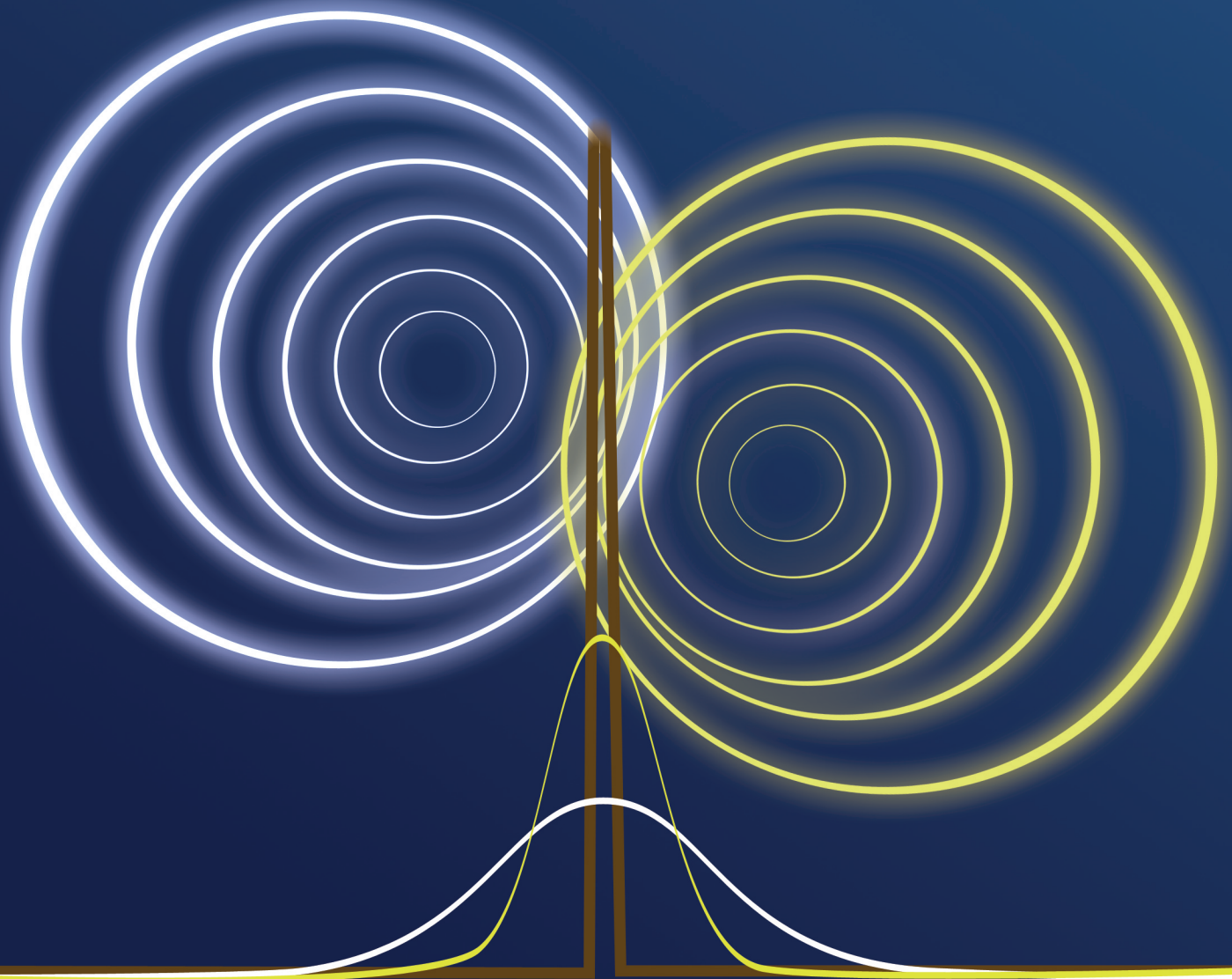


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Open Quantum Physics and Environmental Heat Conversion into Usable Energy



Eliade Stefanescu

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**Open Quantum Physics
and
Environmental Heat Conversion
into
Usable Energy**

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Dedication

To my son Radu, for his understanding

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Foreword

1985 was an important year for us, at Joint Institute for Nuclear Research at Dubna I was the vice director and the director was N. N. Bogoliubov. One year earlier, Rose and Jones discovered a cluster emission process, which was predicted by us a few years earlier, and we were interested in a more rigorous description of the heavy ion collisions. With Horia Scutaru, I succeeded to finalize a paper describing collective coordinate vibrations in the dissipative environment of the nuclear excitations. Though the result was interesting, but somehow doubtful, as it was based on an original generalization of quantum mechanics, performed by Lindblad a few years earlier. I was interested in additional verifications of this theory in other fields of research as the laser theory. In this field, I began to work with Eliade Stefanescu. Two years later, Stefanescu not only re-obtained the Bloch-Feynman equations in the framework of Lindblad's theory, but also obtained a very interesting phenomenon of energy transfer from a disordered environment to a coherent electromagnetic field propagating through this environment. He followed this idea for years, and, finally, he successfully conceived it and in a complex theoretical framework, described a semiconductor device, thus making this operation efficient.

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Preface

Open quantum physics is an interesting field of research, dedicated to realistic systems, which, in the practical cases, are always subjected to the action of the environment. As an example, we have in view the system of active electrons and the electromagnetic field in a laser semiconductor structure, which, besides the useful atom-field interaction, undergoes an important action of the other electrons of the structure, and of the crystal lattice vibrations. Such devices are usually described by models essentially depending on phenomenological parameters as life-times of electrons on excited energy levels, and the absorption coefficients of the electromagnetic fields. A deficiency of these models is given not only by unspecified values of the parameters, but also by forms of quantum equations with dissipation terms, violating the quantum principles. A rigorous study of dissipation in agreement with the quantum principles has been initiated by Sandulescu and Scutaru, more than 25 years ago, based on a general master equation, derived by Lindblad from a generalization of the dynamical groups to semigroups. This theory is in full agreement with the quantum principles, while dissipation parameters satisfy fundamental constraints.

Recently, we developed a fully microscopic theory of the dissipative dynamics, based on a procedure of Ford, Lewis, and O'Connell for reducing the total dynamics of a dissipative system to a master equation for a system of interest. In this framework, we obtained a quantum master equation for a system of particles in a complex dissipative environment of Fermions, Bosons and free electromagnetic field. We also derived master equations for an electromagnetic field propagating in a semiconductor structure, and for the crystal lattice vibrations induced by this field.

We discovered a phenomenon converting environmental heat into usable energy, based on a semiconductor structure (*e.g.*, a $GaAs-Al_xGa_{1-x}As$ heterostructure) in intimate thermal contact with a heat absorbent. While a current is injected into the device, a superradiant power is generated mainly on the account of heat absorption from the environment. This eBook is devoted to sequence the knowledge involved in understanding and modeling such a device, or in similar semiconductor structures. Paraphrasing a famous physicist (Feynman), the summit of this eBook consists in master equations with explicit, microscopic coefficients, for the systems of interest: electrons, photons, and phonons. To ascend this summit is a long one, including basic ideas for describing various aspects of the dissipative dynamics. I believe that, in these older theories, one could still find resources for further developments of the field. To descend this summit is a modeling of a heat converter, having in view the whole active system, of quantum dots, superradiant field, and optical vibrations, and the whole dissipative environment, of quasi-free electrons and holes, crystal vibrations, and free electromagnetic field. Although the reader is supposed to have a knowledge on

quantum mechanics and semiconductor physics, we have also included basic elements of these disciplines for convenience.

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CHAPTER 1

Introduction

Abstract

This eBook is devoted to the domain of physics we call Open Quantum Physics, which seemed important for the new field of research of the environmental heat conversion into usable energy. For this research, a special mathematical tool has been used, consisting of master equations for systems of particles as Fermions, Bosons, and electromagnetic field. This effort was based on the previous results of Lindblad, Sandulescu, and Scutaru for a description of the dissipative coupling of a system of interest in accordance with the quantum principles. We used the method of Ford, Lewis, and O'Connell for reducing the total dynamics to a master equation for a system of interest. The results of our research are presented in this eBook in a more general framework of open physics.

Keywords: Environment, dissipation, system of interest, total system, total dynamics, reduced dynamics, master equation, Lindbladian, Fermion, Boson, electromagnetic field, phonon, density matrix, interaction picture, creation-annihilation operators, coherent state, semiconductor, Fermi level, donor, acceptor, Fabry-Perot cavity.

The field of the open systems of micro-particles has a long history, beginning with Einstein's theory of Brownian motion (1905), based on a friction/mobility coefficient and temperature. In this framework, the diffusion coefficient is found to be proportional to temperature and mobility (Einstein's relation), or inverse proportional to the particle mass and collision rate (theorem of dissipation and fluctuations). Later on, this theory was generalized for taking into account higher-order correlations between the fluctuating forces [1]. Important textbooks have been dedicated to this field [2-4]. Much efforts have been devoted for the description of the dissipative dynamics, by phenomenological parameters in quantum equations of motion [5-7].

However, in an attempt to generalize the quantum mechanics for open systems, by using phenomenological arguments, some serious problems were encountered such as violation of quantum principles as the positivity of the probabilities, uncertainty relations, and the ground state energy. In this way, the quantum phenomenon of tunneling has been found to be suppressed by dissipation [8, 9], while further studies have shown that tunneling on the contrary is enhanced by dissipation [10-13]. A master equation in agreement with all the quantum principles has been derived in an axiomatic framework by generalization of the dynamical groups to completely positive dynamical semigroups [14]. Only ten years later, Lindblad's axiomatic coefficients were interpreted as coefficients of friction, and diffusion in physics [15], and have been used in certain applications [16]. Lindblad's dynamics is

a major subject in some of the important textbooks in open quantum physics [17-19], in controversial discussions on various approaches [20-26], and in the recent developments of open quantum physics [27].

Although the Lindblad theory of open quantum systems is in perfect agreement with the quantum-mechanical principles, it still has shortcomings, including a number of unspecified parameters. Therefore, many authors preferred physical approaches of dissipative dynamics, more or less in agreement with Lindblad's master equation [28-30]. A more rigorous procedure for reducing the system-environment dynamics to a quantum master equation, which is in perfect agreement with Lindblad's theory, was performed, and illustrated for a quantum harmonic oscillator, by Ford, Lewis, and O'Connell [31]. We applied this procedure to a system of Fermions, and obtained a quantum master equation with explicit microscopic coefficients, depending on well known two-body potentials, densities of states, and occupation probabilities of these states according to the Fermi-Dirac and Bose-Einstein distributions, and the principle of detailed balance [32-36]. We obtained similar equations for the electromagnetic field, and crystal vibrations excited by such a field.

This explicit theory of open quantum systems, enabling a detailed description of the energy interchange between a system of interest and environment, seems to be a powerful tool of investigation, suggesting possible applications to the energy production. In this way, a semiconductor device converting environmental heat into usable energy has been conceived [37-39]. This device is based on a new kind of quantum dots [40], where the initial state of a superradiant system is reached by heat absorption, when a current is injected into the semiconductor structure. It is interesting to note that the radiation power delivered by the device, on the account of the environmental heat, is much larger than the power dissipated by the injected current. The device operation has been described in the framework of a microscopic theory [41]. By calculating the entropy evolution of the matter-field system [42], we observed a decrease in entropy away from equilibrium state, corresponding to the device operation, while the entropy increase of the second principle of thermodynamics refers only to equilibrium states [43].

