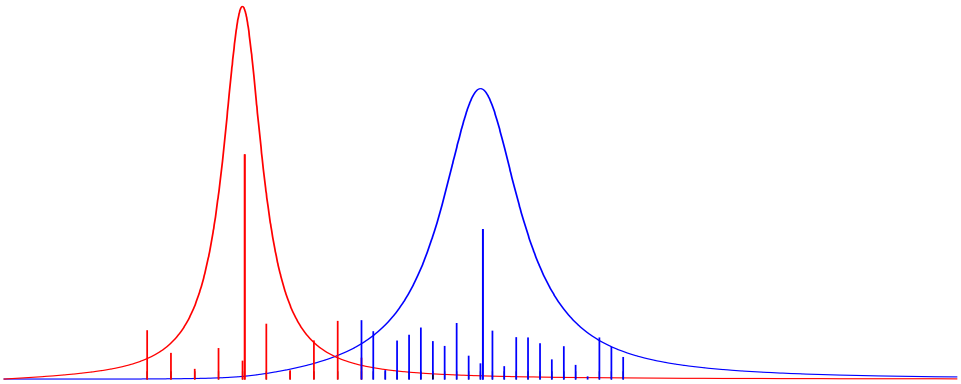
DISSERTATION

zur Erlangung des akademischen Grades
Doktor der Naturwissenschaften
(Dr. rer. nat.)

Collective Motion in Quantum Many–Body Systems



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Hiermit versichere ich an Eides statt, die vorliegende Dissertation selbstständig, ohne fremde Hilfe und ohne Benutzung anderer als den angegebenen Quellen angefertigt zu haben. Alle aus fremden Werken direkt oder indirekt übernommenen Gedanken sind als solche gekennzeichnet. Die vorliegende Dissertation wurde in keinem anderen Promotionsverfahren eingereicht. Mit dieser Arbeit strebe ich die Erlangung des akademische Grades "Doktor der Naturwissenschaften" (Dr. rer. nat.) an.

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"Physics is like sex. Sure, it may give some practical results, but that's not why we do it."
Richard P. Feynman

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Zusammenfassung

Wir untersuchen das Entstehen von kollektiver Dynamik in einem integrablen Modell bestehend aus zwei Ensembles mit einer endlichen Anzahl von gekoppelten Oszillatoren. Nachdem wir einen kollektiven Freiheitsgrad identifiziert haben, wird der Hamiltonian auf ein Caldeira-Leggett-artiges Modell abgebildet, bei dem die Kollektivkoordinate an ein internes Bad von Phononen gekoppelt ist. Im Gegensatz zum gewöhnlichen Caldeira-Leggett Modell ist das vorhandene Bad Teil des Gesamtsystems. Wir leiten eine Bewegungsgleichung für die Kollektivkoordinate ab, die einem gedämpften harmonischem Oszillator entspricht. Wir demonstrieren dann, dass die Verteilung der quantenmechanischen Übergangsstärken für die Kollektivmode durch seine klassische Dynamik bestimmt ist.

Nachfolgend untersuchen wir das Zusammenspiel zwischen Kollektivbewegung und den inkohärenten Einteilchenbewegungen in einem Modell bestehend aus zwei Ensembles von Teilchen deren Wechselwirkung einen nichtintegrablen Teil enthält. Im störungstheoretischen Bereich, aber für eine allgemeine Form der Wechselwirkung, berechnen wir die Fouriertransformation des Zeitkorrelators für die kollektiven Anregungen. Wir erhalten das bemerkenswerte Resultat, dass diese immer eine semiklassische Interpretation besitzt. Wir zeigen dies unter Durchführung einer geeigneten Renormalisierungsvorschrift, welche es uns unter anderem erlaubt, das nichtintegrable System ebenfalls auf ein Caldeira-Leggett-artiges Modell abzubilden, in dem wiederum das Bad Teil des Gesamtsystems ist.

Abstract

We study the emergence of collective dynamics in the integrable Hamiltonian system of two finite ensembles of coupled harmonic oscillators. After identification of a collective degree of freedom, the Hamiltonian is mapped onto a model of Caldeira-Leggett type, where the collective coordinate is coupled to an internal bath of phonons. In contrast to the usual Caldeira-Leggett model, the bath in the present case is part of the system. We derive an equation of motion for the collective coordinate which takes the form of a damped harmonic oscillator. We show that the distribution of quantum transition strengths induced by the collective mode is determined by its classical dynamics. This allows us to derive the spreading for the collective coordinate from first principles.

After that we study the interplay between collective and incoherent single–particle motion in a model of two chains of particles whose interaction comprises a non–integrable part. In the perturbative regime, but for a general form of the interaction, we calculate the Fourier transform of the time correlation for the collective coordinate. We obtain the remarkable result that it always has a unique semi-classical interpretation. We show this by a proper renormalization procedure which also allows us to map the non-integrable system to the integrable model of Caldeira–Leggett–type considered previously in which the bath is part of the system.

Contents

Chapter 1

Prelude

We study collective motion in quantum many particle systems which is defined as coherent collective behavior of single particle degrees of freedom. Below we give a short overview regarding the major issues of collective degrees of freedom in the context of nuclear physics. Although this represents an important example for collective motion in quantum many body systems we stress that the investigation of collective behavior in this thesis was motivated in a much broader context because collective degrees of freedom appear in many different branches of physics.

In 1947 it was observed in photon-induced reactions that at high excitation energies of about 15 to 20 MeV, the atomic nucleus acts as a strong absorber of the incident photons [1]. This phenomenon was called giant dipole resonance (GDR) and described as an excitation of the nucleus in which the protons coherently move against the neutrons [2]. Such a collective shift of the nucleons against each other separates the centers of mass and charge and effectively causes a dipole moment. This behavior can schematically be displayed in the form of figure (1.1). In all studied atomic nuclei these resonances were found to exist.

GDR excitations can be modeled as harmonic oscillators and the quantization of these vibrations introduces the concept of phonons. One therefore refers to a first (giant resonance) excitation of the nucleus from the ground state as the 1-phonon state and the second excitation as the 2-phonon state. In figure (1.2) we show the cross section of one-phonon and two-phonon giant dipole resonances that was obtained by scattering with relativistic ^{208}Pb on a xenon nucleus. Most of the empirical information regarding these modes was obtained from photo-nuclear reactions (photoabsorbtion) and heavy ion inelastic scattering experiments. Besides the GDR there is also a wealth of other collective excitations of atomic nuclei like the giant quadrupole resonance (GQR), breathing modes, scissor modes and others [3], [4], [5].

The atomic nucleus is a complicated many-body system that is very difficult to describe on a microscopic level. The reasons for this are diverse.

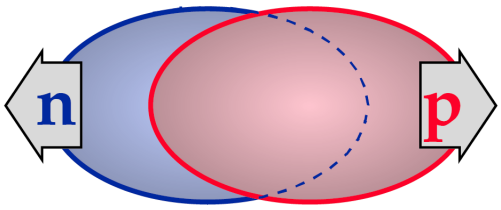

Figure 1.1: The protons and neutrons are schematically represented by red and blue areas respectively, the figure was taken from [10].

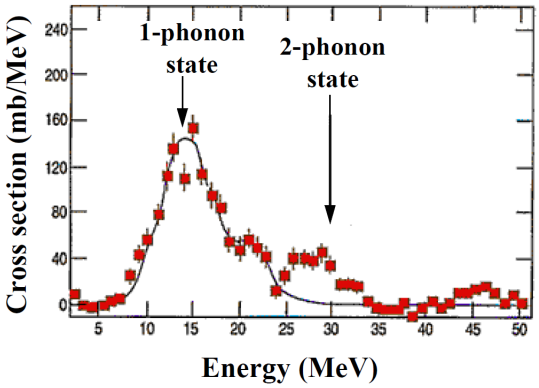

Figure 1.2: Scattering cross section of ^{208}Pb on a Xenon nucleus. The black line represents a theoretical prediction and the red points correspond to measurements. The figure was taken from [10].

On the one hand protons and neutrons which are the constituents of atomic nuclei have to be described themselves as composite particles. These fundamental building blocks of matter are the quarks and gluons that obey the rules of quantum chromodynamics (QCD) which is currently the most fundamental theory for the strong interaction that physicists possess (for a detailed introduction to QCD, see Refs. [6, 7, 8]). Numerous analytical and numerical studies have supplied us with fascinating details regarding the physics of atomic nuclei. Although tested to very high degrees of accuracy in high energy and low energy experiments it is nevertheless a tremendously difficult task to obtain the exact physical behavior of nucleons from first principles (*i.e.* starting from QCD). The problem does not simplify sufficiently even if taken to the next highest level of abstraction where effective interactions between nucleons are considered. To put it differently, although the picture of an atomic nucleus consisting of protons and neutrons reduces the amount of complexity it is still a Herculean task to address questions

regarding collective behavior due to the fact that one has to deal with a quantum many particle problem governed by very complicated interactions (*i.e.* nuclear forces) between the constituents.

Because of the above reasons many nuclear models use to a certain extent a phenomenological framework where the collective dynamics is introduced ad hoc without direct connection to the microscopic structure of the atomic nucleus. In order to illustrate some of the motivations involved in our studies related to collective behavior in complex systems we will outline some of the main issues related to collective motion in atomic nuclei. In this survey of collective aspects in nuclear physics we follow Refs. [5, 9, 10].

