a set of eigenstates as $H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$, a general state is

$$|\psi(t)\rangle = \sum_{n=1}^{D} a_n(t) e^{-i\int_0^t \mathrm{d}s\, E_n(s)} |n(t)\rangle. \tag{5.1}$$

The equations of motion for the weight functions $a_k(t)$ are then

$$\partial_t a_k = -a_k\langle k|\partial_t k\rangle - \sum_{n\neq k} a_n \frac{\langle k|\partial_t H|n\rangle}{E_n - E_k} e^{-i\int_0^t \mathrm{d}s\,[E_n(s)-E_k(s)]}. \tag{5.2}$$

In adiabatic evolution the latter term inducing transitions between the momentary eigenstates vanishes, which is guaranteed by a condition

$$\max_{0\leq t\leq T}\left|\frac{\langle k(t)|\partial_t H(t)|n(t)\rangle}{E_n(t)-E_k(t)}\right| \ll \min_{0\leq t\leq T}|E_n(t)-E_k(t)|. \tag{5.3}$$

With degenerate energy levels, the adiabaticity means that the Hilbert space can be decomposed into decoupled eigenspaces with distinct, time-continuous, and non-crossing instantaneous eigenvalues of Hamiltonian $H(t)$. As is known from the level-crossing models, see e.g. [92], if the crossings, at which $E_n(t) \simeq E_k(t)$, are encountered fast enough, a complete transfer of population occurs while a slow approach mixes the amplitudes. In paper **I** we engineer situations, in which there are clearly separating timescales, such that fast (avoided) energy-level crossings occur during otherwise adiabatic evolution.

As a curiosity, let us look at the open quantum systems, where the state is necessarily expressed as a density operator $\rho(t)$, whose dynamics is governed by the master equation $\partial_t\rho(t) = \mathcal{L}(t)\rho(t)$. In this case, the notion of the Hamiltonian eigenstates is lost and the adiabaticity condition has to be reformulated. Sarandy *et al.* [84] extend the treatment by expressing ρ as a vector $|\rho\rangle\rangle = (\rho_1, \rho_2, \ldots, \rho_{D^2})$ in Hilbert–Schmidt space, cf. the Bloch vector representation, such that the master equation is $\partial_t|\rho(t)\rangle\rangle = \mathcal{L}(t)|\rho(t)\rangle\rangle$, where $\mathcal{L}(t)$ is a non-Hermitian matrix. Looking at the time-dependent Jordan canonical block form of the generator $\mathcal{L}(t)$, the adiabaticity in open quantum systems means that the Hilbert–Schmidt space can be divided into decoupled Lindblad–Jordan eigenspaces with distinct, time-continuous, and noncrossing instantaneous eigenvalues of $\mathcal{L}(t)$.

5.2 Entanglement

Entanglement is a quantum correlation feature without correspondence in classical mechanics. This peculiar character was highlighted in 1935 by the collaboration of Einstein, Podolsky, and Rosen [30], but it took until 1980's before the effect could be experimentally verified by Aspect *et al.* [3, 4]. Formally, if the state $\rho_{AB\ldots} \in S(\mathcal{H})$, where the Hilbert space is divided in parts $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \ldots$, can be expressed as a probability distribution of product states, $\rho_{AB\ldots} = \sum_i p_i \rho_A^i \otimes \rho_B^i \otimes \ldots$, where $p_i > 0$, $\sum_i p_i = 1$, and $\rho_\alpha^i \in S(\mathcal{H}_\alpha)$, the state is separable according to the division $AB\ldots$; otherwise the state entangles the parts $AB\ldots$ [50]. The amount of entanglement is quantified by an entanglement measure $E : S(\mathcal{H}) \to \mathbb{R}_+$.

Several such measures exists in the literature [2, 50, 76], such as entanglement of formation, negativity, and geometric measure of entanglement, each of which approaches the feature from their own perspective. A particularly accessible characterization for bipartite binary systems is provided by the concurrence defined by Wootters [102]. This quantity is straightforwardly evaluated as $C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$, where the λ_j are the eigenvalues of an Hermitian matrix $\sqrt{\sqrt{\rho}(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)\sqrt{\rho}}$ in decreasing order; σ_y is the Pauli spin operator. The concurrence is an auxiliary parameter from which the proper measure, entanglement of formation, can be calculated, but since the dependence is monotonic, it is often used on its own to characterize entanglement in a system. Concurrence takes values between zero and one, such that for separable states it is zero, while for maximally entangled states it is unity. In paper **IV** the appearance of entanglement is monitored by looking at the concurrence.