In this eBook, we have discussed basic ideas of open quantum physics, and the application of the theory of the environmental heat conversion into coherent electromagnetic energy. The eBook is structured on nine chapters. Chapter 2 contains basic elements of the quantum mechanics, including quantum states and operators, Fermions (the exclusion principle) and Bosons (coherent states). We derive electromagnetic field operators, and the statistical distributions of Fermi-Dirac and Bose-Einstein. In chapter 3, we present basic ideas of open physics, from Einstein's theory of the Brownian motion to the concepts as decay, broadening, stability, bifurcation, self-organization, and chaos. We derived stochastic equations, and the quantum master equation obtained by the method of projection operators. In chapter 4, after a presentation of Lindblad's master equation, we gave an alternative demonstration of Alicki and Lendi, and another demonstration relating to Lindblad's coefficients with the environment operators. We demonstrated the conservation of the density matrix positivity. We present the theory of Sandulescu and Scutaru, for relating the Lindblad axiomatic coefficients to physical coefficients of quantum friction and diffusion, satisfying fundamental constraints. In chapter 5, we gave a more detailed description of tunneling in quantum wells, which are basic elements in nanostructures. We demonstrated the Gamov formula for tunneling from an excited state, Brink's formula for tunneling from a ground state, and the Caldeira and Leggett formula for the dissipative tunneling. Finally, we derived the tunneling spectrum by openness according to the Lindblad-Sandulescu-Scutaru theory. In chapter 6, we derived the Maxwell-Bloch equations in their classical form, with decay

and dephasing terms, and in a more general form, with a polarization-population coupling obtained by openness according to the Lindblad-Sandulescu-Scutaru theory. As an application, we studied the optical bistability of an atomic system in a Fabry-Perot resonator, in Carmichael's description, with McCall coefficients, and Bonifacio's cooperativity. In chapter 7, we obtained master equations with explicit microscopic coefficients, for a system of electrons interacting with an electromagnetic field, for this field, and for the crystal lattice vibrations. In chapter 8, we considered an open hydrogen atom, and, for life-times of lower excited states, we found a good agreement of the calculated values with the experimental data. In chapter 9, we studied a semiconductor structure which, while a current is injected in the device, radiates an infrared coherent electromagnetic energy, by heat absorption. We study the superradiant dynamics of the active electrons and the propagation of the superradiant electromagnetic field in the Fabry-Perot cavity of the device. The crystal lattice vibrations, excited by this field, and by the active electron decay, are taken into account. We calculated the superradiant power as a function of physical characteristics of the device, and found operation conditions.

CHAPTER 2

Quantum dynamics

Abstract

In this chapter, we derived some elements of quantum mechanics, which are essential for the further development of our theory: the momentum of a system of Fermions in the second quantization, the coordinate and momentum of a harmonic oscillator as a unique operator at two different moments of time, Boson and Fermion operator algebra, coherent states, the electron-field interaction, the quantization of the electromagnetic field, Boson and Fermion distributions, and densities of states in a degenerate, or a non-degenerate system of Fermions. Our starting point is the wave nature of a quantum particle, the Hamiltonian equations were obtained as group velocities in the two conjugate spaces of the wave, of the coordinates and of the momentum. In this way, the Schrödinger equation and the electron-field potential of interaction are obtained from quantum equations generated by the particle wave function.

Keywords: Wave-function, group velocity, state vector, Schrödinger equation, eigenstate, eigenvector, density matrix, operator, Hermitian conjugate, representation, Maxwell equations, Fermion, Boson, Fermi-Dirac distribution, Bose-Einstein distribution, Fourier transform, Hamiltonian, Lagrangian, Hamilton equations, Lagrange equation.

2.1 Quantum particles

2.1.1 Wavefunctions

An essential discovery concerning the electrons is their wave-like behavior, with diffraction models when they are scattered on the periodic lattice of a crystal. The conclusion was that any quantum particle, as electron, proton, or neutron, is characterized by a wave function, describing its localization in space \vec{r} , and time t . Such a wave function may be represented as a packet of plane waves, depending on a momentum \vec{p} :

$$\psi_0(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi_0(\vec{p}, t) e^{\frac{i}{\hbar} \{\vec{p}\vec{r} - [T(\vec{p}) - U(\vec{r})]t\}} d^3\vec{p}, \quad (2.1)$$

where $T(\vec{p})$ and $U(\vec{r})$ are scalar functions defining this wave function, while \hbar is the Planck constant. With the relations (Appendix A)

$$\delta(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int e^{\frac{i}{\hbar} \vec{p}(\vec{r} - \vec{r}')} \frac{d^3 \vec{p}}{\hbar^3} \quad (2.2a)$$

$$\delta(\vec{p} - \vec{p}') = \frac{1}{(2\pi)^3} \int e^{-\frac{i}{\hbar} \vec{r}(\vec{p} - \vec{p}')} \frac{d^3 \vec{r}}{\hbar^3}, \quad (2.2b)$$

we get the inverse transform

$$\phi_0(\vec{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi_0(\vec{r}, t) e^{-\frac{i}{\hbar} \{\vec{p}\vec{r} - [T(\vec{p}) - U(\vec{r})]t\}} d^3 \vec{r}, \quad (2.3)$$

and the normalization conditions:

$$\int |\psi_0(\vec{r}, t)|^2 d^3 \vec{r} = 1 \quad (2.4a)$$

$$\int |\phi_0(\vec{p}, t)|^2 d^3 \vec{p} = 1. \quad (2.4b)$$

These equations yield evident equivalent relations:

$$\psi_0(\vec{r}, t) = \frac{1}{(2\pi\hbar)^3} \int \psi_0(\vec{r}', t) e^{\frac{i}{\hbar} [U(\vec{r}) - U(\vec{r}')]t} e^{\frac{i}{\hbar} \vec{p}(\vec{r} - \vec{r}')} d^3 \vec{p} d^3 \vec{r}' \quad (2.5)$$

$$\phi_0(\vec{p}, t) = \frac{1}{(2\pi\hbar)^3} \int \phi_0(\vec{p}', t) e^{\frac{i}{\hbar} [T(\vec{p}) - T(\vec{p}')]t} e^{-\frac{i}{\hbar} \vec{r}(\vec{p} - \vec{p}')} d^3 \vec{r} d^3 \vec{p}' \quad (2.6)$$

$$\begin{aligned} \int |\psi_0(\vec{r}, t)|^2 d^3 \vec{r} &= \frac{1}{(2\pi\hbar)^3} \int \phi_0(\vec{p}, t) \phi_0^*(\vec{p}', t) e^{-\frac{i}{\hbar} [T(\vec{p}) - T(\vec{p}')]t} e^{\frac{i}{\hbar} \vec{r}(\vec{p} - \vec{p}')} d^3 \vec{r} d^3 \vec{p}' d^3 \vec{p} \\ &= \int |\phi_0(\vec{p}, t)|^2 d^3 \vec{p} = 1. \end{aligned} \quad (2.7)$$

For the two wave-packets (2.1) and (2.3), we have the group velocities

$$\frac{d}{dt} \vec{r} = \frac{\partial}{\partial \vec{p}} T(\vec{p}) = \frac{\partial}{\partial \vec{p}} H_0(\vec{r}, \vec{p}) \quad (2.8a)$$

$$\frac{d}{dt} \vec{p} = -\frac{\partial}{\partial \vec{r}} U(\vec{r}) = -\frac{\partial}{\partial \vec{r}} H_0(\vec{r}, \vec{p}), \quad (2.8b)$$

where

$$H_0(\vec{r}, \vec{p}) = T(\vec{p}) + U(\vec{r}). \quad (2.9)$$

From these equations, we get

$$\frac{d}{dt} H_0(\vec{r}, \vec{p}) = 0, \quad (2.10)$$

during the time-evolution of the system, which means that the quantity

$$H_0(\vec{r}, \vec{p}) = E. \quad (2.11)$$

is conserved. The Hamiltonian equations (2.8) and the conservation relation (2.11) mean that the function (2.9) represents the classical Hamiltonian of the particle described by the wave-functions (2.1) and (2.3), while $T(\vec{p})$ is the kinetic energy and $U(\vec{r})$ is the potential

energy of this particle with the total energy E . From (2.11) and (2.8), we also obtain an equation

$$dL_0(\vec{r}, \dot{\vec{r}}) = \dot{\vec{p}}d\vec{r} + \vec{p}d\dot{\vec{r}} \quad (2.12)$$

for the Lagrangian

$$L_0(\vec{r}, \dot{\vec{r}}) = \vec{p}\dot{\vec{r}} - H_0(\vec{r}, \vec{p}). \quad (2.13)$$

We obtain expressions for momentum and force,

$$\vec{p} = \frac{\partial}{\partial \dot{\vec{r}}} L_0(\vec{r}, \dot{\vec{r}}) \quad (2.14a)$$

$$\vec{F} = \dot{\vec{p}} = \frac{\partial}{\partial \vec{r}} L_0(\vec{r}, \dot{\vec{r}}), \quad (2.14b)$$

and the Lagrange equation:

$$\frac{d}{dt} \frac{\partial}{\partial \dot{\vec{r}}} L_0(\vec{r}, \dot{\vec{r}}) = \frac{\partial}{\partial \vec{r}} L_0(\vec{r}, \dot{\vec{r}}). \quad (2.15)$$

For a momentum proportional to velocity and mass,

$$\vec{p} = M\dot{\vec{r}}, \quad (2.16)$$

from the Hamilton equation (2.8a), we obtain the kinetic energy

$$T(\vec{p}) = \frac{\vec{p}^2}{2M}. \quad (2.17)$$

With these equations and (2.9), from (2.13) we get the Lagrangian

$$L_0(\vec{r}, \dot{\vec{r}}) = T(\vec{p}) - U(\vec{r}). \quad (2.18)$$

With this equation, from (2.1) and (2.3) we get wave functions of a simpler form:

$$\psi_0(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi_0(\vec{p}, t) e^{\frac{i}{\hbar}[\vec{p}\vec{r} - L(\vec{r}, \dot{\vec{r}})t]} d^3\vec{p} \quad (2.19a)$$

$$\phi_0(\vec{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi_0(\vec{r}, t) e^{-\frac{i}{\hbar}[\vec{p}\vec{r} - L(\vec{r}, \dot{\vec{r}})t]} d^3\vec{r}. \quad (2.19b)$$

Such a wave function representing a particle of mass M in a potential $U(\vec{r})$ can be generalized for the case of an interaction with a field of a potential $V(\vec{r}, \vec{p}, t)$:

$$\psi(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi(\vec{p}, t) e^{\frac{i}{\hbar}\{\vec{p}\vec{r} - [T(\vec{p}) - U(\vec{r}) + V(\vec{r}, \vec{p}, t)]t\}} d^3\vec{p} \quad (2.20)$$

$$\phi(\vec{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r}, t) e^{-\frac{i}{\hbar}\{\vec{p}\vec{r} - [T(\vec{p}) - U(\vec{r}) + V(\vec{r}, \vec{p}, t)]t\}} d^3\vec{r}. \quad (2.21)$$