As a first phenomenological model one can imagine atomic nuclei as self-bound systems of protons and neutrons. The broader theoretical framework in which this model is embedded is the so called liquid drop model of atomic nuclei. Basically it treats the nucleus as a drop of a uniformly dense liquid. Such an approach in particular serves as a useful tool since it gives an illustrative description for different contributions to the binding energy $B(A)$ of nuclei which can be modeled by the semi-empirical Bethe-Weizsäcker formula:

$$B(A) = a_{\rm vol}A + a_{\rm surf}A^{2/3} + a_{\rm coul}Z^2A^{-1/3} + a_{\rm sym}\frac{(N-Z)^2}{A}, \qquad (1.1)$$

with empirical constants given by

$$a_{\rm vol} \approx -16 \text{ MeV}, \qquad a_{\rm surf} \approx 20 \text{ MeV} \qquad (1.2)$$

$$a_{\rm coul} \approx 0.751 \text{ MeV}, \qquad a_{\rm sym} \approx 21.4 \text{ MeV}. \qquad (1.3)$$

Here A is the total number of nucleons, Z the number of protons and N the number of neutrons. The first term models the binding energy per nucleon under the assumption that the density of protons coincides with the density of neutrons. The term is known as volume term. The second term is known as the surface term. It describes the decrease/increase of a nucleon's binding energy caused by the nuclear forces due to its geometrical position in the nucleus. For example, a nucleon at the center of the atomic nucleus has a bigger binding energy than nucleons on the surface because it interacts with more other particles. Term three stands for the Coulomb energy which originates from the electric charges of the protons. The last term is called symmetry energy and it is strongly related to the fermionic properties of nucleons (*i.e.* Pauli principle).

Contrary to the first three terms in (1.1) the understanding of the nuclear symmetry energy requires taking into account the single-particle nature of nuclei. In a first approximation the last term can be explained qualitatively using the Fermi-gas model, where the atomic nucleus is described as a gas of

noninteracting fermions. These free particles are put in a box with lengths a and are thus described by the wave functions

$$\Psi_{\mathbf{k}}(\mathbf{r}) \sim \sin(\mathbf{k} \cdot \mathbf{r}) \tag{1.4}$$

with

$$k_x = \frac{\pi}{a} n_x, \qquad k_y = \frac{\pi}{a} n_y, \qquad k_z = \frac{\pi}{a} n_z, \tag{1.5}$$

and

$$\mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}, \tag{1.6}$$

with the variables taking values from

$$n_x, n_y, n_z = 1, 2, ... \tag{1.7}$$

as well as

$$x, y, z = 0, ..., a. \tag{1.8}$$

The energies of those states are then given by

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2). \tag{1.9}$$

The Pauli principle determines the distribution of identical particles among the energy levels, filling them up with growing density. In the limit of large a we obtain for the density of particles

$$\rho = \frac{1}{\pi^2 \sqrt{2}} \left(\frac{m}{\hbar^2} \right)^{3/2} \int_0^{E_\mathrm{F}} \sqrt{E} \; dE, \tag{1.10}$$

where E_F is the Fermi energy. Taking into account degeneracy (due to the spin all states can be filled twice) by using a degeneracy factor g we obtain

$$E_\mathrm{F} = \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{\rho / g} \right)^{3/2}. \tag{1.11}$$

In this simplified model there is no binding potential because the particles move freely. However for our purpose it will be sufficient to stay in the above framework of a free Fermi-gas. The average energy per particle in that case is then given by

$$\bar{E} = \frac{3}{5} E_\mathrm{F} \sim \rho^{2/3}. \tag{1.12}$$

The total nucleon density of the nucleus is given by

$$\begin{aligned}\rho_0 &= \rho_\mathrm{p} + \rho_\mathrm{n} = \frac{Z\rho_0}{A} + \frac{N\rho_0}{A} \\ &= \frac{\rho_0}{2}\left(1 + \frac{Z-N}{A}\right) + \frac{\rho_0}{2}\left(1 - \frac{Z-N}{A}\right), \end{aligned} \tag{1.13}$$

with the proton and neutron densities ρ_p, ρ_n. Since ρ_p and ρ_n can be different it is necessary to change (1.12) accordingly. Taking differing proton and neutron densities into account we obtain for the average energy

$$\bar{E} = \frac{3}{5}\frac{NE_\mathrm{F}^n + ZE_\mathrm{F}^p}{A}, \tag{1.14}$$

where E_F^n and E_F^p represent the Fermion energy of the protons and neutrons respectively. Inserting the expression for proton and neutron density from (1.13) into their corresponding Fermi energies and expanding in $(Z-N)/A$ we obtain

$$\bar{E} \approx \underbrace{\frac{3}{5}\frac{\hbar^2}{2m}\left(\frac{3\pi^2\rho_0}{2}\right)^{2/3}}_{\approx 21\mathrm{MeV}}\left(1 + \frac{5}{9}\frac{(Z-N)^2}{A^2}\right). \tag{1.15}$$

Comparing this expression with the part describing the symmetry energy in (1.1) one recognizes the $(Z-N)^2$-dependency. That explains qualitatively the appearance of the nuclear symmetry energy from its single-particle properties. However quantitatively the two energies do not agree, which is due to the too simplistic assumption of a noninteracting Fermi-gas. The difference can be accounted for in more refined models. The Bethe-Weizsäcker formula is only one example in the list of so called semi-empirical mass formulae.

As already mentioned the theoretical framework in which it can be embedded is the liquid drop model in which the nucleus is described as a charged classical liquid drop with constant density. Due to its phenomenological character the liquid drop model is far from fully extensive regarding the physical behavior of atomic nuclei but can still be used to describe various nuclear collective excitations. Apart from the GDR which needs *two* liquid drops corresponding to protons and neutrons that oscillate *against* each other, there are resonances that can be described by a simple *single* liquid drop model (*e.g.* GQR). In this context the distortion of the atomic nucleus is modeled by an expansion of the quantity $R(\theta,\phi,t)$ (which determines points on the drop surface) in spherical harmonics

$$R(\theta,\phi,t) = R_0\left(1 + \sum_{\lambda\mu} Q_{\lambda\mu}(t) Y_{\lambda\mu}^*(\theta,\phi)\right) \tag{1.16}$$

where $Q_{\lambda\mu}(t)$ are timed-dependent shape parameters, $Y_{\lambda\mu}(\theta,\phi)$ spherical harmonics and R_0 is the radius of an undeformed (*i.e.* spherical) nucleus

when all $Q_{\lambda\mu}(t) = 0$, and the indices run from $\lambda = 0, ..., \infty$ and $\mu = -\lambda, ..., \lambda$. The coefficients $Q_{\lambda\mu}(t)$ account for the time evolution (change of geometry) of the nuclear surface and may therefore serve as collective coordinates. The different modes $Q_{\lambda\mu}(t)$ of $R(\theta, \phi, t)$ give rise to a diverse spectrum of geometrical deformations. We will mention here some of the most important. The first mode is the so called breathing mode (monopole mode) $\lambda = 0$. Since $R(\theta, \phi, t)$ does not depend on θ and ϕ and

$$Q_{\mu\nu} = 0, \qquad \forall\ \mu, \nu \neq 0, \tag{1.17}$$

Q_{00} can be interpreted as a homogeneous changing (breathing) of the nuclear radius. Since this mode is responsible for a change of volume it does not appear in the incompressible liquid model.

For $\lambda = 1$ we do not obtain a deformation of the drop but translation of the entire drop, see figure 1.3.

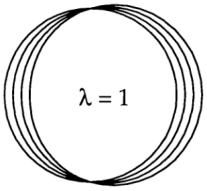

Figure 1.3: Multipole deformation for $\lambda = 1$, translation of the nucleus. The figure was taken from [5].

Collective excitations with $\lambda = 2$ are the so called quadrupole deformations of the nuclear surface. These degrees of freedom are illustrated in figure 1.4.

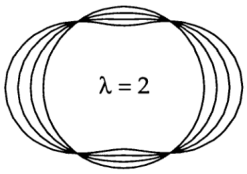

Figure 1.4: Multipole deformation for $\lambda = 2$, quadrupole deformation. The figure was taken from [5].

The next step in the treatment of the liquid drop model is the quantization of the multipole modes $Q_{\mu\nu}$, which is performed in the usual way. For the quantization procedure we need to set up a Hamiltonian for the liquid drop energy. The total energy of a classical drop of liquid is

$$E = T + V \tag{1.18}$$

with T being the kinetic energy and V the potential energy of the liquid. In the hydrodynamical description (liquid drop model) the forces that interplay with each other are the surface tension that attempts to restore a spherical configuration of a perturbed drop of liquid and the Coulomb forces of the protons that act as a deforming net force of the nucleus. Correspondingly, the potential energy is given by

$$V = E_{\mathrm{S}} + E_{\mathrm{Coul}}, \tag{1.19}$$

where

$$E_{\mathrm{S}} = \sigma \int\limits_{\mathrm{surface}} dS \tag{1.20}$$

is the surface energy with the surface tension σ and the surface element dS and

$$E_{\mathrm{Coul}} = \frac{1}{2}\rho_q^2 \int\limits_{\mathrm{Vol}} dr^3 \int\limits_{\mathrm{Vol}} dr'^3 \frac{1}{|\mathbf{r}-\mathbf{r}'|} \tag{1.21}$$

represents the Coulomb energy with proton charge density ρ_q. The integration is performed over a finite volume.

An increase of the drops surface causes an increase of the surface energy. Since the increase of the surface is given by the deformation parameter $Q_{\lambda\mu}$ one obtains for the increase of surface energy E_{S} to first order in Q

$$\Delta E_{\mathrm{S}} = \frac{\sigma}{2}\sum_{\lambda\mu}(\lambda-1)(\lambda+2)|Q_{\lambda\mu}|^2. \tag{1.22}$$

The change of the Coulomb energy that is due to a geometrical deformation of the (uniformly-charged) drop of liquid is at lowest order α given by

$$\Delta E_{\mathrm{Coul}} = -\frac{4\pi\rho_q^2 R_0^5}{3}\sum_{\lambda\mu}\frac{(\lambda-1)}{(2\lambda+1)}|Q_{\lambda\mu}|^2. \tag{1.23}$$

Putting these expressions together we obtain for the total change of energy in a geometrically perturbed drop,

$$V = \Delta E_{\mathrm{S}} + \Delta E_{\mathrm{Coul}} = \frac{1}{2}\sum_{\lambda\mu} K_\lambda |Q_{\lambda\mu}|^2 \tag{1.24}$$

with coefficients K_λ expressed through Z, σ and R_0.