5.3 Wave packets

Wave-packet formalism provides an intuitive means to solve the evolution of the coordinate representation, or the wave function, of a quantum state $\psi(\mathbf{r}, t)$, with $\psi \in L^2(\mathbb{R}^D)$ (square-integrable function), whose dynamics is generated by a time-dependent Schrödinger equation of form $i\partial_t\psi(\mathbf{r}, t) = H\psi(\mathbf{r}, t) = [T(\mathbf{p}) + V(\mathbf{r})]\psi(\mathbf{r}, t)$. Rather than diagonalizing the Hamiltonian and working out the time-dependent coefficients in the eigenstate basis, such that $\psi(\mathbf{r}, t) = \sum_i c_i(t)\phi_i(\mathbf{r}, t)$, the wave packet solution generates the function as a single time-evolving entity. The solution $\psi(\mathbf{r}, t)$ has semiclassical properties, such that the average phase-space quantities behave in a way which is familiar from the classical mechanics: $\partial_t\langle\mathbf{p}\rangle = -\langle\nabla V\rangle$ and $\partial_t\langle\mathbf{r}\rangle = \langle\mathbf{p}\rangle/m$. The formalism fits directly to investigation of dynamical behavior of the spatial probability distribution of a trapped atom or a cloud of atoms, e.g., Bose–Einstein condensates [73, 74], as well as molecular dynamics in Born–Oppenheimer potential surfaces [35, 71]. In paper **I** the dynamics of the motional state of an atom is studied in a time-dependent potential surface $V(\mathbf{r}, t)$.

The additional internal degrees of freedom, such as an angular momentum structure in paper **VI**, suggest treating the state as a multi-component spinor system $\boldsymbol{\psi} = (\psi_1, \psi_2, \ldots \psi_N) \in \bigoplus_{i=1}^{N} L^2(\mathbb{R}^D) \cong L^2(\mathbb{R}^D) \otimes \mathbb{C}^N$, such that the total state $\boldsymbol{\psi}(\mathbf{r}, t) = \sum_i \psi_i(\mathbf{r}, t)|i\rangle$. The resulting group of wave packets are interdependent via internal couplings as well as possible contact interactions which are effectively proportional to the local density.

5.4 Decoherence and dissipation

As we have seen in Chapter 3, the dynamics of an open quantum system is non-unitary, i.e., it cannot be described as a Liouville–von Neumann equation. Thereby, pure quantum states evolve into statistical mixtures. This dynamical destruction of quantum coherence, i.e., decoherence, is an artifact of the enforced reduction of state space and is a counterpart for the unitary evolution. The formalism of open quantum systems gives a direct access to sources of decoherence: the Lindblad structure (3.7) of a standard master equation separates readily into parts generating unitary and non-unitary dynamics. Non-Markovian dynamics (cf. Sec. 3.5) enables a reverse process, i.e., recoherence, where the preceding decoherence is partially canceled. In papers **II** and **III** we study this in the example systems.

Dissipative processes remove energy from the system. Spontaneous emission of radiation is a typical example of such mechanism. Decoherence does not require dissipation: non-dissipative decoherence is also called dephasing. In paper **IV** some of the decoherence processes are of this nature. Furthermore, in the presence of a thermal environment, cf. Sec. 3.3.2, the system may even absorb energy, but being a quantum analog of a classical random field [78], the bath also leads to decoherence.

Decoherence provides the mechanism to transfer from quantum to classical description of a state [17, 104]. However, even in the presence of such processes, not all states unavoidably evolve into classical mixtures. This is the concept of a decoherence-free subspace [70], which is unaffected by the environment. In paper **IV** we utilize such robust states in order to create stable entanglement.

5.5 Superradiance and subradiance

The Dicke model [25, 95] introduced in Sec. 2.1.2 describes the interaction of N identical two-level systems and a quantized EM field. If the collection of atoms is arranged in a spatially regular pattern within a sample size smaller than the wavelength of the field, the model is symmetric (homogeneous) and the atoms behave collectively as a single spin object [47, 49]. In these Dicke modes contributions by individual atoms interacting with the field interfere. In the permutationally symmetric maximal spin state $|J = N/2, M\rangle$ the interference is strongly constructive. On the contrary, in the antisymmetric singlet spin state $|J = 0, M\rangle$ the destructive interference suppresses the

interaction with the field completely. More generally, the superradiant and the subradiant states can be found also in an inhomogeneous single-mode Dicke model, where the atom-field couplings are not equal [5, 18].