From these equations we obtain the evident relations:

$$\psi(\vec{r}, t) = \frac{1}{(2\pi\hbar)^3} \int \psi(\vec{r}', t) e^{\frac{i}{\hbar}[U(\vec{r}) - U(\vec{r}') - V(\vec{r}, \vec{p}, t) + V(\vec{r}', \vec{p}, t)]t} e^{\frac{i}{\hbar}\vec{p}(\vec{r} - \vec{r}')} d^3\vec{p} d^3\vec{r}' \quad (2.22)$$

$$\phi(\vec{p}, t) = \frac{1}{(2\pi\hbar)^3} \int \phi(\vec{p}', t) e^{\frac{i}{\hbar}[T(\vec{p}) - T(\vec{p}') + V(\vec{r}, \vec{p}, t) - V(\vec{r}, \vec{p}', t)]t} e^{-\frac{i}{\hbar}\vec{r}(\vec{p} - \vec{p}')} d^3\vec{r} d^3\vec{p}' \quad (2.23)$$

$$\int |\psi(\vec{r}, t)|^2 d^3\vec{r} = \frac{1}{(2\pi\hbar)^3} \int \phi(\vec{p}, t) \phi^*(\vec{p}', t) e^{-\frac{i}{\hbar}[T(\vec{p}) - T(\vec{p}') + V(\vec{r}, \vec{p}, t) - V(\vec{r}, \vec{p}', t)]t} e^{\frac{i}{\hbar}\vec{r}(\vec{p} - \vec{p}')} d^3\vec{r} d^3\vec{p}' d^3\vec{p} = \int |\phi(\vec{p}, t)|^2 d^3\vec{p} = 1. \quad (2.24)$$

CHAPTER 3

Dissipative dynamics

Abstract

In this chapter, we describe various mechanisms and characteristics of dissipation, mostly in physical terms, as they have been perceived at the beginning. We get a microscopic understanding of temperature, and of the main dissipation effects. We obtain the entropy dynamics, according to principle two of thermodynamics, from the Pauli master equation, as the simplest description of a system defined by states, occupation probabilities, and transition probabilities. For various expansions of these probabilities as functions of coordinates, stochastic equations are obtained for the time evolutions of these coordinates. In this framework, we describe the electron and hole transport in semiconductors. We present various trials for completing a Schrödinger equation with dissipative terms, and the method of projection operators for a description of a system coupled to a dissipative environment.

Keywords: Friction, diffusion, decay rate, entropy, spectral line broadening, correlation, autocorrelation, memory, quality factor, self-organization, chaos, Brownian motion, Markov process, mean free path, collision mean time, mobility, occupation probability, transition probability, field current, diffusion current.

3.1 Brownian motion

3.1.1 Heavy particle in a molecular environment (Einstein-Smoluchowski)

For the beginning, we consider the simplest dissipative system: a particle P , with the position vector \vec{r} , and a single property - the inertia, described by the particle mass m , which is assumed much larger than the masses m_e of the environment particles ($m \gg m_e$) (figure 3.1). When the Brownian particle P is immersed in this environment, composed of the particles P_i at temperature T , the environment particles are scattered on the Brownian particle, thrusting this particle into a random motion, usually called Brownian motion [1]. A Brownian particle in a three dimensional space, according to the equipartition theorem (2.345), has the same energy mean value as a particle of the environment:

$$\left\langle \frac{m\vec{v}^2}{2} \right\rangle = \left\langle \frac{m_e\vec{v}_e^2}{2} \right\rangle = \frac{3}{2}T. \quad (3.1)$$

We notice that the mean square of the Brownian particle velocity is much smaller than that of an environment particle,

$$\frac{\langle \vec{v}^2 \rangle}{\langle \vec{v}_e^2 \rangle} = \frac{m_e}{m} \ll 1, \quad (3.2)$$

while the mean square of the Brownian particle momentum is much bigger than that of an environment particle:

$$\frac{\langle \vec{p}^2 \rangle}{\langle \vec{p}_e^2 \rangle} = \frac{m}{m_e} \gg 1. \quad (3.3)$$

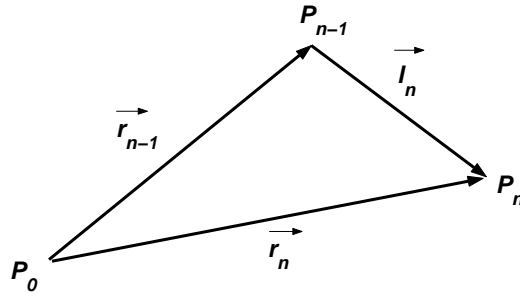


Figure 3.1: A Brownian particle with the initial position P_0 , in the n -th high-energy collision process is scattered from the position P_{n-1} to the position P_n , where it stops by collisions with the environment particles.

However, due to the momentum conservation, the momentum variation of a Brownian particle in a collision with a light environmental particle, is in the order which is double to the momentum of this particle, $|\Delta \vec{p}| \sim 2|\vec{p}_e| \ll |\vec{p}|$. This means that a Brownian particle reaches its momentum root mean square through a number of collisions with environment particles. Obviously, small displacements of a Brownian particle, produced by collisions with environmental particles, are assumed as not being observed in a conventional experiment of Brownian motion. In such an experiment, only the much larger fluctuations of the Brownian particle are observed. Evidently, these position fluctuations, which are much larger than the mean free path of an environment particle, are caused by rare collisions with environment particles of energies much larger than a particle energy mean value at the system temperature T . Thus, in the Brownian motion, we distinguish two classes of processes:

- collisions with high energy particles of the environment, causing displacements \vec{l}_n much larger than the mean free path of an environment particle, usually described by a random force called Langevin force [46], and
- collisions with low energy particles of the environment, usually described by a friction force F_f , when the energy obtained by the Brownian particle in a high energy collision is dissipated in the environment.

For a Brownian particle with the initial position P_0 , we consider the n -th high energy collision, when this particle is scattered from the position P_{n-1} to a position P_n , as it is represented in figure 3.1. This process is described by a relation of the form:

$$\vec{r}_n = \vec{r}_{n-1} + \vec{l}_n. \quad (3.4)$$

When this relation is squared, and averaged over all the probable states,

$$\langle \vec{r}_n^2 \rangle = \langle \vec{r}_{n-1}^2 \rangle + \langle \vec{l}_n^2 \rangle + 2 \langle \vec{r}_{n-1} \vec{l}_n \rangle, \quad (3.5)$$

since the scattering directions \vec{l}_n are independent on particle positions \vec{r}_{n-1} , $\langle \vec{r}_{n-1} \vec{l}_n \rangle = 0$, which means a position vector mean square

$$\langle \vec{r}_n^2 \rangle = \sum_{m=1}^n \langle \vec{l}_m^2 \rangle = n l^2, \quad l^2 = \langle \vec{l}_m^2 \rangle, \quad (3.6)$$

as an integer number of mean squares of the scattering distance l^2 . Since the number of scatterings is proportional to time t , from this expression we obtain the time evolution of the Brownian particle, considered as a quasi-continuous process:

$$\langle \vec{r}^2 \rangle = \langle x^2(t) \rangle + \langle y^2(t) \rangle + \langle z^2(t) \rangle = 3\alpha t. \quad (3.7)$$

The friction force \vec{F}_f , can be described as the momentum variation by two collisions with environment particles with opposed velocities \vec{v}_e and $-\vec{v}_e$, $-2m_e(\vec{v}_e + \vec{v}) + 2m_e(\vec{v}_e - \vec{v}) = -4m_e\vec{v}$, in the mean time $2\langle t_c \rangle$ of the two collisions,

$$\vec{F}_f = m \frac{d^2 \vec{r}}{dt^2} = -\frac{2m_e \vec{v}}{\langle t_c \rangle} = -\mu_e^{-1} \frac{d\vec{r}}{dt}. \quad (3.8)$$

The coefficient μ_e , of proportionality of the velocity with the friction force

$$\vec{v} = -\mu_e \vec{F}_f \quad (3.9)$$

is called mobility, as ratio of the collision mean time $\langle t_c \rangle$ to the double of the environment particle mass m_e :

$$\mu_e = \frac{\langle t_c \rangle}{2m_e}. \quad (3.10)$$

From this equation, we obtain:

$$\begin{aligned} m \vec{r} \frac{d^2 \vec{r}}{dt^2} + \mu_e^{-1} \vec{r} \frac{d\vec{r}}{dt} &= 0 \\ m \left[\frac{d}{dt} \left(\vec{r} \frac{d\vec{r}}{dt} \right) - \left(\frac{d\vec{r}}{dt} \right)^2 \right] + \frac{1}{2\mu_e} \frac{d}{dt} (\vec{r}^2) &= 0 \\ m \left[\frac{1}{2} \frac{d^2}{dt^2} \langle \vec{r}^2 \rangle - \langle \vec{v}^2 \rangle \right] + \frac{1}{2\mu_e} \frac{d}{dt} \langle \vec{r}^2 \rangle &= 0. \end{aligned} \quad (3.11)$$

With equation (3.7), this equation becomes:

$$-\langle m \vec{v}^2 \rangle + \frac{3\alpha}{2\mu_e} = 0. \quad (3.12)$$

Comparing this relation with (3.1), we obtain the coefficient α as a function of temperature and mobility,

$$\alpha = 2\mu_e T, \quad (3.13)$$

CHAPTER 4

Axiomatic open quantum physics

Abstract

This chapter is devoted to Lindblad master equation, obtained by a generalization of the quantum dynamic group to a time dependent semigroup. For this equation, we present a demonstration of Alicki and Lendi, obtained by a linear approximation of the openness operator, which describes the time evolution of a system of interest in an environment. We re-obtain this equation by taking the total dynamic equation with a bilinear dissipative potential in system and environment operators, and tracing over the environment states. In this way, we get physical expressions of the dissipation coefficients, as functions of the system operators. We present the quantum theory of Sandulescu and Scutaru, where the dissipative dynamics is described by friction and diffusion processes, with coefficients which satisfy fundamental constraints.

Keywords: Hilbert space, Banach space, evolution operator, dynamic map, dynamic group, dynamic semigroup, superoperator, openness operator, Born-Markov approximation, Lindblad's generator, dissipative dynamics, dissipation coefficient, hermiticity, positivity, convexity, normalization, Gibbs distribution, friction, diffusion, fundamental constraint.