If we assume an irrotational flow and an incompressible fluid then for small values of Q one obtains

$$T = \sum_{\lambda\mu}\frac{M_\lambda}{2}|\dot{Q}_{\lambda\mu}|^2, \tag{1.25}$$

with a collective mass parameter

$$M_\lambda = \frac{\rho_m R_0^5}{\lambda} \tag{1.26}$$

and the mass density ρ_m. With this the Hamiltonian becomes

$$H = \sum_{\lambda\mu} \frac{M_\lambda}{2}|P_{\lambda\mu}|^2 + \frac{1}{2}K_\lambda|Q_{\lambda\mu}|^2, \tag{1.27}$$

with the momentum $P_{\lambda\mu} = M_\lambda \dot{Q}^*_{\lambda\mu}$. We recognize this as the Hamiltonian for harmonic oscillators with frequencies $\Omega_\lambda = \sqrt{K_\lambda/M_\lambda}$ which can be brought to canonical form using raising and lowering operators

$$\hat{Q} = \sqrt{\Omega/2K}\ (\hat{B}^\dagger + \hat{B}) \tag{1.28}$$

and

$$\hat{P} = i\sqrt{\Omega M/2}\ (\hat{B}^\dagger - \hat{B}), \tag{1.29}$$

with creation and annihilation operators, $\hat{B}^\dagger$ and $\hat{B}$, see Refs. [11, 12]. The spectrum of the Hamiltonian (1.27) can be interpreted as single and multiple phonon excitations. This model gives a qualitative explanation for the giant resonances within the liquid drop model framework. Within this paradigm it is also possible to understand the emergence of the widths of resonances like the GDR in figure 1.2. If there is no friction between the two drops of protons and neutrons that vibrate collectively against each other one would expect just a single spike in the absorption spectra corresponding to a sharp excitation energy of the collective state. The broad width of the 1-phonon excitation of the GDR in atomic nuclei can be modeled by introducing the concept of viscosity into the liquid drop model.

Probably one of the most influential attempts to describe the dynamics of collective motion alongside the single particle degrees of freedom in an atomic nucleus was made by A.Bohr in his paper [13]. Bohr modeled the coupling of single particle and collective excitations by an interaction Hamiltonian

$$H_{\text{int}} = -\sum_{\lambda\mu} c_{\lambda\mu} Q_{\lambda\mu} \sum_i f(r_i) Y_{\lambda\mu}(\theta_i, \phi_i), \tag{1.30}$$

where $Q_{\lambda\mu}$ describes the strength of the nuclear deformation (collective coordinate), $c_{\lambda\mu}$ are the coupling constants mediating the interaction between collective modes and single particle modes and $f(r_i)Y_{\lambda\mu}(\theta_i, \phi_i)$ representing the multipole moment of the i-th (valence) nucleon. Such a coupling was introduced in order to account for the splitting of the collective vibrational levels. The degeneracy of the collective states is lifted by an interaction between collective degrees and single particle degrees of freedom of the atomic nucleus.

Although very successful in describing (qualitatively) quantum properties of atomic nuclei such an approach poses certain problems on a conceptual level since there is no logical reason why one should start with a classical drop model and quantize it when the underlying system is composed of single quantum particles.

An important disadvantage of such an analysis is that one does not obtain couplings of the form (1.30) from first principles. Rather one postulates the existence (a priori there is no collective degree) of the collective mode and introduces its coupling with the single particle excitations in a phenomenological manner. We already mentioned that it is a horrendous difficult task to derive this form of the interaction from first principles in nuclear physics. As we have seen here as well, there is a certain kind of ambiguity in the treatment of collective and single particle modes in nuclear physics. While these two kinds of excitation are often observed at the same energies, a common theoretical approach describing both phenomena is currently lacking.

It would be much more desirable to obtain the collective coordinate and a justification for effective models like the liquid drop model from a microscopic starting point that only involves the single particles which build complex systems like nuclei and their interactions. In such a framework the above mentioned viscosity of the liquid drops has also effectively to emerge out of the interaction between individual degrees of freedom. The basic physical picture is that the nucleons move around coherently and transfer their collective energy within a certain time to incoherent single particle motion. The width is thus connected to the question of how fast the energy is transfered from the collective degree to the single particle degrees of freedom. Although too difficult for any realistic system like an atomic nucleus we studied a simple model where we were able to derive the collective coordinate and its coupling with the coexisting single particle degrees of freedom. Furthermore we were able to show that the equations of motion for the quantum system have a certain classical interpretation which might be seen as a microscopic justification of the usage of phenomenological (*e.g.* liquid-drop-like) effective models in complex systems.

Chapter 2

Introduction

Many-body systems show incoherent, single-particle-motion, as well as coherent collective motion. Historically this phenomenon received much attention in nuclear physics where there is a wealth of data providing information on the coexistence of collective excitations, such as the Giant Dipole Resonance (GDR), and single particle excitations [14]. There is also strong experimental [15] and theoretical [16] evidence that similar effects occur in fermionic systems different from atomic nuclei. Other examples for collective motion are vortex-generating rotations and oscillations in Bose-Einstein condensates [17, 18, 19]. Furthermore collective behavior can also be present in confined systems such as quantum dots [20, 21].

Coherent, collective motion emerges out of incoherent, single-particle motion whenever favored by energy conditions. Statistical analysis of spectra in nuclei indicates that chaotic fluctuations are due to single-particle motion, while collective motion is predominantly regular, for a review see Ref. [22] and more recent results in Refs. [23, 24]. This generic occurrence and the coexistence of the two forms of motion pose a fundamental challenge. Strictly speaking, in a generic many-body system there is not an *a priori* separation of the collective motion from the single-particle dynamics. Taking the three-dimensional Boltzmann gas with hard-wall interactions as an example, one observes that the dynamics in the phase space of the system is completely chaotic [25]. Still, we know that the system exhibits regular collective motion in the form of sound waves. The deep and fascinating question in this context is therefore to understand from first principles how the regular motion emerges out of the full phase space chaos [26].

Whenever collective dynamics arises on the classical level one might expect on the basis of quantum-classical correspondence that this phenomena should be reflected in the spectral properties of the corresponding quantum many-body Hamiltonian. One way to probe the existence of collective excitations is to couple the system to a weak external periodic potential $V(X)\exp(i\omega t)$ depending on a collective mode X. The presence of a collec-

tive excitation can then be usually registered as a spike at certain energies in the distribution of the transition strengths $T(E_n)$ between the ground and other states of the system. Such a large peak can be observed, for instance, in the cross section of electric dipole radiation in atomic nuclei at high excitation energies, when the GDR is excited. On a phenomenological level one can obtain such a distribution of the transition strengths from a doorway-type of Hamiltonian [14, 27]:

$$H = \sum_{n_c=1}^{N_0} E_{n_c}|n_c\rangle\langle n_c| + \sum_{n,m=1}^{N} H_{nm}|n\rangle\langle m| + \sum_{n_c,n} V_{nn_c}|n_c\rangle\langle n| + c.c. \; . \quad (2.1)$$

Here, the first term describes N_0 collective states $|n_c\rangle$ with energies E_{n_c}, the second term describes the environment of single particle states $|n\rangle$ with H_{nm} typically modeled by a random matrix. The last term models the interaction V_{nn_c} between collective and single-particle excitations. The collective states act as doorways into the other levels of the system. A recent discussion can be found in Ref. [28]. Although successful in the qualitative description of collective excitation in nuclei, this model does not provide any explanation of the physical reasons that lead to the collective behavior. We notice that the collective and single-particle excitations are separated here from the start, while collectivity is in fact an emergent phenomena.

Having a classical Hamiltonian whose dynamics exhibits collective motion, what can be stated about the distribution of the transition strengths $T(E_n)$ for the corresponding quantum problem? In particular, it makes sense to ask under what conditions it is possible to use models like (2.1) and how the parameters there are related to the classical problem. It is also of considerable interest to understand the role of chaos in this context [29]. Unfortunately, at present we are lacking a genuine "semi-classical theory" for the emergence of collective excitations which would allow us to tackle the problem starting from the corresponding classical dynamics. The main goal of this thesis is to provide answers to some of the questions posed above in the framework of a simple integrable model of linearly coupled harmonic oscillators and its non-integrable extension. Integrability of the system simplifies the treatment immensely. It allows for a clear identification of a collective coordinate X and an investigation of its dynamical evolution employing an analogy with the Caldeira-Leggett model [30]. After we fix the collective coordinate the remaining degrees of freedom are considered as a bath which is internal, not external as in standard models of the Caldeira-Leggett-type [31, 32, 33, 34]. As a result, it turns out that the time evolution of $X(t)$ is fully governed by the equation of motion for a damped harmonic oscillator of some frequency Ω_0 determined by the parameters of the many-body Hamiltonian. After this we show that under certain conditions on the Hamiltonian of the system the averaged distribution of $T(E_n)$ is directly connected to the corresponding classical problem for time evolution

of $X(t)$. In particular, the distribution of the transition strengths $T(E_n)$ exhibit spikes at energies E_n which are close to the energies $E_n = E_0 + n\hbar\Omega_0$ — where E_0 is the ground state energy — of the collective oscillations, while the width of these spikes is controlled by the classical decay rate γ of these oscillations. Even though the considered model does not involve chaotic features it serves as a testing ground to address the emergence of collective dynamics in a many-body system. Furthermore, it allows to see the effect of the absence of dynamical chaos on the distribution of $T(E_n)$ and to set up the ground for a perturbative analysis of a non-integrable model.