The terms superradiance (constructive interference) and subradiance (destructive) come historically from the radiative measurements of the field, which is excited by the atomic system: the subradiant state does not excite the vacuum at all and hence no radiation occurs, while the superadiant one couples strongly and an enhanced radiation burst is observed. However, observing the collective behavior in free space is very difficult because of the symmetry and size constraints. On the other hand, in a cavity resonator the spectrum is dominated by the standing wave cavity mode, to which all the atoms couple. The first experimental observation of superradiant behavior was achieved in early 1980's by Raimond *et al.* [80] using Rydberg atoms with a millimeter-wave cavity. In the presence of photonic losses from the cavity, the superradiant component of the initial state decays to the global ground state $|J, -J\rangle$ while the subradiant component remains intact, i.e., it belongs to a decoherence-free subspace (cf. Sec. 5.4). The collective atomic Dicke modes are in general entangled, and in paper **IV** we study entanglement generation utilizing these modes.

Chapter 6

Numerical methods

As is often the case in physics, even the very compactly formulated mathematical models are not analytically soluble. In this chapter we review concisely some practical aspects about the implementation of the numerical methods, which have been used in the papers **I**–**VI** and **VI**.

6.1 Closed quantum systems

6.1.1 Split operator FFT-method

The time evolution of a Schrödinger equation (papers **I** and **VI**) and corresponding Gross–Pitaevskii equation for interacting atoms [73, 74] (paper **VI**) is solved numerically by splitting the propagator $U(t+\delta t,t) \simeq \exp\{-i[T(\mathbf{p})+V(\mathbf{r},t)]\delta t/\hbar\}$ [notice that the time step δt is chosen small enough such that $[H(t),H(t')] \simeq 0$ for $|t-t'| < \delta t$ and $\int_t^{t+\delta t} \mathrm{d}s\, H(s) \simeq H(t)\delta t$] into a product of parts corresponding to operations exclusively in momentum and position spaces. Therefore, applying a Fourier transform $\mathcal{F}$ [see, e.g., Ref. [72] for numerical implementation of the fast Fourier transform (FFT)] in between, the action of the propagator on the state is always purely multiplicative and, consequently, numerically efficient to apply. Since the kinetic and the potential parts do not commute, the splitting $U \simeq U_1 = e^{-iT\delta t/\hbar}e^{-iV\delta t/\hbar}$ is accurate only in the first order of δt. The approximative evolution is then given by $\psi(\mathbf{r},t) \mapsto \psi(\mathbf{r},t+\delta t) = \mathcal{F}^{-1}e^{-iT(\mathbf{p})\delta t/\hbar}\mathcal{F}e^{-iV(\mathbf{r},t)\delta t/\hbar}\psi(\mathbf{r},t)$. Alternatively, the splitting $U_2 = e^{-iV(\mathbf{r},t)\delta t/2\hbar}e^{-iT(\mathbf{p})\delta t/\hbar}e^{-iV(\mathbf{r},t)\delta t/2\hbar}$ is accurate to the second order, but requires on the other hand slightly more computational effort.

The stable initial state $\psi(\mathbf{r},0)$ in the wave-packet simulations is found

by imaginary time evolution setting $\delta t = -i\delta\tau$ and renormalizing the state after each iteration. This procedure projects an arbitrary ansatz state $\phi(\mathbf{r})$ to the lowest energy eigenstate, with which it has a finite initial overlap; with numerical noise the method finds the global ground state in practice always. It should be noted that the numerical eigenstates differ slightly from the analytical ones because of the spatial discretization.

6.1.2 Numerov algorithm

The Numerov algorithm [72] is a numerical method to solve linear differential equations of form

$$u''(x) + q(x)u(x) = s(x). \tag{6.1}$$

Using notation $v_i = v(x_i)$, where $v = u, q, s$, and a uniform spatial discretization $x_{i+1} - x_i = h$, the solution is achieved recursively by identity

$$c_{i+1}u_{i+1} + c_{i-1}u_{i-1} = c_i u_i + d_i + \mathcal{O}(h^6), \tag{6.2}$$

where the coefficients are

$$c_{i\pm1} = 1 + \frac{h^2}{12}q_{i\pm1}, \quad c_i = 2 - \frac{5h^2}{6}q_i, \quad d_i = \frac{h^2}{12}(s_{i+1} + 10s_i + s_{i-1}). \tag{6.3}$$