4.1 Lindblad's master equation

4.1.1 Lindblad's master equation as a generator of a dynamic semigroup

In the previous chapter, we described the dissipative dynamics of a quantum system based on various phenomenological assumptions regarding possible effects of the system-environment coupling. Thus, the quantum equations of motion have been modified, without taking into account the preservation of the quantum relations, as the positivity of the density matrix, the uncertainty relations, and the ground-state energy. The Schrödinger equation of motion

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = -\frac{i}{\hbar}H|\Psi(t)\rangle \quad (4.1)$$

defines a system of operators

$$U_t = e^{-\frac{i}{\hbar}Ht}, \quad (4.2)$$

which describes the dynamics of the system:

$$|\Psi(t)\rangle = U_t|\Psi(0)\rangle. \quad (4.3)$$

This system is a dynamic group $\mathcal{D} = \{U_t\}$, for the product

$$U_t U_{t'} = U_{t+t'}, \quad (4.4)$$

of any two operators $U_t, U_{t'} \in \mathcal{D}$, with a unity element

$$U_0 = \hat{1}, \quad (4.5)$$

while any element $U_t \in \mathcal{D}$ has an inverse $U_t^{-1} = U_{-t}$,

$$U_t^{-1} U_t = U_t U_t^{-1} = \hat{1}. \quad (4.6)$$

Since

$$U_t^{-1} = U_t^+, \quad (4.7)$$

this is a unitary group, defined by the relation $U_t U_t^+ = \hat{1}$, in agreement with the relations (2.83)-(2.84) of a unitary matrix. Similarly, the Schrödinger equation of the density matrix

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H, \rho(t)] \quad (4.8)$$

defines a system of time-dependent superoperators $\tilde{\mathcal{D}} = \{\tilde{U}_t\}$,

$$\rho(t) = \tilde{U}_t \rho(0) = U_t \rho(0) U_t^{-1}. \quad (4.9)$$

This system has also a group structure:

$$\tilde{U}_t \in \tilde{\mathcal{D}}, \quad \tilde{U}_{t'} \in \tilde{\mathcal{D}} \quad \Rightarrow \quad \tilde{U}_t \tilde{U}_{t'} = \tilde{U}_{t+t'} \in \tilde{\mathcal{D}} \quad (4.10)$$

$$\tilde{U}_0 = \hat{1} \quad (4.11)$$

$$\tilde{U}_t \in \tilde{\mathcal{D}} \quad \Rightarrow \quad \tilde{U}_t^{-1} = \tilde{U}_{-t} \in \tilde{\mathcal{D}}, \quad \tilde{U}_t^{-1} \tilde{U}_t = \tilde{U}_t \tilde{U}_t^{-1} = \hat{1}. \quad (4.12)$$

The space of the density matrix $\rho(t) = \tilde{U}_t \rho(0)$ generated by the dynamic superoperator \tilde{U}_t over the space of the density matrix $\rho(0)$ is called dynamic map. Lindblad's idea was to describe the dissipative dynamics by an equation similar to (4.8),

$$\frac{d}{dt} \rho(t) = Z \rho(t), \quad (4.13)$$

with Z as the generator of the dynamic superoperators \tilde{T}_t ,

$$\rho(t) = \tilde{T}_t \rho(0), \quad (4.14)$$

by considering the simplest generalization from the dynamic group $\tilde{\mathcal{D}} = \{\tilde{U}_t\}$ to a semigroup of dynamic superoperators $\tilde{\mathcal{D}}_T = \{\tilde{T}_t\}$:

$$\tilde{T}_t \in \tilde{\mathcal{D}}_T, \quad \tilde{T}_{t'} \in \tilde{\mathcal{D}}_T \quad \Rightarrow \quad \tilde{T}_t \tilde{T}_{t'} = \tilde{T}_{t+t'} \in \tilde{\mathcal{D}}_T \quad (4.15)$$

$$\tilde{T}_0 = \hat{1}. \quad (4.16)$$

These superoperators must preserve Von Neumann's conditions during the hole evolution of the physical system [15]:

$$\tilde{T}_t(\lambda_1 \rho_1 + \lambda_2 \rho_2) = \lambda_1 \tilde{T}_t \rho_1 + \lambda_2 \tilde{T}_t \rho_2 \quad \text{for } \lambda_1, \lambda_2 \geq 0 \quad \text{with } \lambda_1 + \lambda_2 = 1 \quad (4.17)$$

(convexity)

$$\tilde{T}_t \rho^+ = [\tilde{T}_t \rho]^+ \quad \text{(hermiticity)} \quad (4.18)$$

$$\tilde{T}_t \rho > 0 \quad \text{(positivity)} \quad (4.19)$$

$$\text{Tr}(\tilde{T}_t \rho) = 1. \quad \text{(normalization)}. \quad (4.20)$$

In this axiomatic framework, for a physical system with N states, described by a system of independent operators F_n , $n = 1, 2, \dots, N^2 - 1$, Lindblad obtained a generator of the dynamic semigroup of the form

$$Z\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] + \frac{1}{2\hbar} \sum_{n=1}^{N^2-1} ([V_n\rho(t), V_n^+] + [V_n, \rho(t)V_n^+]), \quad (4.21)$$

where the openness operators V_n are linear combinations of the system operators

$$V_n = \sum_{k=1}^{N^2-1} c_{kn} F_k. \quad (4.22)$$

In the following, we shall derive this equation in more physical approaches [17, 48, 49].

4.1.2 Lindblad's master equation as generator of a dynamic map with linear openness operators (Alicki and Lendi)

Although Lindblad's demonstration of the dissipative generator (4.21) is a mathematically rigorous one, it is based on an unphysical assumption, of quantum-dynamical semigroups, without any assumption on the environment, or on the system coupling to this environment. In the quantum mechanics, this assumption could be considered only as an approximate description of the dissipative dynamics, usually called the Born-Markov approximation. In section 7.1, it is shown that, besides the Born-Markov, or Lindbladian local in time terms, which describe correlated transitions of the system and environment particles, the quantum dynamics also includes non-local in time terms [36, 41], due to the self-consistent field of the environmental particles, which means that the semigroup assumption can not be considered as a basic quantum-mechanical principle. In this subsection, and in the following one, we derive Lindblad's master equation by reducing the total dynamics, in two linear approximation modes of the system-environment coupling.

Following an approach of Alicki and Lendi [17], we consider a physical system of interest S , with the following characteristics:

- 1) $X = \{x\}$ - coordinate space
- 2) $\mathcal{H} = \{|\psi_i\rangle\}$ - Hilbert space of the state vectors
- 3) $\mathcal{B}(\mathcal{H}) = \{s_k\}$ - Banach space of the system observables
- 4) $\mathcal{T}(\mathcal{H}) = \{\rho(t)\}$ - Banach space of the density trace-class operators.

Similarly, we consider the dissipative environment E of this system defined by

- 1) $Y = \{y\}$ - coordinate space of the environment
- 2) $\mathcal{H}^E = \{|\phi_\nu\rangle\}$ - Hilbert space of the environment state vectors
- 3) $\mathcal{B}^E(\mathcal{H}^E) = \{\Gamma_\mu\}$ - Banach space of the environment observables
- 4) $\mathcal{T}^E(\mathcal{H}^E) = \{\rho^E(t)\}$ - Banach space of the environment density trace-class operators.

We take the total system as

CHAPTER 5

Quantum tunneling with dissipative coupling

Abstract

This chapter is devoted to quantum tunneling, as a basic quantum process, essential for important applications. Tunneling between two wells, of the double well potential of a one particle system of interest, makes sense only when a second system, capable to distinguish between the presence of the particle in a well, or in the other well, is present. The potential of interaction between such two systems is called tunneling operator. We treat a few problems of interest as tunneling in a quasi-continuum of states, the energy shift in a well by the proximity of another well, dissipation effects, and tunneling spectrum.

Keywords: Probability distribution, probability flow, potential well, potential barrier, double well potential, tunneling operator, Wronskian, interaction picture, ground state, excited state, density of states, golden rule, WKB approximation, action, wave vector, penetrability, Lindbladian, dissipative tunneling, tunneling spectrum.

5.1 Quantum tunneling and states

5.1.1 Tunneling operator

The wave nature of a particle means a probability variation in a volume \mathcal{V}_Σ , and a probability flow from this volume:

$$\frac{\partial}{\partial t} \int_{\mathcal{V}_\Sigma} |\psi(\vec{r}, t)|^2 d^3\vec{r} = - \oint_\Sigma \vec{J}_\psi(\vec{r}, t) d^2\vec{r}, \quad (5.1)$$

where $\vec{J}_\psi(\vec{r}, t)$ is the particle flow density. If the volume \mathcal{V}_Σ is situated inside a barrier with the maximum on the surface Σ , the particle passage through the barrier is called tunneling. With the Schrödinger equation

$$\begin{cases} H_0\psi(\vec{r}, t) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial \vec{r}^2}\psi(\vec{r}, t) + U(\vec{r})\psi(\vec{r}, t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) & / \psi^*(\vec{r}, t) \\ H_0\psi^*(\vec{r}, t) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial \vec{r}^2}\psi^*(\vec{r}, t) + U(\vec{r})\psi^*(\vec{r}, t) = -i\hbar\frac{\partial}{\partial t}\psi^*(\vec{r}, t) & / \psi(\vec{r}, t), \end{cases} \quad (5.2)$$

the probability conservation equation (5.1) takes a form

$$\begin{aligned}
 \frac{\partial}{\partial t} \int_{V_\Sigma} \psi^*(\vec{r}, t) \psi(\vec{r}, t) d^3\vec{r} &= \int_{V_\Sigma} \left[\frac{\partial}{\partial t} \psi^*(\vec{r}, t) \psi(\vec{r}, t) + \psi^*(\vec{r}, t) \frac{\partial}{\partial t} \psi(\vec{r}, t) \right] d^3\vec{r} \\
 &= -\frac{i}{\hbar} \frac{\hbar^2}{2M} \int_{V_\Sigma} \left[\psi(\vec{r}, t) \frac{\partial^2}{\partial \vec{r}^2} \psi^*(\vec{r}, t) - \psi^*(\vec{r}, t) \frac{\partial^2}{\partial \vec{r}^2} \psi(\vec{r}, t) \right] d^3\vec{r} \\
 &= -\frac{i\hbar}{2M} \int_{V_\Sigma} \frac{\partial}{\partial \vec{r}} \left[\psi(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi^*(\vec{r}, t) - \psi^*(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi(\vec{r}, t) \right] d^3\vec{r} \\
 &= -\frac{i\hbar}{2M} \oint_\Sigma \left[\psi(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi^*(\vec{r}, t) - \psi^*(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi(\vec{r}, t) \right] d^2\vec{r},
 \end{aligned}$$

with the flow density:

$$\vec{J}_\psi = \frac{i\hbar}{2M} \left[\psi(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi^*(\vec{r}, t) - \psi^*(\vec{r}, t) \frac{\partial}{\partial \vec{r}} \psi(\vec{r}, t) \right]. \quad (5.3)$$

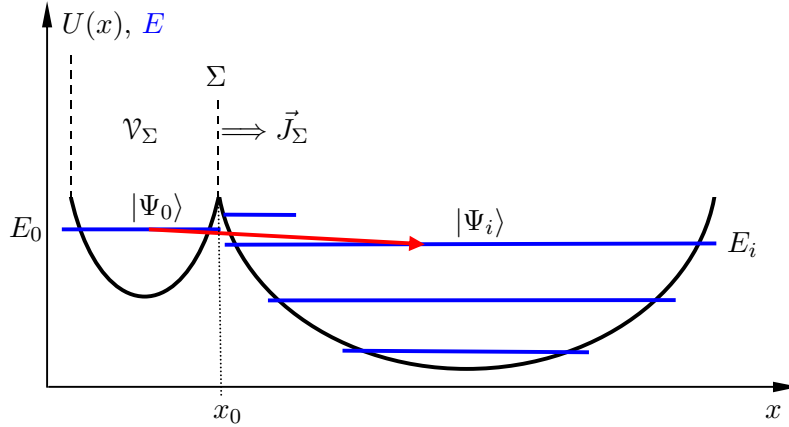


Figure 5.1: Quantum tunneling in a double-well potential.