Beyond the integrable case it turns out that the quantum-classical correspondence can also be established for the non-integrable model as long as one studies perturbation theory to linear order. The non-integrable model can in linear order perturbation theory be mapped to the integrable Caldeira-Leggett model with renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. This means that the renormalized spreading kernel $\gamma^{\mathrm{R}}(t)$, the oscillator frequency Ω_0^{R} and the spectral density of the perturbed non-integrable case are fully determined by the *classical* dynamics of a renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. Since higher order terms in the perturbative treatment of the correlation function $S(t)$ come with higher powers of $\hbar$ we take the point of view that the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$ provides the first semi-classical correction to the spectrum of the collective modes. It is thus possible for us to study the emergence of collectivity from first principles instead of starting from an effective model. We actually obtain an effective description of collective phenomena by relating the time correlator of the collective operator and its Fourier transform to a purely *classical* equation. At the same time we keep full control over the original degrees of freedom. Even though we do this with a simple model it can be viewed as a justification of the routinely used strategy in nuclear physics, where effective models are set up classically and then quantized (*e.g.* the liquid drop model). Therefore we consider our investigation as an essential step towards an understanding of the interplay between chaos and regularity in quantum many body systems.

The thesis is organized as follows. In Sec. 3.1 we introduce our model and map it to a Caldeira-Leggett-like system. In order to illustrate the general procedure we treat the special configuration of two simple coupled chains in Sec. 3.2. In Sec. 3.3 we derive the equation of motion for the collective coordinate and obtain an expression for the spectral density which encodes the crucial physical properties of our model. In Sec. 3.4 we investigate the distribution of transition strengths between the ground state and excited states and relate the result to the dynamics of collective motion. In Sec. 4.1 we derive a generally valid expression for the correlation function $S(t)$ up to second order perturbation theory in λ and test the formalism in the Caldeira-Legget case in Sec. 4.2. After that, in Sec. 4.3 follows a general discussion about the treatment of a non-integrable model in that framework. In chapter 5 we investigate the full non-integrable case up to leading order perturbation

theory and analyze its connection to classical dynamics. In appendix A we introduce the Feynman-Vernon theory which was used for the analysis of the Caldeira-Leggett model in appendix B. In appendix C we calculate the Fourier transform of the correlation function $S(t)$ for the Caldeira-Leggett model as a test case. In appendix D we calculate the Fourier transform of $S(t)$ in an alternative way in order to identify the information regarding the spreading kernel in a perturbative framework.

Chapter 3

Integrable model

In Sec. 3.1 we introduce our model and map it to a Caldeira-Leggett-like system. For the convenience of the reader the Caldeira-Leggett model is briefly reviewed in appendix B. In order to illustrate the general procedure we treat the special configuration of two simple coupled chains in Sec. 3.2. In Sec. 3.3 we derive the equation of motion for the collective coordinate and obtain an expression for the spectral density which encodes the crucial physical properties of our model. In Sec. 3.4 we investigate the distribution of transition strengths between the ground state and excited states and relate the result with the dynamics of collective motion.

3.1 Coupled chains of oscillators

In Sec. 3.1.1 we define the model. After defining a collective coordinate we map the system onto a Caldeira-Leggett-like model in Sec. 3.1.2.

3.1.1 The model

We consider two identical chains of one-dimensional coupled harmonic oscillators each consisting of N particles with positions $x_j^{(1)}$, $j = 1 \dots N$ and momenta $p_j^{(1)}$, $j = 1 \dots N$ as well as $x_j^{(2)}$ and $p_j^{(2)}$, respectively. They are ordered in vectors $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$, $\mathbf{p}^{(1)}$ and $\mathbf{p}^{(2)}$. The chains are coupled by an interaction H_{int}. When the coupling is "switched off" i.e., $H_{\text{int}} = 0$ these two chains are governed by the Hamiltonians

$$\begin{aligned} H_{\text{I}} &= \frac{1}{2m}\left(\mathbf{p}^{(1)}, \mathbf{p}^{(1)}\right) + \left(\mathbf{x}^{(1)}, W\ \mathbf{x}^{(1)}\right), \\ H_{\text{II}} &= \frac{1}{2m}\left(\mathbf{p}^{(2)}, \mathbf{p}^{(2)}\right) + \left(\mathbf{x}^{(2)}, W\ \mathbf{x}^{(2)}\right), \end{aligned} \tag{3.1}$$

where the notation $(\cdot,\cdot)$ stands for the scalar product. In the coordinate representation, we have

$$\left(\mathbf{p}^{(1)},\mathbf{p}^{(1)}\right)=\sum_{i=1}^{N}(p_i^{(1)})^2,\qquad \left(\mathbf{p}^{(2)},\mathbf{p}^{(2)}\right)=\sum_{i=1}^{N}(p_i^{(2)})^2, \tag{3.2}$$

while the potential terms describing the interactions of different particles within the chains can be written as

$$\begin{aligned}\left(\mathbf{x}^{(1)},W\ \mathbf{x}^{(1)}\right)&=\sum_{i,j=1}^{N}x_i^{(1)}W_{ij}x_j^{(1)},\\ \left(\mathbf{x}^{(2)},W\ \mathbf{x}^{(2)}\right)&=\sum_{i,j=1}^{N}x_i^{(2)}W_{ij}x_j^{(2)}.\end{aligned} \tag{3.3}$$

We assume that such interactions are given by a shift invariant matrix $W_{ij}=W_{(i+n)\mathrm{mod}N\ (j+n)\mathrm{mod}N}$ which, in addition, satisfies translational symmetry condition $\sum_{i=1}^{N}W_{ij}=0$. This implies that for uncoupled chains the non-interacting degrees of freedom are phonons.

After introducing the coupling between the two chains the total Hamiltonian of the system becomes

$$H=H_{\mathrm{I}}+H_{\mathrm{II}}+H_{\mathrm{int}}, \tag{3.4}$$

where the interaction term

$$\begin{aligned}H_{\mathrm{int}}&=\sum_{i,j=1}^{N}K_{ij}\left(x_i^{(1)}-x_j^{(2)}\right)^2\\ &=\sum_{i,j=1}^{N}K_{ij}\left((x_i^{(1)})^2+(x_j^{(2)})^2\right)-2\sum_{i,j=1}^{N}K_{ij}x_i^{(1)}x_j^{(2)}\end{aligned} \tag{3.5}$$

is determined by positive symmetric coupling constants K_{ij}. In what follows, we assume that $H(\mathbf{x}^{(1)},\mathbf{p}^{(1)},\mathbf{x}^{(2)},\mathbf{p}^{(2)})$ is a non-negative function. This guarantees that the motion of the whole system remains bounded for all times. We notice that we do not make a similar requirement for $H_{\mathrm{I}}(\mathbf{p}^{(1)},\mathbf{x}^{(1)})$ and $H_{\mathrm{II}}(\mathbf{p}^{(2)},\mathbf{x}^{(2)})$.

3.1.2 Mapping onto a Caldeira-Leggett-like model

In what follows we study the dynamics of the collective coordinate X defined as the difference between the center of masses of two chains scaled with the factor $\sqrt{N/2}$

$$X=\frac{1}{\sqrt{2N}}\sum_{i=1}^{N}x_i^{(1)}-\frac{1}{\sqrt{2N}}\sum_{i=1}^{N}x_i^{(2)}. \tag{3.6}$$

To this end we map the general problem (3.4) of two coupled chains of harmonic oscillators to a model of Caldeira-Leggett type, where X is coupled to the "bath" provided by the remaining degrees of freedom. This formulation provides an intuitive description for the dynamics of the collective coordinate in the process of transferring energy from X to the bath coordinates. Such an interpretation, however, has to be used carefully because the energy transfer happens inside the full system and a precise definition of the bath depends not only on the form of the Hamiltonian (3.4), but also on the choice of the collective coordinate.

As a first step, we introduce the new set of canonical coordinates and momenta

$$c_i^{(1)} = \sum_{n=1}^{N} A_{in} x_n^{(1)}, \quad \chi_i^{(1)} = \sum_{n=1}^{N} A_{in} p_n^{(1)}, \tag{3.7}$$

$$c_i^{(2)} = \sum_{n=1}^{N} A_{in} x_n^{(2)}, \quad \chi_i^{(2)} = \sum_{n=1}^{N} A_{in} p_n^{(2)}, \tag{3.8}$$

such that H_{I} and H_{II} become diagonal

$$H_{\mathrm{I}} = \sum_{i=1}^{N} \left(\frac{(\chi_i^{(1)})^2}{2m} + \frac{m\omega_i^2 (c_i^{(1)})^2}{2} \right), \tag{3.9}$$

$$H_{\mathrm{II}} = \sum_{i=1}^{N} \left(\frac{(\chi_i^{(2)})^2}{2m} + \frac{m\omega_i^2 (c_i^{(2)})^2}{2} \right) , \tag{3.10}$$

where A_{in} are the elements of the matrix A that diagonalizes W

$$AWA^T = \frac{m}{2}\, \Omega^2, \qquad \Omega = \mathrm{diag}(\omega_1, \ldots, \omega_N). \tag{3.11}$$

For the translational invariant matrix W used in this model the diagonalization matrix A is given by [35]

$$A_{j1} = \sqrt{\frac{1}{N}}, \; A_{jm} = \sqrt{\frac{2}{N}} \cos\left(\frac{\pi(m-1)}{N} \left(j - \frac{1}{2} \right) \right), \tag{3.12}$$

with indices $m = 2, \ldots N$ and $j = 1, \ldots N$.

We express the interaction part of the two chains in the new coordinates.

