EBERHARD KARLS UNIVERSITÄT TÜBINGEN
&
UNIVERSIDAD DE GRANADA

MASTER THESIS

Master thesis

Author:
Leopold BODAMER

Supervisor:
Prof. Dr. Daniel Manzano Diosdado

A thesis submitted in fulfillment of the requirements for the degree of Master of Science

in

Theoretical Atomic Physics and Synthetic Quantum Systems
Institut für Theoretische Physik

March 11, 2025

Declaration of Authorship

I, Leopold BODAMER, declare that this thesis titled, "Master thesis" and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while applying for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed:

Date:

Chapter 1

Introduction

1.1 Coherence and Excitation Transport

In this chapter, we aim to explain the phenomena of long coherences (lifetimes) and the excitation transport of light on a microtubule. The proposed model takes the following approach:

- The microtubule is modeled as a cylindrical structure consisting of nodes. Each node represents an atom, which is modeled as a two-level system. The number of atoms, N_{atoms}, is determined by the number of chains (n_{chains}) and the number of rings (n_{rings}), assuming fixed positions for these nodes.
- The system is restricted to a single excitation.
- A time-dependent coupling to an electric field is proposed, which may be either classical or quantum in nature. This coupling is intended to facilitate spectroscopy.
- Two types of Lindblad operators are introduced to model dissipation processes. Specifically:
  1. Spontaneous decay
  2. Dephasing

The Lindblad operators introduced to model the spontaneous decay and dephasing processes for each individual atom are defined as follows:

$$C_{\text{decay}}^{(i)} = \sqrt{\gamma_0}\,\sigma_-^{(i)}, \tag{1.1}$$

$$C_{\text{dephase}}^{(i)} = \sqrt{\gamma_\phi}\,\sigma_z^{(i)}, \tag{1.2}$$

where:

- $C_{\text{decay}}^{(i)}$ describes the spontaneous decay of the i-th atom, with a rate given by γ_0.
- $C_{\text{dephase}}^{(i)}$ describes the dephasing of the i-th atom, with a rate given by γ_ϕ.
- $\sigma_-^{(i)}$ is the lowering operator for the i-th atom, and $\sigma_z^{(i)}$ is the Pauli z-operator for the i-th atom.

1.2 Motivation

Quantum computing, an exceptionally promising area of study in modern physics, offers a fundamentally new way to process and transmit information. Applications of this, not yet scalable technology range from cryptography to drug research. Quantum computers would especially outperform classical computers in quantum simulations of chemical / physical systems [**Eddins2022**]. Qubits, the analog to classical bits, for example, photons or atoms play a crucial role in harnessing this quantum technology [**Ramakrishnan2023**]. The area which describes photons and their interaction with matter is quantum optics. One essential goal of this filed is to build efficient and controllable interactions between photons and atoms. A challenge for this is unwanted (spontaneous) emission, where photons are scattered into channels out of control. This spontaneous emission hampers the development of quantum technologies, especially in quantum information processing. Subradiant states are a promising concept for this field of study. These states appear when many emitters interact via light-mediated resonant dipole-dipole interactions and inherit lifetimes magnitudes larger than that of a single emitter [**AsenjoGarcia2017**]. Insights into information transport within complex systems are of utmost interest, as they could lead to advances in quantum computing. Especially with subradiant states, as they also offer ultrafast readout [**Scully2015**].

It is widely assumed that one of the crucial tasks currently facing quantum theorists is to understand and characterize the behaviour of realistic quantum systems. In any experiment, a quantum system is subject to noise and decoherence due to the unavoidable interaction with its surroundings. The theory of open quantum systems aims at developing a general framework to analyze the dynamical behaviour of systems that, as a result of their coupling with environmental degrees of freedom, will no longer evolve unitarily. [1]

2DES> [2], [3], [4]

NONlinear Optics> [5], [6]

Spectroscopy investigates the interaction between matter and electromagnetic radiation, offering a means to analyze composition and structure. Central to this analysis is the understanding of how molecules respond to specific frequencies of light, revealing information about their energy levels and bonding. Key concepts include wavelength (λ), wavenumber ($\bar{\nu}$), and frequency (ν). Wavelength, the distance between successive wave crests, is typically measured in nanometers or micrometers. Wavenumber, expressed in inverse centimeters (cm^{-1}), represents the number of waves per unit distance and is directly proportional to energy, defined as $\bar{\nu} = 1/\lambda$ (where λ is in cm). Frequency, the number of wave cycles per second, is measured in Hertz (Hz), and the angular frequency (ω) is related to frequency by $\omega = 2\pi\nu$. The relationship between angular frequency and wavenumber is given by $\omega = 2\pi c\bar{\nu}$, where c is the speed of light.