Generally, this particle flow describes a quantum tunneling through a potential barrier. However, when a double-well potential is considered, there is a difficulty, namely, the steady states have no particle flow, a particle in such a state remaining in this state. However a quantum tunneling arises just in this case, from another reason. In figure 5.1, we considered a finite domain for a double-well potential, where normalized eigenfunctions can be defined:

$$\begin{aligned}
 H_0 |\Psi_0\rangle &= E_0 |\Psi_0\rangle \\
 H_0 |\Psi_i\rangle &= E_i |\Psi_i\rangle.
 \end{aligned} \quad (5.4)$$

The wave function $|\Psi_0\rangle$ defined in a rigid potential $U(\vec{r})$, being a steady state, does not describe any tunneling. However, a tunneling process arises if this wave function is under the action of a perturbation V inside the barrier,

$$(H_0 + V) |\Psi_0\rangle = E_0 |\Psi_0\rangle. \quad (5.5)$$

That means that the initial and the final states of a tunneling process satisfy the Schrödinger equations:

$$\begin{cases} -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \vec{r}^2} \Psi_0(\vec{r}) + [U(\vec{r}) + V] \Psi_0(\vec{r}) = E_0 \Psi_0(\vec{r}) & / \Psi_i^*(\vec{r}) \\ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \vec{r}^2} \Psi_i^*(\vec{r}) + U(\vec{r}) \Psi_i^*(\vec{r}) = E_i \Psi_i^*(\vec{r}). & / \Psi_0(\vec{r}) \end{cases} \quad (5.6)$$

For a process with energy conservation, $E_i \approx E_0$, from these equations, we get the matrix elements of the perturbation operator V :

$$\begin{aligned} V_{i0} &= \frac{\hbar^2}{2M} \int_{V_\Sigma} \left[\Psi_i^*(\vec{r}) \frac{\partial^2}{\partial \vec{r}^2} \Psi_0(\vec{r}) - \Psi_0(\vec{r}) \frac{\partial^2}{\partial \vec{r}^2} \Psi_i^*(\vec{r}) \right] d^3 \vec{r} \\ &= \frac{\hbar^2}{2M} \oint_\Sigma \left[\Psi_i^*(\vec{r}) \frac{\partial}{\partial \vec{r}} \Psi_0(\vec{r}) - \Psi_0(\vec{r}) \frac{\partial}{\partial \vec{r}} \Psi_i^*(\vec{r}) \right] d^2 \vec{r}, \end{aligned} \quad (5.7)$$

which, for a one-dimensional system, is

$$V_{i0} = \frac{\hbar^2}{2M} \left[\Psi_i^*(x) \frac{d}{dx} \Psi_0(x) - \Psi_0(x) \frac{d}{dx} \Psi_i^*(x) \right]_{x=x_0}. \quad (5.8)$$

Due to the Hermiticity condition, $V_{0i} = V_{i0}^*$, we obtain the tunneling operator represented by the tunneling matrix:

$$V = \begin{pmatrix} 0 & V_{01} & V_{02} & \dots & V_{0N} \\ V_{10} & 0 & 0 & \dots & 0 \\ V_{20} & 0 & 0 & \dots & 0 \\ \vdots & & & & \\ V_{N0} & 0 & 0 & \dots & 0 \end{pmatrix}. \quad (5.9)$$

A perturbation V of a potential $U(\vec{r})$ is always present in the practical cases, such potential being always generated by a system of particles, which are always in motion at a certain temperature T . It is interesting that although such a perturbation is an arbitrary one, its matrix elements are essentially determined by wave-functions in a rigid potential, without depending on this perturbation. However, a tunneling process effectively arises only when the energy is conserved, which means that, for tunneling to a different energy from the initial one, a coupling to another system is necessary. Such a coupling is present in open systems.

5.1.2 Fermi's golden rule

A problem of interest is the transition of a particle from a state of energy E_0 to a quasi-continuum of states with a density $g(E)$ (figure 5.2). To calculate the total transition probability determined by the perturbation matrix (5.9), in a system with the Hamiltonian H_0 , one has to sum up the transition probabilities from the initial state $|0\rangle = |\Psi_0\rangle$ to the final states $|i\rangle = |\Psi_i\rangle$. The quantum dynamics determined by this operator is described by the Schrödinger equation (2.108), which, with a perturbation operator V , takes the form

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H_0 + V, \rho(t)]. \quad (5.10)$$

Atom-field interaction with dissipative coupling

Abstract

In this chapter, we treat the basic quantum process of electromagnetic field propagation through an atomic system in a resonant Fabry-Perot cavity. We obtain the transmission characteristic of such a cavity, which is a basic element for a quantum heat converter. When the system is opened only by a population decay and a polarization dephasing, we get only an optical bistability characteristic. By openness according to the Lindblad-Sandulescu-Scutaru theory, we get also a coupling through environment between population and polarization, which, in some conditions, leads to an energy transfer from the disordered environment to the coherent electromagnetic field. We find that this phenomenon, which has experimental evidence, is an effect of an atom-atom coupling.

Keywords: pseudo-spin operators, Pauli matrices, Bloch vector, population, polarization, dipole moment, coupling coefficient, Rabi frequency, decay, dephasing, atomic detuning, homogeneous broadening, inhomogeneous broadening, Lorentzian shape, Gaussian shape, optical bistability, nonlinear detuning, saturation, McCall coefficients, cooperativity.

6.1 Maxwell-Bloch equations (Feynman, Vernon, and Hellwarth)

6.1.1 Quantum atom-field system

We consider a system of N two-level atoms occupying a volume \mathcal{V} , with the ground state $|0\rangle$ of energy E_0 and an excited state $|1\rangle$ of energy E_1 , in interaction with a coherent electromagnetic field \vec{E} of quasi-resonant frequency $\omega \sim \omega_0 = \frac{E_1 - E_0}{\hbar}$ (see figure 6.1). For a rather large intensity of this field, we can consider the electric dipole interaction described by the potential

$$V = e\vec{r}\vec{E}, \quad (6.1)$$

where the electron charge is $-e$, and \vec{r} is the electron coordinate. This potential can be understood physically, or in more rigorous terms by using the second quantization expression (2.319) with (2.320), (2.321), and (2.325). For a two-level system with a transition frequency

ω_0 , interacting with an electromagnetic field of frequency ω and polarization \vec{l}_ω , we get

$$V = ie\vec{l}_\omega\vec{r}_{01}\sqrt{\frac{\hbar}{2\varepsilon\mathcal{V}\omega}}\omega_0(c_1^\dagger c_0 - c_0^\dagger c_1)(a + a^\dagger), \quad (6.2)$$

while the electric dipole interaction potential (6.1) is of the form

$$V = ie\vec{l}_\omega\vec{r}_{01}\sqrt{\frac{\hbar\omega}{2\varepsilon\mathcal{V}}}(c_1^\dagger c_0 + c_0^\dagger c_1)(a - a^\dagger). \quad (6.3)$$

With the resonance condition $\omega \approx \omega_0$, and taking into account only single-particle processes, *i.e.* an electron excitation $c_1^\dagger c_0$ coupled to a photon absorption a , and an electron decay $c_0^\dagger c_1$ coupled to a photon creation a^\dagger , both these relations give the same result:

$$V = ie\vec{l}_\omega\vec{r}_{01}\sqrt{\frac{\hbar\omega}{2\varepsilon\mathcal{V}}}(c_1^\dagger c_0 a - c_0^\dagger c_1 a^\dagger). \quad (6.4)$$

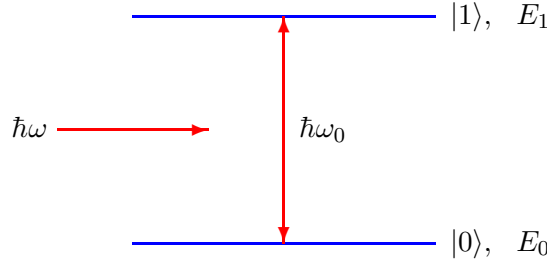


Figure 6.1: A photon of energy $\hbar\omega$ of a coherent electromagnetic field interacting with a two-level system of quasi-resonant transition frequency $\omega_0 = \frac{E_1 - E_0}{\hbar} \sim \omega$.

With this potential, the system dynamics is described by the equation of the density matrix

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H_0 + V, \rho(t)], \quad (6.5)$$

where H_0 is the Hamiltonian of the isolated two-level system. The idea of Feynman, Vernon, and Hellwarth was to describe a two-level system by the three real functions defined by the two complex probability amplitudes of the eigenstates of the system (Bloch vector) [55]. These functions are the mean-values of the three operators that can be defined for a system with two states $|0\rangle$ and $|1\rangle$:

$$\sigma_x = |1\rangle\langle 0| + |0\rangle\langle 1| \quad (6.6)$$

$$\sigma_y = \frac{|1\rangle\langle 0| - |0\rangle\langle 1|}{i} \quad (6.7)$$

$$\sigma_z = |1\rangle\langle 1| - |0\rangle\langle 0|. \quad (6.8)$$

These operators are represented by the Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6.9)$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (6.10)$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (6.11)$$

while their mean values are

$$\langle \sigma_x \rangle = \text{Tr} \{ \sigma_x \rho(t) \} = \rho_{10}(t) + \rho_{01}(t) \quad (6.12)$$

$$\langle \sigma_y \rangle = \text{Tr} \{ \sigma_y \rho(t) \} = i [\rho_{10}(t) - \rho_{01}(t)] \quad (6.13)$$

$$\langle \sigma_z \rangle = \text{Tr} \{ \sigma_z \rho(t) \} = \rho_{11}(t) - \rho_{00}(t). \quad (6.14)$$

With the operator σ_z , we can express the Hamiltonian of a two-level system as

$$H_0 = \frac{\hbar\omega_0}{2} \sigma_z. \quad (6.15)$$

If the two wave-functions $\psi_0(\vec{r}) = \langle \vec{r}|0\rangle$ and $\psi_1(\vec{r}) = \langle \vec{r}|1\rangle$ are of different parities, the electric dipole potential (6.1) has the matrix elements

$$\begin{aligned} V_{11} &= e\langle 1|\vec{r}|1\rangle\vec{E} = 0 & V_{10} &= e\langle 1|\vec{r}|0\rangle\vec{E} = -\vec{\mu}\vec{E} \\ V_{01} &= e\langle 0|\vec{r}|1\rangle\vec{E} = -\vec{\mu}\vec{E} & V_{00} &= e\langle 0|\vec{r}|0\rangle\vec{E} = 0, \end{aligned} \quad (6.16)$$

where we used the notation

$$\vec{\mu} = -e\langle 1|\vec{r}|0\rangle = -e\langle 0|\vec{r}|1\rangle \quad (6.17)$$

for the atomic electric dipole moment. Thus, the interaction potential has the expression

$$V = -\vec{\mu}\vec{E}\sigma_x. \quad (6.18)$$

With (6.15) and (6.18), the equation of motion (6.18) takes the form

$$\frac{d}{dt}\rho(t) = -i \left[\frac{\omega_0}{2} \sigma_z - \bar{\chi} \sigma_x, \rho(t) \right], \quad (6.19)$$

where we used the notation

$$\bar{\chi} = \frac{\vec{\mu}}{\hbar} \vec{E}. \quad (6.20)$$

From this equation, we obtain equations for the elements of the density matrix:

$$\begin{aligned} \frac{d\rho_{11}}{dt} &= -i\bar{\chi}(\rho_{10} - \rho_{01}) & \frac{d\rho_{10}}{dt} &= -i\omega_0\rho_{10} - i\bar{\chi}(\rho_{11} - \rho_{00}) \\ \frac{d\rho_{01}}{dt} &= i\omega_0\rho_{01} + i\bar{\chi}(\rho_{11} - \rho_{00}) & \frac{d\rho_{00}}{dt} &= i\bar{\chi}(\rho_{10} - \rho_{01}). \end{aligned} \quad (6.21)$$