For the first term in equation (3.5) we obtain

$$\begin{aligned}\sum_{i,j=1}^{N} K_{ij}((x_i^{(1)})^2+(x_j^{(2)})^2) &= \sum_{i,j=1}^{N} K_{ij}(x_i^{(1)})^2 + \underbrace{\sum_{i,j=1}^{N} K_{ji}(x_j^{(2)})^2}_{\sum_{i,j=1} K_{ij}(x_i^{(2)})^2} \\ &= \sum_{i,j,m,n=1}^{N} K_{ij}(A_{in}A_{im}c_n^{(1)}c_m^{(1)} + A_{in}A_{im}c_n^{(2)}c_m^{(2)}) \\ &= \sum_{n,m=1}^{N}\sum_{i=1}^{N} \hat{k}_i A_{in}A_{im}(c_n^{(1)}c_m^{(1)} + c_n^{(2)}c_m^{(2)}) \quad (3.13)\end{aligned}$$

where we introduced $\hat{k}_i = \sum_{j=1}^{N} \hat{K}_{ij}$ and $\hat{K}_{ij} = \delta_{ij}\hat{k}_j$. Simplifying this further via

$$\begin{aligned}\sum_{i=1}^{N} \hat{k}_i A_{in}A_{im} &= \sum_{i=1}^{N} \hat{k}_i A_{ni}^T A_{im} = \sum_{i=1}^{N} A_{ni}^T \hat{k}_i A_{im} \\ &= \sum_{i,l=1}^{N} A_{ni}^T \delta_{il}\hat{k}_l A_{lm} = \sum_{i,l=1}^{N} A_{ni}^T \hat{K}_{il} A_{lm} \\ &= A^T \hat{K} A = \tilde{K}^{\alpha} \quad (3.14)\end{aligned}$$

we get

$$\sum_{i,j=1}^{N} K_{ij}((x_i^{(1)})^2+(x_j^{(2)})^2) = \sum_{n,m=1}^{N} \tilde{K}_{n,m}^{\alpha}(c_n^{(1)}c_m^{(1)} + c_n^{(2)}c_m^{(2)}). \quad (3.15)$$

Treating the second term in equation (3.5) in an analogous way we obtain

$$\begin{aligned}\sum_{i,j=1}^{N} K_{ij}x_i^{(1)}x_j^{(2)} &= \sum_{i,j,n,m=1}^{N} K_{ij}A_{ni}A_{jm}\; c_n^{(1)}c_m^{(2)} \\ &= \sum_{i,j=1}^{N} \underbrace{\sum_{n,m=1}^{N} K_{ij}A_{ni}A_{jm}}_{\tilde{K}_{nm}^{\beta}=\sum_{i,j=1} K_{ij}A_{ni}^T A_{jm}} \; c_n^{(1)}c_m^{(2)} \\ &= \sum_{n,m=1}^{N} \tilde{K}_{nm}^{\beta} c_n^{(1)}c_m^{(2)} \\ &= \frac{1}{2}\sum_{n,m=1}^{N} \tilde{K}_{nm}^{\beta}(c_n^{(1)}c_m^{(2)} + c_m^{(1)}c_n^{(2)}) \\ &= \frac{1}{2}\big((\mathbf{c}^{(1)}, A^T K A\; \mathbf{c}^{(2)}) + (\mathbf{c}^{(1)}, A^T K A\; \mathbf{c}^{(2)})\big) \\ &= \frac{1}{2}\big((\mathbf{c}^{(1)}, \tilde{K}^{\beta}\; \mathbf{c}^{(2)}) + (\mathbf{c}^{(1)}, \tilde{K}^{\beta}\; \mathbf{c}^{(2)})\big), \quad (3.16)\end{aligned}$$

where we used that $\sum_{n,m=1}^{N} \tilde{K}^{\beta}_{nm} c^{(1)}_n c^{(2)}_m = \sum_{i,j=1}^{N} \tilde{K}^{\beta}_{nm} c^{(1)}_m c^{(2)}_n$.

Thus we get for the interaction part of the Hamiltonian

$$H_{\rm int} = \left(\mathbf{c}^{(1)}, \tilde{K}^{\alpha}\mathbf{c}^{(1)}\right) + \left(\mathbf{c}^{(2)}, \tilde{K}^{\alpha}\mathbf{c}^{(2)}\right) - \left(\mathbf{c}^{(1)}, \tilde{K}^{\beta}\mathbf{c}^{(2)}\right) - \left(\mathbf{c}^{(1)}, \tilde{K}^{\beta}\mathbf{c}^{(2)}\right), \tag{3.17}$$

where $\mathbf{c}^{(1)}, \mathbf{c}^{(2)}$ are vectors with components $c^{(1)}_n$, $c^{(2)}_n$ and $\tilde{K}^{\alpha}, \tilde{K}^{\beta}$ are the matrices defined by

$$\tilde{K}^{\alpha} = A^T \hat{K} A, \qquad \tilde{K}^{\beta} = A^T K A, \tag{3.18}$$

with $\hat{K}_{ij} = \delta_{ij}\hat{k}_j$. After transforming the coordinates and momenta according to

$$d^{(1)}_n = \frac{\left(c^{(1)}_n - c^{(2)}_n\right)}{\sqrt{2}}, \quad d^{(2)}_n = \frac{\left(c^{(1)}_n + c^{(2)}_n\right)}{\sqrt{2}}, \tag{3.19}$$

$$\eta^{(1)}_n = \frac{\left(\chi^{(1)}_n - \chi^{(2)}_n\right)}{\sqrt{2}}, \quad \eta^{(2)}_n = \frac{\left(\chi^{(1)}_n + \chi^{(2)}_n\right)}{\sqrt{2}} \tag{3.20}$$

we obtain

$$\begin{aligned} c^{(1)}_n c^{(2)}_m + c^{(1)}_m c^{(2)}_n &= \frac{1}{2}\big((d^{(1)}_n + d^{(2)}_n)(d^{(2)}_m - d^{(2)}_m) + (d^{(1)}_m + d^{(2)}_m)(d^{(2)}_n - d^{(2)}_n)\big) \\ &= d^{(2)}_m d^{(2)}_n - d^{(1)}_n d^{(1)}_m. \end{aligned} \tag{3.21}$$

The momenta transform in an analogous way. With this we get

$$\sum_{ij=1}^{N} K_{ij}\big((x^{(1)}_i)^2 + (x^{(2)}_i)^2\big) = \sum_{nm=1}^{N} \tilde{K}^{\alpha}_{nm}\big(d^{(1)}_n d^{(1)}_m - d^{(2)}_n d^{(2)}_m\big) \tag{3.22}$$

and

$$\sum_{ij=1}^{N} K_{ij}\; x^{(1)}_i x^{(2)}_j = \frac{1}{2}\sum_{nm=1}^{N} \tilde{K}^{\beta}_{nm}\big(d^{(2)}_m d^{(2)}_n - d^{(1)}_n d^{(1)}_m\big). \tag{3.23}$$

From this we obtain for $H_{\rm int}$

$$\begin{aligned} &\sum_{ij=1}^{N} K_{ij}\big((x^{(1)}_i)^2 + (x^{(2)}_i)^2\big) - 2\sum_{ij=1}^{N} K_{ij}\; x^{(1)}_i x^{(2)}_j \\ &\quad = \sum_{nm=1}^{N} \tilde{K}^{\alpha}_{nm}\big(d^{(1)}_n d^{(1)}_m - d^{(2)}_n d^{(2)}_m\big) - \sum_{nm=1}^{N} \tilde{K}^{\beta}_{nm}\big(d^{(2)}_m d^{(2)}_n - d^{(1)}_n d^{(1)}_m\big) \\ &\quad = \sum_{nm=1}^{N} \big(\tilde{K}^{\alpha}_{nm} + \tilde{K}^{\beta}_{nm}\big)\; d^{(1)}_n d^{(1)}_m + \big(\tilde{K}^{\alpha}_{nm} - \tilde{K}^{\beta}_{nm}\big)\; d^{(2)}_n d^{(2)}_m, \end{aligned} \tag{3.24}$$

where we defined $\tilde{K} = \tilde{K}^{\alpha} + \tilde{K}^{\beta}$, $\bar{K} = \tilde{K}^{\alpha} - \tilde{K}^{\beta}$, hence the interaction term can be cast into the form

$$H_{\rm int} = \left(\mathbf{d}^{(1)}, \tilde{K}\mathbf{d}^{(1)}\right) + \left(\mathbf{d}^{(2)}, \bar{K}\mathbf{d}^{(2)}\right). \tag{3.25}$$

With this new set of canonical coordinates the Hamiltonian becomes

$$\begin{aligned} H &= \sum_{i=1}^{N}\left(\frac{(\eta_i^{(1)})^2}{2m} + \frac{(\eta_i^{(2)})^2}{2m}\right) + \frac{m}{2}\sum_{i=1}^{N}\left(\omega_i^2 (d_i^{(2)})^2 + \omega_i^2 (d_i^{(1)})^2\right) \\ &\quad + \sum_{n,m=1}^{N}\tilde{K}_{nm} d_n^{(1)} d_m^{(1)} + \sum_{n,m=1}^{N}\bar{K}_{nm} d_n^{(2)} d_m^{(2)} \\ &= \frac{1}{2m}\left(\eta^{(1)}, \eta^{(1)}\right) + \left(\mathbf{d}^{(1)}, \frac{m}{2}\Omega^2 + \tilde{K}\mathbf{d}^{(1)}\right) \\ &\quad + \frac{1}{2m}\left(\eta^{(2)}, \eta^{(2)}\right) + \left(\mathbf{d}^{(2)}, \frac{m}{2}\Omega^2 + \bar{K}\mathbf{d}^{(2)}\right). \end{aligned} \tag{3.26}$$