In contrast to the local sixth order accuracy, globally the solution is accurate to the fourth order in discretization step h. In paper **I** this algorithm was used for finding the eigenstates and corresponding eigenvalues of a Schrödinger equation $[-\frac{\hbar^2}{2m}\nabla^2 + V(x)]\psi(x) = \epsilon\psi(x)$. The idea is to test a proposed eigenvalue ϵ by integrating the corresponding equation $\psi''(x) - \frac{2m}{\hbar^2}[V(x) - \epsilon]\psi(x) = 0$ by the Numerov algorithm from left and right, giving solutions $\psi_L(x)$ and $\psi_R(x)$. The solutions are then compared at the classical turning point x_C [defined by $V(x_C) = \epsilon$], where the correct solution is necessarily finite. The continuity equations

$$\psi_L(x_C) = \psi_R(x_C), \qquad \psi'_L(x_C) = \psi'_R(x_C), \tag{6.4}$$

give an estimate for the validity of the proposed eigenvalue ϵ. Rescaling the solutions to match at x_C, $\psi_L(x_C) = \psi_R(x_C) = \psi(x_C)$, the continuity of the derivative gives a error estimate

$$f(\epsilon) = \frac{\psi'_L(x_C) - \psi'_R(x_C)}{\psi(x_C)}. \tag{6.5}$$

A root search algorithm for ϵ can then be used in order to determine a proper eigenvalue ϵ_0, and a corresponding eigenstate, for which $f(\epsilon_0) = 0$.

6.2 Open quantum systems

6.2.1 Monte Carlo wavefunction simulation

Finding the solution of a master equation with a (time-dependent) positive Lindblad structure in paper **IV** is done using the variant of Monte Carlo wavefunction simulation method by Dum *et al.* [27, 28] and Carmichael [19]. In this approach, the delay τ between the consecutive quantum jumps is decided randomly according to a waiting-time distribution $F_T(\tau)$. This quantity is related to the change of norm due to non-unitary propagator $U(t,t') = \mathcal{T}_{\leftarrow} \exp[-\frac{i}{\hbar}\int_{t'}^{t} \mathrm{d}s\, H_{\mathrm{eff}}(s)]$, where the non-Hermitian Hamiltonian $H_{\mathrm{eff}}(t)$ is defined in Eq. (4.6). Defining an unnormalized auxiliary state $|\tilde{\psi}_T(s)\rangle = U(T+s,T)|\psi(T)\rangle$, where T is the time of the previous jump due to which the state became $|\psi(T)\rangle$, the waiting time distribution is $F_T(\tau) = 1 - \|\tilde{\psi}_T(\tau)\|^2$.

The algorithm for generating a single trajectory $|\psi(t)\rangle$ is summarized as follows:

1. Start with an initial condition $|\psi(0)\rangle$ and $T = 0$.

2. Draw a uniformly distributed random number $\eta \in [0,1]$, and evolve $|\tilde{\psi}_T(s)\rangle$ deterministically by a method of choice until $s = \tau$, for which $\eta = F_T(\tau) = 1 - \|\tilde{\psi}_T(\tau)\|^2$. Meanwhile, $|\psi(T+s)\rangle = |\tilde{\psi}_T(s)\rangle / \|\tilde{\psi}_T(s)\|$.

3. Form the relative jump probability densities at the instant of jump, $t = T + \tau$, by

$$p_k = \frac{\Delta_k(T+\tau)\|C_k(T+\tau)\psi(T+\tau)\|^2}{\sum_j \Delta_j(T+\tau)\|C_j(T+\tau)\psi(T+\tau)\|^2} \tag{6.6}$$

   and select randomly a channel K among them. Apply the corresponding Lindblad operator on the state, $|\psi(T+\tau)\rangle \mapsto C_K(T+\tau)|\psi(T+\tau)\rangle / \|C_K(T+\tau)\psi(T+\tau)\|$ and update the jump time $T \mapsto T + \tau$.

4. Repeat steps 2–3 until the requested time interval is covered.

In paper **IV** the master equation is manipulated such that H_{eff} is time independent, and therefore the propagator is given by the exponential $U(t,t_0) = \exp[-\frac{i}{\hbar}(t-t_0)H_{\mathrm{eff}}]$, which is evaluated accurately for large time intervals as a matrix exponential.