Using the expressions (6.12)-(6.12), we get the Bloch-Feynman equations

$$\frac{d}{dt}\langle \sigma_x \rangle + \omega_0 \langle \sigma_y \rangle = 0 \quad (6.22)$$

$$\frac{d}{dt}\langle \sigma_y \rangle - \omega_0 \langle \sigma_x \rangle - 2\bar{\chi} \langle \sigma_z \rangle = 0 \quad (6.23)$$

$$\frac{d}{dt}\langle \sigma_z \rangle + 2\bar{\chi} \langle \sigma_y \rangle = 0. \quad (6.24)$$

CHAPTER 7

Microscopic open quantum physics

Abstract

In this chapter, we derive quantum master equations with explicit, microscopic coefficients, for the systems of interest of a superradiant semiconductor structure: the active electrons, the electromagnetic field, and the optical crystal vibrations. These vibrations determine an important retardation in the field propagation (refractive index), and a spectrum splitting (the Raman effect). For the active electrons we consider three environmental systems: the quasi-free electrons/holes of the conduction regions, the crystal lattice vibrations excited by electron transitions, and the free electromagnetic field. For the electromagnetic field, we consider the absorption by coupling to the conduction electrons/holes, and to the optical vibrations of the crystal, while these vibrations are damped by coupling with the valence electron transitions to thermally released states. For the electron-field coupling we consider the potential derived in chapter 2 from the Lorentz force, while the momentum difference is supposed to be taken by the crystal lattice. For the coupling of the crystal vibrations to the electromagnetic field and electron transitions we consider potentials obtained from the momentum conservation. For the active electrons, we find a quantum master equation with a Markovian term describing correlated transitions with the environmental particles, and a non-Markovian term given by the self-consistent field of the environmental particles. Since the dissipative environment of the electromagnetic field is contained inside the quantization volume of this field, which is taken as a unit volume, its quantum master equation includes a dissipative term of a space integral form. For the field mean values, the dissipation integral, of propagation through the dissipative environment, can be divided in two parts: an integral from the initial coordinate up to the boundary of the quantum uncertainty region, taken for a coherent wave, which describes dephasing, and an integral over the uncertainty region, which describes absorption. Similar equations are obtained for the optical vibration field. When the vibrational field is eliminated from these equations, we obtain a frequency splitting, corresponding to the Raman effect, and an absorption rate, including the absorption of the electromagnetic waves by conduction electrons/holes, and the absorption of the vibrational waves by the valence electrons, excited by the crystal deformations in the thermally released states.

Keywords: Total dynamics, reduced dynamics, Gibbs statistics, Fermi-Dirac statistics, Bose-Einstein statistics, Markovian dynamics, non-Markovian dynamics, dipole moment, interaction picture, transition operator, two-body potential, self-consistent field, decay, dephasing, creation-annihilation operators, Fermion operators, anticommutation relations, commutation relations, optical phonon, field-dressed electron.

7.1 Dissipative dynamics of Fermions

7.1.1 Reduced quantum dynamics (Ford, Lewis, and O'Connell)

We approach a problem somehow similar to that represented in figure 2.1, but with a difference that, now, the system of interest S is coupled to an electromagnetic field F (figure 7.1). With the potential of interaction V between these two systems, the Hamiltonian of the system S can be considered as a perturbed form

$$H = H_0^S + V, \quad (7.1)$$

of the Hamiltonian

$$H_0^S = \sum_k \varepsilon_k c_k^\dagger c_k. \quad (7.2)$$

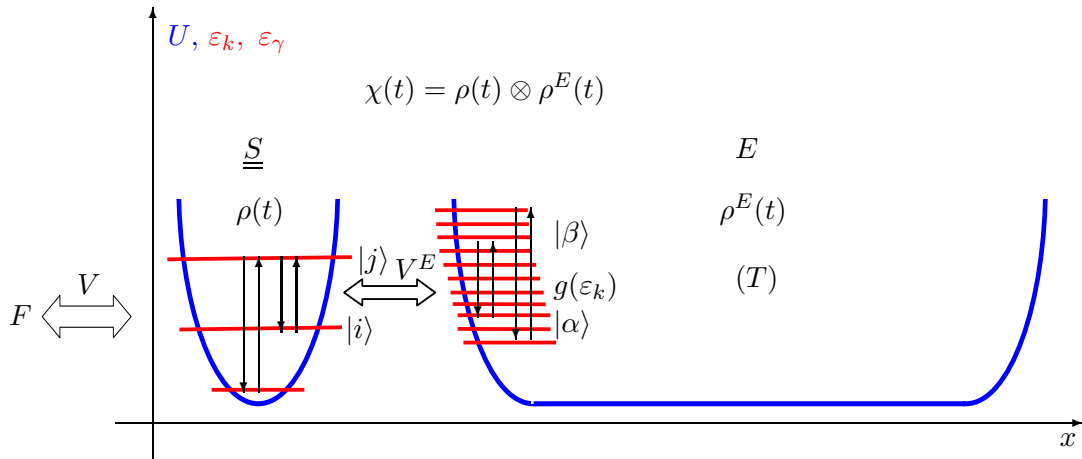


Figure 7.1: Fermion system S , described by the density $\rho(t)$, in an environment E , with the density $\rho^E(t)$, at a temperature T , in interaction with a field F . While this field is acting on the system S , by the potential V , transitions $|i\rangle \leftrightarrow |j\rangle$ of this system, correlated to transitions $|\alpha\rangle \leftrightarrow |\beta\rangle$ in the quasi-continuum of the environmental states, arise due to the dissipative coupling potential V^E , in the dynamics of the total system.

While in section 2.3 we were interested only in the statistical distribution at equilibrium (statistical quantum physics), now we are interested in a more difficult problem of the system dynamics (open quantum physics).

In chapter 3, we described various characteristics of the dissipative dynamic, as friction, diffusion, mobility, decay, broadening, etc. Dynamical equations have been obtained as functions of the occupation and transition probabilities. From the Pauli master equation, we obtained the entropy increase as a general property of the dissipative dynamics. Here, we describe the dissipative dynamics of a system S by the density matrix in the second quantization:

$$\rho(t) = \sum_{i,j} \rho_{ij}(t) c_i^\dagger c_j. \quad (7.3)$$

According to the theory developed in chapter 4, this dynamics is described by a quantum master equation of the form

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] + \sum_{i,j} \lambda_{ij}([c_i^+ c_j \rho(t), c_j^+ c_i] + [c_i^+ c_j, \rho(t) c_j^+ c_i]), \quad (7.4)$$

which depends on the phenomenological coefficients λ_{ij} .

In this chapter, we obtain a similar equation with microscopic coefficients [32, 36, 41]. On this purpose, we consider the equation of motion of the total system,

$$\frac{d}{dt}\tilde{\chi}(t) = -\frac{i}{\hbar} \left[\varepsilon \tilde{V}(t) + \varepsilon \tilde{V}^E(t), \tilde{\chi}(t) \right], \quad (7.5)$$

where tilde denotes operators in the interaction picture, as the total density

$$\tilde{\chi}(t) = e^{\frac{i}{\hbar}(H^E + H_0^S)t} \chi(t) e^{-\frac{i}{\hbar}(H_0^S + H^E)t}. \quad (7.6)$$

For this density, we consider a series expansion [31]:

$$\tilde{\chi}(t) = R \otimes \tilde{\rho}(t) + \varepsilon \tilde{\chi}^{(1)}(t) + \varepsilon^2 \tilde{\chi}^{(2)}(t) + \dots, \quad (7.7)$$

with a zero-order term $R \otimes \tilde{\rho}(t)$ corresponding to the Born-Markov approximation, when the environment with the equilibrium density R is not influenced by the system of Fermions with the density $\rho(t)$, while the environment evolution is taken into account by higher-order terms $\tilde{\chi}^{(1)}(t), \tilde{\chi}^{(2)}(t), \dots$. To handle the orders of magnitude, we use the strength parameter ε which is set to 1 in the final results. In these equations, the density matrix of the system is considered as a reduced form of the total density,

$$\tilde{\rho}(t) = Tr_E\{\tilde{\chi}(t)\}, \quad (7.8)$$

while the higher-order terms of the expression (7.7) satisfy the conditions

$$Tr_E\{\tilde{\chi}^{(1)}\} = Tr_E\{\tilde{\chi}^{(2)}\} = \dots = 0. \quad (7.9)$$

For the system density matrix $\tilde{\rho}(t)$, described by the total dynamic equation (7.5), we consider a generator of the form

$$\frac{d}{dt}\tilde{\rho}(t) = \varepsilon \tilde{B}^{(1)}(\tilde{\rho}(t), t) + \varepsilon^2 \tilde{B}^{(2)}(\tilde{\rho}(t), t) + \dots. \quad (7.10)$$

In this way, from equations (7.5), (7.7), and (7.10), we obtain equations for the powers of the parameter ε :

$$R \otimes \tilde{B}^{(1)}(\tilde{\rho}(t), t) + \frac{d}{dt}\tilde{\chi}^{(1)}(t) = -\frac{i}{\hbar} \left[\tilde{V}(t) + \tilde{V}^E(t), R \otimes \tilde{\rho}(t) \right] \quad (7.11)$$

$$R \otimes \tilde{B}^{(2)}(\tilde{\rho}(t), t) + \frac{d}{dt}\tilde{\chi}^{(2)}(t) = -\frac{i}{\hbar} \left[\tilde{V}(t) + \tilde{V}^E(t), \tilde{\chi}^{(1)}(t) \right] \quad (7.12)$$

$$R \otimes \tilde{B}^{(3)}(\tilde{\rho}(t), t) + \frac{d}{dt}\tilde{\chi}^{(3)}(t) = -\frac{i}{\hbar} \left[\tilde{V}(t) + \tilde{V}^E(t), \tilde{\chi}^{(2)}(t) \right] \quad (7.13)$$

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CHAPTER 8

Open hydrogen atom

Abstract

In this chapter, we apply our quantum master equation for a system of Fermions in free electromagnetic field to a hydrogen atom. We obtain a quantum master equation describing transitions between the eigenstates of a hydrogen atom, with coefficients depending on the hydrogen wave functions. We find that these coefficients are in agreement with published experimental data for life times of the lower excited states.

Keywords: spherical coordinates, effective mass, momentum, angular momentum, spin, total angular momentum, commutation relation, eigenfunction, eigenvalue, spectroscopic constant, Laguerre polynomial, Legendre polynomial, orthogonality, Bohr radius, transition operator, degenerate states, radial function, spherical function, decay rate, life time.