We notice that the collective coordinate and momentum are just

$$X = d_1^{(1)}, \qquad P = \eta_1^{(1)} \tag{3.27}$$

and the corresponding frequency is $\omega_1 = 0$. We therefore find

$$\begin{aligned} \sum_{m,n=1}^{N}\tilde{K}_{nm}\, d_n^{(1)} d_m^{(1)} &= \sum_{m=1}^{N}\left(\tilde{K}_{1m}\, d_1^{(1)} d_m^{(1)} + \sum_{n=2}^{N}\tilde{K}_{nm}\, d_m^{(1)} d_n^{(1)}\right) \\ &= \tilde{K}_{11} d_1^{(1)} d_1^{(1)} + \sum_{n=2}^{N}\tilde{K}_{n1} d_1^{(1)} d_n^{(1)} + \sum_{m=2}^{N}\underbrace{\tilde{K}_{1m}}_{\tilde{K}_{m1}} d_1^{(1)} d_m^{(1)} \\ &\quad + \sum_{m,n=2}^{N}\tilde{K}_{nm} d_m^{(1)} d_n^{(1)} \\ &= \tilde{K}_{11}(d_1^{(1)})^2 + 2\sum_{n=2}^{N}\tilde{K}_{n1} d_1^{(1)} d_n^{(1)} + \sum_{m=2}^{N}\tilde{K}_{nm} d_m^{(1)} d_n^{(1)} \\ &= \tilde{K}_{11} X^2 + X\sum_{n=2}^{N}\tilde{K}_{n1} d_n^{(1)} + \sum_{m=2}^{N}\tilde{K}_{nm} d_m^{(1)} d_n^{(1)}. \end{aligned} \tag{3.28}$$

Since X couples only to the coordinates $d_n^{(1)}$, the part of H which depends on $\mathbf{d}^{(2)}, \eta^{(2)}$ can be disregarded when the dynamics of the collective mode is considered. Consequently, the relevant part of the Hamiltonian is given by

$$\begin{aligned} H' &= \frac{P^2}{2m} + \tilde{K}_{11} X^2 + X\sum_{n=2}^{N}\tilde{K}_{n1} d_n^{(1)} + \sum_{n=2}^{N}\frac{(\eta_n^{(1)})^2}{2m} \\ &\quad + \sum_{m,n=2}^{N}\left(\tilde{K}_{nm} + \frac{m\omega_n^2\delta_{nm}}{2}\right) d_n^{(1)} d_m^{(1)}., \end{aligned} \tag{3.29}$$

This already strongly resembles the Caldeira-Legget model but with the non-diagonal bath Hamiltonian

$$H_{\rm bath} = \sum_{n=1}^{N-1} \frac{(\eta_{n+1}^{(1)})^2}{2m} + \sum_{n,m=1}^{N-1} B_{nm} d_{n+1}^{(1)} d_{m+1}^{(1)}, \tag{3.30}$$

where the elements of the $(N-1)\times(N-1)$ matrix B are given by

$$B_{(n-1)(m-1)} = \tilde{K}_{nm} + \frac{m\omega_n^2 \delta_{nm}}{2}, \qquad n,m = 2,\dots N. \tag{3.31}$$

To cast the bath Hamiltonian into diagonal form, we introduce yet another set of the coordinates $\xi_i = \sum_{j=1}^{N-1} U_{ji} d_{j+1}^{(1)} \Leftrightarrow d_{i+1}^{(1)} = \sum_{j=1}^{N-1} U_{i,j}\xi_j$ and $\nu_i = \sum_{j=1}^{N-1} U_{ji}\eta_{j+1}^{(1)} \Leftrightarrow \eta_{i+1}^{(1)} = \sum_{j=1}^{N-1} U_{i,j}\nu_j$, where U is the orthogonal matrix ($U_{ji} = U_{ij}^T$) diagonalizing B,

$$U^T B U = \frac{m}{2}\,\tilde{\Omega}^2, \tag{3.32}$$

$\tilde{\Omega} = \mathrm{diag}(\tilde{\omega}_1, \dots \tilde{\omega}_{N-1})$. With this choice of coordinates $H_{\rm bath}$ reads

$$\begin{aligned}
H_{\rm bath} &= \sum_{n=1}^{N-1} \frac{(\eta_{n+1}^{(1)})^2}{2m} + \frac{m}{2}\sum_{n,m=1}^{N-1} B_{nm} d_{n+1}^{(1)} d_{m+1}^{(1)} \\
&= \sum_{n,l,k=1}^{N-1} \frac{U_{n,l}\nu_l\; U_{n,k}\nu_k}{2m} + \frac{m}{2}\sum_{n,m,l,k=1}^{N-1} \Big(B_{nm} U_{m,l}\xi_l U_{n,k}\xi_k \Big) \\
&= \sum_{n,l,k=1}^{N-1} \frac{U_{n,l}\; U_{n,k}\nu_l\nu_k}{2m} + \frac{m}{2}\sum_{n,m,l,k=1}^{N-1} U_{k,n}^T B_{nm} U_{m,l}\xi_l\xi_k \\
&= \sum_{n,l,k=1}^{N-1} \frac{1}{2m} \overbrace{\sum_{n=1}^{N-1} U_{l,n}\; U_{n,k}}^{\delta_{lk}} \nu_l\nu_k \\
&\qquad + \frac{m}{2}\sum_{n,m,l,k=1}^{N-1} \xi_k^T \underbrace{U_{k,n}^T B_{nm} U_{m,l}}_{\tilde{\omega}_n^2\;\delta nm} \xi_l \\
&= \sum_{l=1}^{N-1} \frac{\nu_l^2}{2m} + \frac{m}{2}\sum_{n,m,l,k=1}^{N-1} \tilde{\omega}_n^2 \delta_{nm} \xi_l^2 \delta_{lk} \\
&= \sum_{l=1}^{N-1} \frac{\nu_l^2}{2m} + \frac{m}{2}\sum_{n,m=1}^{N-1} \tilde{\omega}_n^2 \delta_{nm} \sum_{l,k=1}^{N-1} \xi_l^2 \delta_{lk} \\
&= \sum_{n=1}^{N-1} \frac{\nu_n^2}{2m} + \frac{m}{2}\sum_{n=1}^{N-1} \tilde{\omega}_n^2 \sum_{l=1}^{N-1} \xi_l^2 = \sum_{n=1}^{N-1} \frac{\nu_n^2}{2m} + \frac{m}{2}\sum_{n=1}^{N-1} \tilde{\omega}_n^2 \xi_n^2,
\end{aligned}$$

which gives us

$$H_{\rm bath} \;=\; \sum_{n=1}^{N-1}\left(\frac{\nu_n^2}{2m}+\frac{m}{2}\,\tilde{\omega}_n^2\xi_n^2\right). \tag{3.33}$$

Now we have to perform the transformation in the part of the Hamiltonian that represents the interaction between the bath coordinates and the collective degree of freedom,

$$X\sum_{n=1}^{N-1}k_n d_{n+1} = X\sum_{n,m=1}^{N-1}U_{nm}k_n\xi_m = X(\mathbf{l},\xi)\,, \tag{3.34}$$

where we defined the vectors $\mathbf{k}$ and $\mathbf{l}=U^T\mathbf{k}$ with the components

$$l_m=\sum_{n=1}^{N-1}U^T_{mn}k_n, \qquad k_n=\tilde{K}_{1(n+1)}, \quad n=1,\dots N-1. \tag{3.35}$$

Putting all the expressions together we finally arrive at the following Caldeira-Legget form for our model

$$H'=\frac{P^2}{2m}+\tilde{K}_{11}X^2+X\sum_{m=1}^{N-1}l_m\xi_m+\sum_{n=1}^{N-1}\left(\frac{\nu_n^2}{2m}+\frac{1}{2}m\tilde{\omega}_n^2\xi_n^2\right). \tag{3.36}$$

This Hamiltonian describes an effective particle moving in a harmonic potential and also interacting with a heat bath. We emphasize again that contrary to the Caldeira-Legget model the bath is part of the system and not an external configuration of particles. The spreading of the collective motion is a result of a redistribution of energy and not an actual loss of energy as in models with an external bath. Furthermore, our model possesses only a finite number of degrees of freedom which eventually causes a return of energy into the collective mode. However, since the volume of available phase space grows exponentially, the recurrence time will be much longer than the spreading time for a sufficiently large number of particles.

3.2 Chain with next neighbor coupling

Below we illustrate the above mapping procedure for a simple example, where the resulting Hamiltonian (3.36) can be written down explicitly. We consider a system of two chains with next neighbor interaction coupled at one point. The Hamiltonian for that system reads

$$\begin{aligned}H=&\sum_{j=1}^{N}\frac{1}{2m}\left((p_j^{(1)})^2+(p_j^{(2)})^2\right)+\frac{\alpha}{2}\left(x_1^{(1)}-x_1^{(2)}\right)^2\\&+\frac{m\omega_0^2}{2}\sum_{j=1}^{N}\Big((x_j^{(1)}-x^{(1)}_{(j+1)\mathrm{mod}N})^2+(x_j^{(2)}-x^{(2)}_{(j+1)\mathrm{mod}N})^2\Big)\,,\end{aligned} \tag{3.37}$$

where $K_{ij} = (\alpha/2)\delta_{i1}\delta_{j1}$ are the coupling constants.