Then I turned everything into fs^{-1}.

Spectrometers are instruments designed to measure the intensity of light as a function of wavelength or frequency. Different types of spectrometers are employed for various regions of the electromagnetic spectrum. Notably, UV-Vis spectrometers analyze absorption and transmission of ultraviolet and visible light, while infrared (IR) spectrometers measure the absorption of infrared light, providing insights into molecular vibrations. Nuclear Magnetic Resonance (NMR) spectrometers probe the magnetic properties of atomic nuclei, revealing molecular structure.

Conversion from Discrete Sum to Continuous Spectral Density

In the theory of open quantum systems, one often moves from a discrete description of the bath to a continuous one. This is summarized by the transformation:

$$\sum_{j=1}^{M} g_j^2\, \delta(\omega - \omega_j) \quad \longrightarrow \quad J(\omega).$$

1. Discrete Modes

The bath is initially described as a set of M harmonic oscillators:

- Each oscillator has frequency ω_j.
- Each oscillator couples to the system with coupling constant g_j.

The spectral contribution of each oscillator is:

$$\sum_{j=1}^{M} g_j^2\, \delta(\omega - \omega_j).$$

2. Density of States

As $M \to \infty$ and the frequencies $\{\omega_j\}$ become dense, replace the sum by an integral:

$$\sum_{j=1}^{M} \quad \longrightarrow \quad \int d\omega'\, \rho(\omega'),$$

where $\rho(\omega')$ is the density of states, indicating how many modes lie near frequency ω'.

3. Frequency-Dependent Coupling

In the continuum limit, the coupling g_j becomes a function of frequency, $g(\omega')$. Hence:

$$g_j^2 \quad \longrightarrow \quad g(\omega')^2.$$

4. Form of $J(\omega)$

Putting these together, one obtains

$$\sum_{j=1}^{M} g_j^2\, \delta(\omega - \omega_j) \quad \longrightarrow \quad \int_0^{\infty} d\omega'\, \rho(\omega')\, g(\omega')^2\, \delta(\omega - \omega').$$

Using the sifting property of the delta function, this becomes

$$J(\omega) \; = \; \rho(\omega)\, g(\omega)^2.$$

5. Ohmic Spectral Density with Exponential Cutoff

A commonly used form in open quantum system models is the Ohmic spectral density with an exponential cutoff:

$$J(\omega) \; = \; \alpha\, \omega\, e^{-\omega/\omega_c},$$

where:

- α is a coupling constant,
- ω_c is the cutoff frequency.

"Ohmic" means $J(\omega) \propto \omega$ for small ω, and the exponential cutoff ensures convergence at large ω.

Bibliography

[1] Ángel Rivas et al. *Markovian master equations: a critical study* New Journal of Physics **12** p. 113032 (2010)

[2] Jannis Krumland et al. *Two-dimensional electronic spectroscopy from first principles* Applied Physics Reviews **11** p. 011305 (2024)

[3] Javier Segarra-Martí et al. *Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy* Topics in Current Chemistry **376** p. 24 (2018)

[4] Haoran Sun et al. *Two-dimensional spectroscopy of open quantum systems*. Dec. 2024. DOI: 10.48550/arXiv.2412.10931.

[5] Peter Hamm. *Principles of Nonlinear Optical Spectroscopy: A Practical Approach*. or: Mukamel for Dummies. Zurich, Switzerland: University of Zurich, Aug. 2005.

[6] Shaul Mukamel. *Principles of Nonlinear Optical Spectroscopy*. New York: Oxford University Press, 1995, p. 543. ISBN: 0-19-509278-3.