8.1 Hydrogen atom

8.1.1 Schrödinger equation and operators

The simplest physical system existing in nature is the hydrogen atom. It consists in a proton of mass $m_p = 1.673 \times 10^{-27} \text{Kg} = 938 \text{MeV}/c^2 = 1.007 \text{amu}$, interacting with an electron of mass $m_e = 9.11 \times 10^{-31} \text{Kg} = 0.511 \text{MeV}/c^2$. That means that, roughly, we have to study the motion of the light particle, the electron, around the much heavier particle, the proton ($m_p/m_e = 1836$). The hydrogen atom, usually studied as a closed system, in fact is always open, interacting with the free electromagnetic field that exists at temperature T of the environment.

From our viewpoint, the importance of hydrogen atom is threefold: (1) we apply our theory of open systems to a well-known system, (2) we compare the numerical results of our theory with well-known experimental data for decay rates, (3) an open hydrogen atom is somehow similar to an impurity atom in a semiconductor structure. Here, we present the hydrogen atom as a closed system, the openness of this system being studied in section 5.2.

For this two-body system in the rest state, we consider the electron-proton distance and the total momentum that is null,

$$\vec{r} = \vec{r}_e - \vec{r}_p, \quad (8.1)$$

$$0 = \vec{p}_e + \vec{p}_p, \quad (8.2)$$

while the interaction potential, given by Coulomb's law, is of the form:

$$U(\vec{r}) = -\frac{\alpha\hbar c}{r}, \quad (8.3)$$

where we distinguish the quantity $\hbar c = 197 \text{ eV} \cdot \text{nm}$, and the coefficient $\alpha\hbar c = 1.44 \text{ eV} \cdot \text{nm}$.

Thus, for the Hamiltonian of the system, we get a simpler, canonic expression:

$$H = \frac{\vec{p}_p^2}{2m_p} + \frac{\vec{p}_e^2}{2m_e} + U(r) = \frac{\vec{p}^2}{2M} + U(r), \quad (8.4)$$

where $\vec{p} = \vec{p}_e$ is the momentum of the electron, and

$$M = \frac{m_p m_e}{m_p + m_e} \quad (8.5)$$

is the effective mass. This quantum system, in an arbitrary state with the wave-function $\Psi(\vec{r}) = \langle \vec{r} | \Psi \rangle$ and the energy E , is described by the Schrödinger equation

$$H\Psi(\vec{r}) = \left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \vec{r}^2} + U(r) \right] \Psi(\vec{r}) = E\Psi(\vec{r}). \quad (8.6)$$

That means that this two-body system can be described by means of a single-particle model, as in the most books of quantum mechanics. In fact, this model describes steady states

$$|\Psi\rangle = \sum_i w_i |\Psi_i\rangle \quad (8.7)$$

with constant occupation probability amplitudes w_i of the eigenstates $|\Psi_i\rangle$ and energy eigenvalues ε_i of the Schrödinger equation (8.6):

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \vec{r}^2} + U(r) \right] \Psi_i(\vec{r}) = \varepsilon_i \Psi_i(\vec{r}). \quad (8.8)$$

The Schrödinger equation (8.8) gets nicer solutions, and enables a deeper physical insight, by investigating the properties of the system observables (2.198), for coordinates, momentum, and angular momentum. From the commutation relations (2.208)-(2.210),

$$[U(r), l_x] = [U(r), l_y] = [U(r), l_z] = 0. \quad (8.9)$$

Thus, we get a system of three commuting observables: the Hamiltonian H , the square of the angular momentum \vec{l}^2 , and the projection l_z of this momentum on an arbitrary axis z :

$$[H, \vec{l}^2] = [\vec{l}^2, l_z] = [l_z, H] = 0. \quad (8.10)$$

8.1.2 Angular momentum in spherical coordinates

The hydrogen atom being a system with spherical symmetry, we study this system in spherical coordinates r, θ, ϕ (figure 8.1), where

$$\vec{r} = \vec{l}_x r \sin \theta \cos \varphi + \vec{l}_y r \sin \theta \sin \varphi + \vec{l}_z r \cos \theta. \quad (8.11)$$

To obtain the observables of the system in these coordinates, we consider the differential of an arbitrary function $f(\vec{r})$ as

$$df(\vec{r}) = \frac{\partial}{\partial \vec{r}} f(\vec{r}) \cdot d\vec{r}, \quad (8.12)$$

while the differential of the position vector

$$d\vec{r} = \vec{1}_r dr + \vec{1}_\theta r d\theta + \vec{1}_\varphi r \sin \theta d\varphi, \quad (8.13)$$

is represented in the system of orthonormal versors

$$\vec{1}_r = \vec{1}_x \sin \theta \cos \varphi + \vec{1}_y \sin \theta \sin \varphi + \vec{1}_z \cos \theta \quad (8.14)$$

$$\vec{1}_\theta = \vec{1}_x \cos \theta \cos \varphi + \vec{1}_y \cos \theta \sin \varphi - \vec{1}_z \sin \theta \quad (8.15)$$

$$\vec{1}_\varphi = -\vec{1}_x \sin \varphi + \vec{1}_y \cos \varphi, \quad (8.16)$$

$$|\vec{1}_r|^2 = |\vec{1}_\theta|^2 = |\vec{1}_\varphi|^2 = 1 \quad (8.17)$$

$$\vec{1}_r \vec{1}_\theta = \vec{1}_\theta \vec{1}_\varphi = \vec{1}_\varphi \vec{1}_r = 0, \quad (8.18)$$

of the spherical coordinates $\vec{r}(r, \theta, \phi)$. From (8.12) and (8.13), we obtain the gradient in these coordinates:

$$\frac{\partial}{\partial \vec{r}} = \vec{1}_r \frac{\partial}{\partial r} + \vec{1}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{1}_\varphi \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi}. \quad (8.19)$$

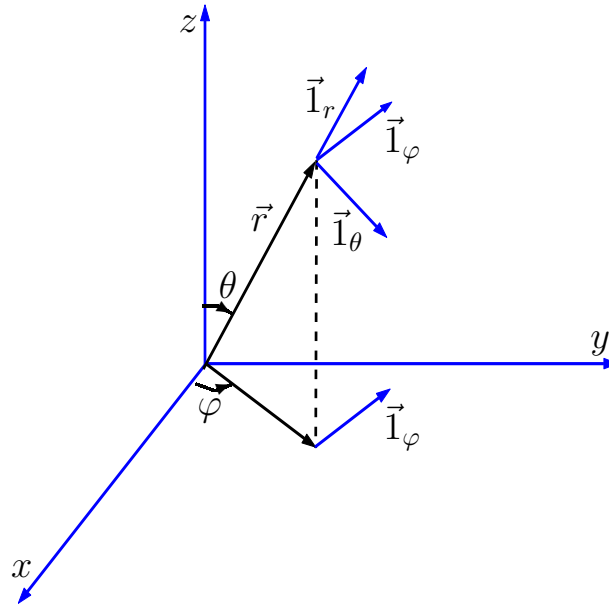


Figure 8.1: Spherical coordinates.

With this operator, we calculate the normalized angular momentum

$$\vec{L} = \vec{1}_x L_x + \vec{1}_y L_y + \vec{1}_z L_z = -ir \vec{1}_r \times \frac{\partial}{\partial \vec{r}} \quad (8.20)$$

CHAPTER 9

Quantum heat converter

Abstract

In this chapter, we apply the theory developed in chapter 7 to a superradiant semiconductor device for the conversion of the environmental heat into coherent electromagnetic energy. The operation principle of the device is formulated in simple terms, as a superradiant flow mainly supplied by heat absorption, only a much smaller part of the energy necessary for producing this flow being supplied from outside. This mechanism seems to counter the second principle of thermodynamics, but in fact does not, because this principle refers to an atomic system, describable by the Pauli master equation, as we showed in subsection 3.2.1. Any modification of this equation, as is our case of interaction with an electromagnetic field, involves a modification of the entropy dynamics. We calculate the wave-function, the corresponding dipole moments, and the dissipation coefficients, and obtain the superradiant power in the mean field approximation. When the field propagation, coupled to the crystal optical vibration, is taken into account, we get a resonance frequency shift with the Raman frequency, and a small decrease of the superradiant power by Raman effect.

Keywords: Coherence, superradiance, conduction band, forbidden band, valence band, deep level, junction, donor, acceptor, transistor, emitter, base, collector, internal field, doping impurity cluster, Poynting vector, Rabi frequency, saturation field, optical phonon, Raman effect.

9.1 Superradiant transistor

A quantum heat converter is based on the concept of superradiant transistor (figure 9.1) [37-41], which can be compared with a conventional bipolar transistor (figure 9.2) [63]: (1) while in a conventional transistor the electrons crossing the emitter-base junction are injected in the conduction band of the base, in a superradiant transistor these electrons are injected in the hole states of the base; (2) while in a conventional transistor the electrons crossing the base-collector junction fall from the conduction band of the base to the much lower states of the collector conduction band by dissipation, *i.e.* with heat production, in a superradiant transistor these electrons go up, from the base valence band to the collector conduction band, with heat absorption. In this way, a coherent electromagnetic field can be generated on the account of the environmental heat. However, such a phenomenon arises only when the superradiance condition is satisfied. Otherwise, a superradiant transistor

behaves more or less as a conventional transistor, and no coherent electromagnetic field is generated. In principle, a connection between two successive superradiant junctions could consist in a mere quasi-ohmic contact, placed in a node of the standing waves in the cavity. However, since these waves still have a significant progressive component, a slope deep level path is considered, to diminish the power dissipation. In this case, the overlap between the higher and the lower wave functions is smaller, which means a weaker coupling with the electromagnetic field. Since by a current injection I the lower states are enhanced, while the higher ones are depleted, the deep level path region becomes colder, leading to heat absorption, which means an electron excitation closing this current.

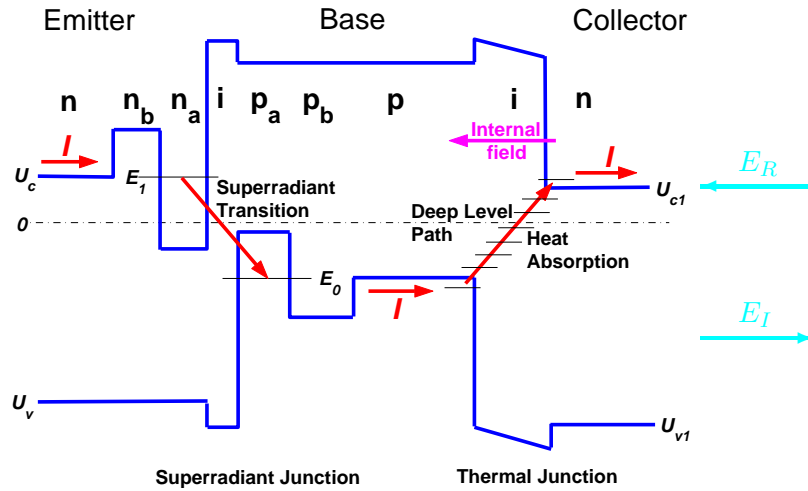


Figure 9.1: Superradiant transistor: when a superradiance condition is satisfied, while a current I is injected in the device, an electromagnetic field is generated by superradiant transitions in the emitter-base junction, and a heat absorption arises in the base-collector junction.