The eigenfrequencies for a free chain of N oscillators with the next-neighbor interaction as in (3.37) are given by [35]

$$\omega_k = 2\omega_0 \left| \sin \frac{\pi(k-1)}{2N} \right| , \quad k = 1, ..., N. \tag{3.38}$$

with the corresponding eigenvectors given by (3.12). As described in section 3.1.2 we define the set of new coordinates d_i and consider the part of the Hamiltonian H' which only contains the couplings between the d_j's and $X = d_1$. Straightforward calculations then yield

$$H' = \frac{P^2}{2m} + \frac{\alpha}{N} X^2 + \frac{\alpha}{\sqrt{N}} X(\mathbf{a}, \mathbf{d}) + H_{\text{bath}} , \tag{3.39}$$

where $\mathbf{a} = (A_{12}, ..., A_{1N})$ and the bath Hamiltonian is given by

$$H_{\text{bath}} = \frac{1}{2m}(\eta, \eta) + \left(\mathbf{d}, \left(\frac{m}{2}\Omega^2 + \alpha \ \mathbf{a} \otimes \mathbf{a}^T \right) \mathbf{d} \right) \tag{3.40}$$

with Ω^2 being the diagonal matrix of the eigenvalues ω_k^2 and "$\otimes$" being the ordinary tensor product. Diagonalization of the bath leads to

$$H' = \frac{P^2}{2m} + \frac{2\alpha}{N} X^2 + X \sum_{n=2}^{N} C_n(\alpha)\xi_n + \sum_{n=2}^{N} \left(\frac{\nu_n^2}{2m} + \frac{m\tilde{\omega}_n^2 \xi_n^2}{2} \right) \tag{3.41}$$

with the coupling coefficients

$$C_n(\alpha) = \frac{\sqrt{2}\alpha}{N} \left(\sum_{k=2}^{N} \frac{\cos^2(\frac{\pi(k-1)}{2N})}{(\tilde{\omega}_n^2 - \omega_k^2)^2} \right)^{-1/2} \sum_{k=2}^{N} \frac{\cos^2(\frac{\pi(k-1)}{2N})}{\tilde{\omega}_n^2 - \omega_k^2} , \tag{3.42}$$

where the implicit equation

$$\frac{4\alpha}{Nm} \sum_{k=2}^{N} \frac{\cos^2\left(\frac{\pi(k-1)}{2N}\right)}{\tilde{\omega}_j^2 - \omega_k^2} = 1 \tag{3.43}$$

yields the eigenfrequencies $\tilde{\omega}_j$.

3.3 Dynamics of the collective coordinate

We return to the general case. So far we mapped the Hamiltonian system of two coupled chains of harmonic oscillators to the Caldeira-Leggett model. The next step is to consider the time evolution of the collective mode $X(t)$ induced by the Hamiltonian (3.36). The full quantum mechanical solution of the problem would require calculating the time evolution for a reduced

density-matrix $\hat{\rho}_{\mathbf{rd}}(X)$ of the collective coordinate. While such an analysis is certainly possible along the lines of Ref. [30, 36, 37, 38] (see also Appendix B), for our purposes it will be sufficient to consider the most basic collective dynamical properties captured by the time evolution of the expectation value for the quantized collective observable $\hat{X}$

$$\langle \hat{X}(t) \rangle := \mathrm{Tr}(\hat{\rho}\hat{X}(t)) \ , \tag{3.44}$$

where $\hat{\rho}$ is the full density matrix. In this case the problem simplifies, since one can deduce the time evolution equation for $\langle \hat{X}(t) \rangle$ from the corresponding equation for the time evolution of the quantum operator $\hat{X}(t)$ [39]. It is worthwhile to mention that, since $\hat{H}'$ contains only quadratic terms, the resulting equation of motion for $\langle \hat{X}(t) \rangle$ coincides with the corresponding equation of motions for the classical observable $X(t)$ obtained for the classical Hamiltonian H'. Below we give a short derivation of this equation and analyze its solution for certain types of initial conditions for $\hat{\rho}$.

The Heisenberg equations for our system read

$$\dot{\hat{X}}(t) = \frac{i}{\hbar}[\hat{H}', \hat{X}(t)] = \frac{\hat{P}}{m}, \tag{3.45}$$

$$\dot{\hat{P}}(t) = \frac{i}{\hbar}[\hat{H}', \hat{P}(t)] = -2\tilde{K}_{11}\hat{X} + \sum_{n=1}^{N-1} l_n \hat{\xi}_n(t), \tag{3.46}$$

$$\dot{\hat{\xi}}_n(t) = \frac{i}{\hbar}[\hat{H}', \hat{\xi}_n(t)] = \frac{\hat{\nu}_n}{m}, \tag{3.47}$$

$$\dot{\hat{\nu}}_n(t) = \frac{i}{\hbar}[\hat{H}', \hat{\xi}_n(t)] = -m\tilde{\omega}_n^2 \hat{\xi}_n(t) + l_n \hat{X}(t). \tag{3.48}$$

From these equations one immediately obtains

$$m\ddot{\hat{X}}(t) + 2\tilde{K}_{11}\hat{X} - \sum_{n=1}^{N-1} l_n \hat{\xi}_n(t) = 0 \tag{3.49}$$

and

$$m\ddot{\hat{\xi}}_n(t) + m\tilde{\omega}_n^2 \hat{\xi}_n(t) - l_n \hat{X}(t) = 0, \qquad n = 1, \ldots N-1. \tag{3.50}$$

We now use the representation of the momentum and coordinate operators at time zero in terms of creation and annihilation operators

$$\hat{\xi}_n(0) = \sqrt{\frac{\hbar}{2m\tilde{\omega}_n}}(\hat{b}_n + \hat{b}_n^\dagger), \qquad \hat{\nu}_n(0) = -i\sqrt{\frac{m\hbar\tilde{\omega}_n}{2}}(\hat{b}_n - \hat{b}_n^\dagger). \tag{3.51}$$

With these initial conditions the solution of equation (3.50) takes the form

$$\begin{aligned}\hat{\xi}_n(t) &= \sqrt{\frac{\hbar}{2m\tilde{\omega}_n}}(e^{-i\tilde{\omega}_n t}\hat{b}_n + e^{i\tilde{\omega}_n t}\hat{b}_n^\dagger) \\ &\quad + \frac{l_n}{m\tilde{\omega}_n}\int_0^t ds\ \sin(\tilde{\omega}_n(t-s))\hat{X}(s). \end{aligned} \tag{3.52}$$

Using this to eliminate the bath-modes from the equation (3.49), we obtain

$$\ddot{\hat{X}}(t) + \frac{2\tilde{K}_{11}}{m}\hat{X} - \frac{2}{m}\int_0^t\int_0^\infty ds\ d\tilde{\omega}\ \sigma(\tilde{\omega})\sin(\tilde{\omega}(t-s))\ \hat{X}(s) = \frac{\hat{F}(t)}{m} \tag{3.53}$$

where

$$\hat{F}(t) = \sum_{n=1}^{N-1} l_n\sqrt{\frac{\hbar}{2m\tilde{\omega}_n}}(e^{-i\tilde{\omega}_n t}\hat{b}_n + e^{i\tilde{\omega}_n t}\hat{b}_n^\dagger) \tag{3.54}$$

is the force operator that acts on the collective coordinate and

$$\sigma(\tilde{\omega}) = \sum_{n=1}^{N-1}\frac{l_n^2}{2m\tilde{\omega}_n}\ \delta(\tilde{\omega}-\tilde{\omega}_n) \tag{3.55}$$

is the spectral density. We further rewrite the part describing the dissipation as

$$-\frac{2}{m}\int_0^t\int_0^\infty ds\ d\tilde{\omega}\ \sigma(\tilde{\omega})\ \sin(\tilde{\omega}(t-s))\hat{X}(s) = \int_0^t\frac{d\gamma(t-s)}{dt}\ \hat{X}(s)ds, \tag{3.56}$$

where we defined the damping-kernel as

$$\gamma(t-s) = \frac{2}{m}\int_0^\infty d\tilde{\omega}\ \frac{\sigma(\tilde{\omega})}{\tilde{\omega}}\ \cos(\tilde{\omega}(t-s)). \tag{3.57}$$

After inserting this term into equation (3.53) we arrive at

$$\frac{d^2\hat{X}(t)}{dt^2} + \frac{2\tilde{K}_{11}}{m}\hat{X}(t) + \int_0^t ds\ \dot{\gamma}(t-s)\hat{X}(s) = \frac{1}{m}\hat{F}(t)\ . \tag{3.58}$$

We now use equation (3.58) to obtain the evolution equation for the expectation value (3.44) of $\hat{X}$ for some class of initial states $\hat{\rho}$. We assume that the initial conditions for $\hat{\rho}$ satisfy

$$\langle\hat{X}(0)\rangle = 0\ , \qquad \langle\hat{P}(0)\rangle = P_0\ , \qquad \langle\hat{b}_n\rangle = \langle\hat{b}_n^\dagger\rangle = 0\ . \tag{3.59}$$

Here we have used the notation $\langle\hat{A}\rangle := \mathrm{Tr}(\hat{\rho}\hat{A})$ for the expectation value of an observable $\hat{A}$. Under these assumptions equation (3.58) yields for the expectation value of $\hat{X}$

$$\frac{d^2\langle\hat{X}(t)\rangle}{dt^2} + \Omega_0^2\langle\hat{X}(t)\rangle + \int_0^t ds\ \gamma(t-s)\frac{d\langle\hat{X}(s)\rangle}{ds} = 0\ , \tag{3.60}$$

where $\Omega_0^2 = 2\tilde{K}_{11}/m - \gamma(0)$ and the term $\gamma(0)$ is a renormalization of the potential resulting from the interaction between the collective mode and the bath. Equation (3.60) is a classical damping equation which together with the initial conditions (3.59) describes the time development of the collective mode. It is straightforward to see that one obtains precisely the same equation for classical time evolution of X under the classical Hamiltonian flow induced by H' if the initial conditions are fixed as

$$X(0) = 0\ , \quad P(0) = P_0\ , \quad \xi_i = 0\ , \quad \nu_i = 0\ , \quad i = 1, \ldots N-1\ . \tag{3.61}$$

We notice that the entire information on the time evolution of $\langle\hat{X}(t)\rangle$ is encoded in the damping kernel γ. If $\gamma(t) = \gamma_0\delta(t)$, that is, if the system has no "memory", the above equation describes the damped harmonic oscillator of frequency Ω_0 with the damping coefficient γ_0.