6.2.2 Non-Markovian quantum jump method

In papers **II** and **III** we apply the NMQJ method (cf. Sec. 4.3) in simple 2- and 3-level-models. As a technical remark appropriate for this Chapter, let us discuss practical aspects of the implementation. In the simple example cases discussed in the papers it is possible to determine a priori the states forming the effective ensemble $\{|\phi_\alpha(t)\rangle\}_{\alpha=1}^{N_{\rm eff}}$ just by examining the structure of the Lindblad operators. Moreover, the connections between the states via jump channels are also then obvious, see Fig. 3 in paper **III**.

Such a connection map simplifies especially the procedure for evaluating the reverse jump probabilities for negative channels k_-: in a general case the possible target states β, given by equivalence $C_{k_-}|\phi_\beta\rangle/\|C_{k_-}\phi_\beta\| \sim |\phi_\alpha\rangle$, would have to be searched by some ultimately inaccurate numerical test of form $f(\alpha,\beta,k_-) = 1 - |\langle\phi_\alpha|C_{k_-}|\phi_\beta\rangle|/\|C_{k_-}\phi_\beta\| < \epsilon$, where ϵ is a small threshold value, separately for every β just in order to form the jump probabilities $P^{k_-}_{\alpha\to\beta}$. The same inconvenience would occur in a milder form for positive channels k_+ after the jump has been decided: the target state $C_{k_+}|\phi_\alpha\rangle/\|C_{k_+}\phi_\alpha\|$ has to be compared against all the other states β in order to keep track on occupation numbers N_α. With a large effective ensemble this would significantly slow down the algorithm. However, until now there are no examples in the literature about realistic master equations with time-dependent operators where this would happen, and the NMQJ method is therefore efficient. Also, a large number of channels (see, e.g., Ref. [81]) actually favors the NMQJ method as compared to methods with extended Hilbert spaces introduced Sec. 4.5.

Chapter 7

Results and conclusions

The original research articles forming this Thesis all deal with the same fundamental phenomenon of atoms interacting with an electromagnetic field. As we have seen in Chapters 2, 3, and 5, this interaction appears mathematically in very different forms depending on the prevailing circumstances, and causes a wide variety of physical phenomena. The research articles cover many aspects of the interaction, mainly used as a tool to generate a desired dynamical effect in the atomic degrees of freedom. We present now a brief summary of the results and conclusion achieved in the research articles and explain in which form the EM field enters the topic.

7.1 Summary of results in the papers

7.1.1 Paper I

Garraway *et al.* [39] and Rodriguez *et al.* [83] discovered a method to manipulate the vibrational state of a multicomponent molecule by strong laser pulses, and explained the dynamics by adiabatic processes in field-dressed electronic states. We apply this idea to the context of the motional state of an atom residing in a time-dependent double-well potential. Such trapping potential for the motional state is provided by an off-resonant semiclassical interaction of the EM field with the internal degrees of freedom (cf. Sec. 2.2): for an optical lattice implementation see, e.g., Ref. [88] and for a radio-frequency-field-dressed magnetic traps see Ref. [86].

A deep asymmetric double-well structure supports essentially two sets of low-energy eigenstates, corresponding to states localized in each well, while at the energies above the central barrier level the eigenstates spread over

the both wells. Therefore, by manipulating the geometry of the double-well potential, the sets move with respect to each other. In this way we introduce sharp (avoided) energy-level crossings, which are passed diabatically, while the evolution is otherwise purely adiabatic (cf. Sec. 5.1). This allows us to selectively transfer the population from one eigenstate to another. Later, essentially the same mechanism has been implemented in experiments by Sebby-Strabley *et al.* [89] and Fölling *et al.* [31].

7.1.2 Paper II

We develop the NMQJ method (see Sec. 4.3). It is a generalization of the MCWF method and unravels the dynamics of an open quantum system, described by a generic time-local master equation with negative rates, by quantum jumps processes within the reduced state space. We apply the method to a simple example case of a 2-level atom interacting with a reservoir of EM modes. In particular, we examine a photonic band gap structure with a sharp edge, which is impossible to solve exactly with the pseudomode method, and verify an exact match with an analytical solution. Later, the method has been applied by Rebentrost *et al.* [81] in context of exciton transfer in biomolecules.