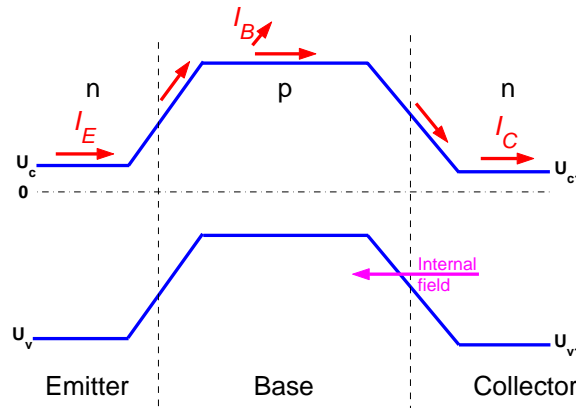


Figure 9.2: Conventional bipolar transistor: while a small current I_B is injected in base, an important part I_C of the emitter current I_E is carried through the base-collector junction by the internal field.

The active quantum dots are separated from the conduction regions by potential barriers, squeezing the active states and diminishing the dissipation, but, at the same time, providing the injection current by quantum tunneling. The electric dipole moments of transition between the two states E_0 and E_1 , which determine the coupling coefficient with the superradiant field mode, are determined by the overlap of the two wave functions in the intrinsic

layer i . The superradiant field flow is determined by the potential difference $U_c - U_{c1}$ created by injecting the current I in the device.

The semiconductor structure includes a succession of n-i-p-i-n superradiant transistors connected in series, in a Fabry-Perot cavity (figure 9.3). For N_t transistors, an electron carried through the structure by a certain injection current I undertakes N_t superradiant transitions, producing N_t photons in the superradiant field mode. In this way, the coupling of the active electrons with the superradiant field is increased, up to a limit beyond which, the electrons cross the superradiant junction only to the valence band, by superradiant transitions, or by energy dissipation. The decay rates are essentially determined

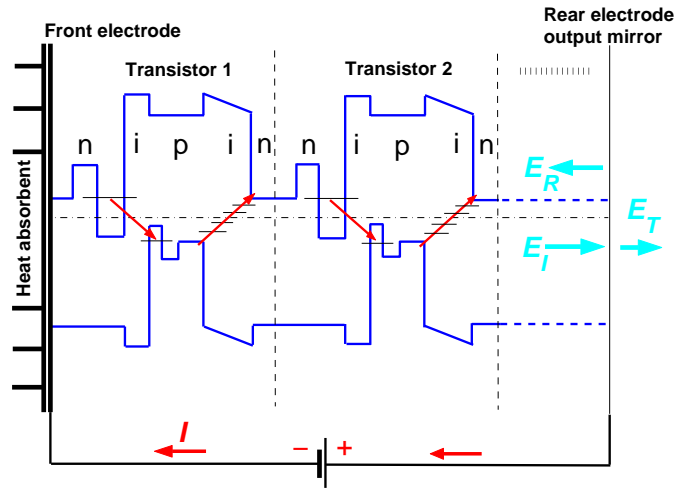


Figure 9.3: Quantum heat converter: while a current I is injected in the device, an electromagnetic field is generated by heat absorption.

by the coupling with the crystal lattice vibrations and the quasi-free electrons/holes of the conduction regions. The ratio between the coupling coefficient and the dissipation rates determines the threshold current for a superradiant operation. It is interesting that, in such an operation, the heat production in the superradiant junction is canceled by heat absorption in the thermal junction.

The proposal of this device could be considered a result of the theoretical framework presented above, and of some investigations on dissipative dynamics [32-36, 48-54, 60, 64], optical bistability [65-79], and superradiant tunneling [80-84]. In the following, we present a theoretical model, which takes into account the electron-field coupling, and the dissipative coupling of the active electrons with the quasi-free electrons in the conduction regions, with the lattice vibrations, and the free electromagnetic field.

In [41], we have taken into account essential dissipative couplings of the system of active electrons with the crystal lattice vibrations and the quasi-free electrons of the conduction regions, but dissipation of the field has been described only phenomenologically, by a decay rate and a refractive index. However, a more detailed description of the electromagnetic field propagation is important, since this propagation involves a strong generation of optical phonons, revealed by a refractive index much larger than 1. That means that the decay of the optical phonons has a contribution to the decay of the field, while the Raman splitting of the generated field modifies the system dynamics. In next section, we consider a quantized electromagnetic field interacting with an active system of quantum dots, the vibrations of the crystal lattice, and the quasi-free electrons of the conduction regions.

Appendix A

Integrals

A.1 Fourier integral

In problems with quasi-continuum of states there are used some integrals depending on time and frequency. A periodic time dependent function, with the period $T = \frac{2\pi}{\omega_0}$, is described by a Fourier series expansion:

$$f(t) = \sum_{n=-\infty}^{\infty} F(n\omega_0) e^{in\omega_0 t}. \quad (\text{A.1})$$

From the integral

$$\int_0^T f(t) e^{-im\omega_0 t} dt = \sum_n F(n\omega_0) \underbrace{\int_0^T e^{i(n-m)\omega_0 t} dt}_{T\delta_{mn}},$$

we get the Fourier transform:

$$F(n\omega_0) = \frac{1}{T} \int_0^T f(t) e^{-i2\pi n \frac{t}{T}} dt. \quad (\text{A.2})$$

With (A.2), from (A.1) we get

$$f(t) = \sum_{n=-\infty}^{\infty} \frac{1}{T} \int_0^T f(t') e^{in\omega_0(t-t')} dt'. \quad (\text{A.3})$$

Considering this equation in the form

$$f(t) = \sum_{n=-\infty}^{\infty} \frac{\omega_0}{2\pi} \int_0^T f(t') e^{in\omega_0(t-t')} dt',$$

with $T = \frac{2\pi}{\omega_0} \rightarrow \infty$, while $\omega_0 = d\omega$ and $n\omega_0 = \omega$, we obtain the Fourier integral

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_0^{\infty} f(t') e^{i\omega(t-t')} dt'. \quad (\text{A.4})$$

A.2 Dirac's function as an integral

From (A.4), we obtain Dirac's function as an integral

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-t')} d\omega. \quad (\text{A.5})$$

Integrating between two limits $-N, N \rightarrow \infty$, we obtain the δ -function as

$$\delta(t - t') = \frac{1}{2\pi} \frac{e^{i\omega(t-t')}}{i(t-t')} \Big|_{-N}^N = \frac{1}{\pi} \frac{\sin[N(t-t')]}{t-t'} \Big|_{N \rightarrow \infty}. \quad (\text{A.6})$$

We notice that Dirac's function can be calculated from a one-parameter integral:

$$I(\lambda) = \int_0^{\infty} e^{-\lambda x} \sin(\omega x) dx, \quad (\text{A.7})$$

while

$$\int_0^{\infty} I(\lambda) d\lambda = \int_0^{\infty} \frac{\sin(\omega x)}{x} dx. \quad (\text{A.8})$$

Integrating by parts,

$$\begin{aligned} I(\lambda) &= -\frac{1}{\lambda} e^{-\lambda x} \sin(\omega x) \Big|_0^{\infty} + \frac{1}{\lambda} \int_0^{\infty} e^{-\lambda x} \omega \cos(\omega x) dx \\ &= \frac{\omega}{\lambda} \left[-\frac{1}{\lambda} e^{-\lambda x} \cos(\omega x) \Big|_0^{\infty} - \frac{\omega}{\lambda} \int_0^{\infty} e^{-\lambda x} \sin(\omega x) dx \right], \end{aligned}$$

we obtain this integral as

$$I(\lambda) = \frac{\omega}{\omega^2 + \lambda^2}. \quad (\text{A.9})$$

With this expression, from (A.8) we get

$$\int_0^{\infty} \frac{\sin(\omega x)}{x} dx = \int_0^{\infty} \frac{\omega d\lambda}{\omega^2 + \lambda^2} = \arctan\left(\frac{\lambda}{\omega}\right) \Big|_0^{\infty} = \frac{\pi}{2}, \quad (\text{A.10})$$

and reobtain expression (A.6) under the form

$$\delta(x) = \frac{1}{\pi} \frac{\sin(\omega x)}{x} \Big|_{\omega \rightarrow \infty}. \quad (\text{A.11})$$

Such an expression of the Dirac function is obtained for the time integral

$$I(\omega) = \int_0^t e^{i\omega(t-t')} dt', \quad (\text{A.12})$$

when the time intervals of interest are much longer than the oscillation period, $t \gg 2\pi/\omega$. Really,

$$\begin{aligned} I(\omega) &= \int_0^t \{ \cos[\omega(t-t')] + i \sin[\omega(t-t')] \} dt' \\ &= -\frac{\sin[\omega(t-t')]}{\omega} \Big|_0^t + i \frac{\cos[\omega(t-t')]}{\omega} \Big|_0^t \approx \frac{\sin(\omega t)}{\omega} \Big|_{t \rightarrow \infty}. \end{aligned} \quad (\text{A.13})$$

We get

$$\int_0^t e^{i\omega(t-t')} dt' \approx \pi \delta(\omega). \quad (\text{A.14})$$

A.3 Gauss integral

The Gaussian integral is defined as

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx. \quad (\text{A.15})$$

This integral can be calculated from

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-x^2-y^2} dx dy = 2\pi \int_0^{\infty} e^{-\rho^2} \rho d\rho = -\pi e^{-\rho^2} \Big|_0^{\infty} = \pi.$$

We get:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}. \quad (\text{A.16})$$

A.4 Fermi-Dirac integrals

With the notation $E^{1/2} = x$, $dE = 2x dx$, the Fermi-Dirac integral (2.374) is

$$I_{1/2}(\xi) = 2 \int_0^{\infty} \frac{x^2 dx}{e^{x^2/T} + \xi} \quad (\text{A.17})$$

For the simpler case $\xi \ll 1$, specific to non-degenerate semiconductors, we can consider

$$\begin{aligned} I_{1/2}(0) &= 2 \int_0^{\infty} x^2 e^{-x^2/T} dx = -T \int_0^{\infty} \frac{-2x}{T} e^{-x^2/T} x dx \\ &= -T e^{-x^2/T} x \Big|_0^{\infty} + T \int_0^{\infty} e^{-x^2/T} dx. \end{aligned} \quad (\text{A.18})$$

With (A.16), we get

$$I_{1/2}(0) = \frac{\sqrt{\pi}}{2} T^{3/2}. \quad (\text{A.19})$$

For $\xi < 1$, the Fermi-Dirac (A.17) can be considered as a series expansion of the form:

$$\begin{aligned} I_{1/2}(\xi) &= 2 \int_0^{\infty} x^2 e^{-x^2/T} \frac{1}{1 + \xi e^{-x^2/T}} dx = I_{1/2}(0) \\ &\quad + 2 \int_0^{\infty} x^2 \left[-\xi e^{-2x^2/T} + \xi^2 e^{-3x^2/T} + \dots + (-\xi)^n e^{-(n+1)x^2/T} + \dots \right] dx. \end{aligned} \quad (\text{A.20})$$

With the notation $\sqrt{n+1}x = y$, an integral

$$I_{1/2}^{(n)} = 2 \int_0^{\infty} x^2 e^{-(n+1)x^2/T} dx \quad (\text{A.21})$$

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