7.1.3 Paper III

This paper presents a detailed proof that the NMQJ method indeed unravels the dynamics described by a master equation with a general Lindblad structure. We present several examples of its use in terms 2- and 3-level systems interacting off-resonantly with a reservoir described by a Lorentzian spectral density, which corresponds to the mode structure of an imperfect cavity resonator in the direction of the cavity axis. Especially, with a 3-level system we examine different coupling geometries (Λ, V, and ladder couplings) such that there are periods where the two independent decay channels have opposite signs. Again, we find a perfect match with the exact solution of the master equation.

In addition, we discuss the physical interpretation of the reverse jump processes introduced by the NMQJ method as a cancellation of a virtual process. The single Markovian Monte Carlo trajectories have a direct interpretation as a periodic measurement sequence for the environment state [75], but such scheme can not be applied directly into the non-Markovian case, since measurements on the environment would erase the

system-reservoir correlations, which are driving the non-Markovian dynamics. Therefore, we conclude that the single NMQJ trajectories may correspond to a real physical state evolution as being possible paths to a given final state, but the evolution can not be measured continuously.

7.1.4 Paper IV

We review the properties of the collective modes in an inhomogeneous Dicke model (cf. Secs. 2.1.2 and 5.5), and present an experimental proposal to realize them in the context of ion-cavity QED. The proposal is based on existing experimental setups [48, 56], where trapped ions are resided inside an optical cavity. The ions are modeled as 3-level systems coupled in a Λ-setup.

Inside the leaky cavity, the ion couples strongly to a continuum of modes in the direction of the cavity axis constituting a Lorentzian spectrum, which is then reformulated in terms of the pseudomode method [37, 38] as a single cavity mode, which couples coherently with an electronic transition of the ion and decays into an effective Markovian reservoir. The second electronic transition is driven by a (classical) laser injected from the side of the cavity. Finally, all the other directions aside the cavity axis correspond to thermal free-space modes, but since the relevant electronic transitions of the ion are in the optical range, the thermal occupation of the modes at the transition frequency is negligibly small (cf. Sec. 3.3) and only spontaneous emission occurs (the transition between the lower states is dipole forbidden and such radiative transitions may be neglected).

In the proposal, we locate two ions simultaneously inside the cavity, and derive an effective master equation by adiabatically eliminating the unstable excited electronic state. Thereby, we arrive at an effective Dicke model disturbed by decay processes. Especially, the decay processes due to the spontaneous emissions are reformulated in terms of interrupted Raman transitions. In the effective model, we show how the parameters scale in terms of physical parameters, and confirm by Monte Carlo simulations that even in the experimentally feasible values a trace of the collective behavior predicted by the idealized Dicke model can be observed. Thereby, the initially uncorrelated ions are driven into an entangled subradiant state because of the interaction with a shared environment provided by the cavity mode.

7.1.5 Paper V

This paper presents a detailed reasoning behind the peculiar structure of jump processes introduced by the NMQJ method. Starting from a general time-local master equation, the paper recognizes the several arbitrary choices which finally lead to the method: the form of the deterministic propagator, the notion of independent channels, and the requirement of proper probability distribution. Especially, the reverse quantum jumps are formulated in terms of ensemble-induced jump operators, which are related to the Lindblad operators. Together with the ensemble-dependent jump probabilities, they underline the role of the ensemble as a memory storage, which is required for the non-Markovian behavior.

7.1.6 Paper VI

We study the interference of overlapping streams of atoms which are output coupled by two weak radio-frequency (rf) fields from a magnetic trap into the linear potential of gravity. A classical non-radiative rf-field in the perpendicular direction to the trapping field couples the internal angular momentum states, such that a trapped low-field-seeking state is transfered to $M_F = 0$ Zeeman sublevel, where the motional state is not trapped and the atoms fall freely under gravity.

The total stream of output coupled atoms is expressed as a convolution of the classical driving fields and a free-fall time evolution of a spatial distribution corresponding to the trapped source cloud. We demonstrate how the interference visibility of the driving rf-fields is washed out because of the finite spatial width of the source and confirm the validity of the approximative analytical solution by wave-packet simulations.

The study is motivated by two seemingly distinct interpretations of the interference patterns in terms of asymptotic (unphysical) atomic distributions [7] or interfering classical rf-fields which are driving the coupling [98]. Our model shows how these points of view are connected.

7.2 General conclusion

As is often the case, the most significant work has to be started by constructing the new tools first. Our emphasis has been in the development of experimental and computational methods. Being general concepts they are readily available for any future applications and further refinement. More-

over, as we have seen, sometimes the methods themselves give new insights into the physical problem and are therefore valuable on their own right.

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