Since (3.60) is a linear equation, we can easily construct its solution for a general kernel $\gamma(t)$. To this end we consider a slightly different equation

$$\frac{d^2\langle\hat{X}(t)\rangle}{dt^2} + \Omega_0^2\langle\hat{X}(t)\rangle + \int_{-\infty}^{\infty} ds\ \Theta(t-s)\gamma(t-s)\frac{d\langle\hat{X}(s)\rangle}{ds} = \frac{P_0}{m}\ \delta(t), \tag{3.62}$$

with the initial conditions

$$\langle\hat{X}(-\infty)\rangle = 0, \qquad \langle\hat{P}(-\infty)\rangle = 0. \tag{3.63}$$

at time $t = -\infty$. $\Theta(t-s)$ denotes the Heaviside step function. Equation (3.62) describes thus the system which stays at rest for all times $t < 0$ and then gets a "kick" at the time $t = 0$. After this it acquires a momentum P_0 and continues to evolve according to equation (3.60). Obviously both, equation (3.60) and equation (3.62), give the same solution for positive times. We can solve equation (3.62) employing the pair of Fourier transforms

$$\langle\hat{X}(t)\rangle = \int_{-\infty}^{\infty} \tilde{X}(\omega)\ e^{-i\omega t}d\omega, \qquad \tilde{X}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\hat{X}(t)\rangle\ e^{i\omega t}dt. \tag{3.64}$$

Applying the Fourier transformation to both sides of equation (3.62) we find the following expression

$$\tilde{X}(\omega) = \frac{P_0}{2\pi m(\Omega_0^2 - \omega^2 - i\omega\tilde{\gamma}(\omega))}, \tag{3.65}$$

where $\tilde{\gamma}(\omega)$ is defined as

$$\tilde{\gamma}(\omega) := \int_0^\infty \gamma(s) e^{i\omega s} ds. \tag{3.66}$$

Therefore the solution of the homogeneous system becomes

$$\langle \hat{X}(t) \rangle = \frac{P_0}{2\pi m} \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\Omega_0^2 - \omega^2 - i\omega\tilde{\gamma}(\omega)} \, d\omega \ . \tag{3.67}$$

As one can see from equations (3.66) and (3.67), the dynamics of the collective mode is encoded in the spectral density $\sigma(\omega)$. It is thus important to relate $\sigma(\omega)$ to the interaction matrix $\tilde{K}$ appearing in the original Hamiltonian (3.29). Recalling the definition (3.55) of σ and using $\mathbf{k} = U\mathbf{l}$ we obtain

$$\begin{aligned} \sigma(\omega) &= -\frac{1}{2\pi m\omega} \mathrm{Im} \left(\sum_{n=1}^{N-1} \frac{l_n l_n^*}{\omega - \tilde{\omega}_n + i\epsilon} \right) \\ &= -\frac{1}{2\pi m\omega} \mathrm{Im} \left(\sum_{n=1}^{N-1} \frac{\left[\mathbf{l} \otimes \mathbf{l}^T \right]_{n,n}}{\omega - \tilde{\omega}_n + i\epsilon} \right) \\ &= -\frac{1}{2\pi m\omega} \mathrm{Im} \mathrm{Tr} \left[\frac{\mathbf{k} \otimes \mathbf{k}^T}{\omega \mathbf{1} - \left(\frac{\mathbf{2}}{\mathbf{m}} \mathbf{B} \right)^{\mathbf{1/2}} + \mathbf{i}\epsilon} \right] \end{aligned} \tag{3.68}$$

where $\mathbf{l} \otimes \mathbf{l}^T$, $\mathbf{k} \otimes \mathbf{k}^T$ stands for the tensor product between $\mathbf{l}$ and $\mathbf{l}^T$ (resp. $\mathbf{k}$ and $\mathbf{k}^T$). The last expression can be rewritten in terms of a scalar product,

$$\sigma(\omega) = -\frac{1}{2\pi m\omega} \mathrm{Im} \left(\mathbf{k}, \ \frac{1}{\omega \mathbf{1} - (\mathbf{\Omega_r^2} + \frac{\mathbf{2}}{\mathbf{m}} \mathbf{\tilde{K}_r})^{\mathbf{1/2}} + \mathbf{i}\epsilon} \ \mathbf{k} \right) \ , \tag{3.69}$$

where Ω_r, $\tilde{K}_r$ are $(N-1) \times (N-1)$ matrices obtained from Ω, $\tilde{K}$ by deleting the first row and the first column, respectively. We have now a formal expression for the spectral density of our general model. Two remarks are in order. First the collective coordinate becomes completely decoupled from the bath if and only if $\mathbf{k} = 0$. Since the components of $\mathbf{k}$ can be written as

$$k_i = \frac{2}{\sqrt{N}} \sum_{j=1}^{N} \hat{k}_j A_{j(i+1)} \ , \tag{3.70}$$

the above condition is equivalent to the requirement that the $\hat{k}_i = \sum_{j=1}^N K_{ij}$ take the same value for all i. In particular, there is no damping if $K_{ij} =$

const. We notice that given a splitting of the interactions: $K_{ij} = \mathcal{K} + \delta K_{ij}$ into "constant" and "fluctuating" parts of the interaction, only δK_{ij} contributes to $\mathbf{k}$. Second, by adding the term $K_0 X^2$ to the Hamiltonian (4.1) one can adjust the collective frequency $\tilde{\Omega}_0$ without changing the spectral density σ. This additional term can be incorporated into H_I, H_{II}, $H_{\rm int}$ such that the overall structural form of H remains intact. Note that this "renormalization" results in a shift of the spectrum Ω_r of the chain Hamiltonians H_I, H_{II} which is compensated by the shift of the interaction term $\tilde{K}_r$ by a diagonal matrix, such that the matrix B (resp. σ) does not change.

The form (3.69) for the density σ hinders an exact treatment for a general form of interaction matrix K. However, if we assume that the fluctuation part of couplings matrix elements are small $|\delta K_{ij}| \ll m|\omega_{n+1}^2 - \omega_n^2|$, we can approximate the density function by

$$\sigma(\omega) = \sum_{n=1}^{N-1} \frac{k_n^2}{2m\omega}\, \delta\left(\omega - \sqrt{\omega_n^2 + 2N\mathcal{K}/m}\right)\ , \tag{3.71}$$

where $\{\omega_n\}$ is the phononic spectrum of the noninteracting chains and the k_n's are determined solely by δK_{ij}. The expression (3.71) can be interpreted to the extent that after introducing the interaction between the two chains the phonons acquire a "mass". Assuming that k_n are uniformly distributed, the behavior of $\sigma(\omega)$ is determined by the spectral density of the phonon frequencies ω_n. In particular, in the case of an Ohmic law distribution for the ω_n this leads to $\sigma(\omega) \sim \omega\Theta(\omega - \frac{2N}{m}\mathcal{K})$ at low frequencies. Furthermore, if $\mathcal{K} = 0$ this in turn implies that $\gamma(t)$ is localized at $t = 0$ and equation (3.60) can be approximated by the differential equation describing time evolution of a harmonic oscillator with a friction.

3.4 Transition strength and collective excitation

In the previous section, we derived an equation of motion that describes the damping of the collective excitation. As we mentioned already, the quantum evolution governed by equation (3.60) coincides with the classical evolution of $X(t)$ if the initial conditions are defined in an appropriate way. In this section we consider the problem of existence of quantum collective states in the spectrum of the system. One way to probe such collective excitations is to couple the system to an external weak periodic potential $v(X,t) \sim A(X)\cos(\omega t)$ depending on the collective variable X. Assuming that the coupling is weak, the energy absorption rate in the first order perturbation theory will be determined by the following spectral function

$$\tilde{S}_A(\omega) = \sum_{n=0}^{\infty} \langle 0|A(\hat{X})|n\rangle|^2\, \delta\left(\omega - \frac{E_n - E_0}{\hbar}\right), \tag{3.72}$$

with $T_n = |\langle 0|A(\hat{X})|n\rangle|^2$ being the transition strengths between the ground state with energy E_0 and n-th state with energy E_n. The collective states can then be defined, as states having large transition strengths T_n. Accordingly, the spectral function (3.72) keeps the information about the existence of collective modes in the system. Equivalently, one can consider the Fourier transform of $\tilde{S}_A(\omega)$, which is given by the time correlation of $A(\hat{X})$

$$S_A(t) = \langle 0|A(\hat{X}(t))A(\hat{X}(0))|0\rangle. \tag{3.73}$$

On an intuitive level one might expect that the averaged transition strengths T_n should exhibit spikes for the energies E_n corresponding to collective motion. Below we show that under certain conditions this is indeed the case and the dynamical equation (3.60), in fact, determines the form of the time correlations $S_A(t)$.

3.4.1 Transition strengths induced by $\hat{X}$

Let us first consider the case of the observable $A(X) = X$. We calculate the time correlator

$$S(t) = \langle 0|\hat{X}(t)\hat{X}(0)|0\rangle. \tag{3.74}$$

Since we are dealing here with a system of coupled harmonic oscillators it is useful to consider the set of normal coordinates (q_n, p_n) where the Hamiltonian (3.26) becomes diagonal [40],

$$\hat{H} = \sum_{i=1}^{2N}\left(\frac{\hat{p}_i^2}{2m} + \frac{m\bar{\omega}_i^2\hat{q}_i^2}{2}\right) = \sum_{i=1}^{2N}\hbar\bar{\omega}_i\left(\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right) \tag{3.75}$$

Here $\hat{q}_i$, $\hat{p}_i$ are the position and the momentum operators corresponding to (q_i, p_i), with $\hat{a}_i^\dagger$, $\hat{a}_i$ being the creation and the annihilation operators, respectively. The frequencies $\bar{\omega}_i$ are the eigenfrequencies of the full system. Since the connection between old coordinates X, $\{d_i\}$, $\{\bar{d}_i\}$ and new $\{q_i\}$ coordinates is given by a linear transformation, we can assume that

$$\hat{X} = \sum_{i=1}^{2N}\tilde{c}_i\hat{q}_i \tag{3.76}$$

with some coefficients $\tilde{c}_i$. Substituting (3.76) into (3.74) we obtain

$$\begin{aligned} S(t) &= \langle 0|\hat{X}(t)\hat{X}(0)|0\rangle \\ &= \langle 0|\exp(i\hat{H}t/\hbar)\hat{X}(0)\exp(-i\hat{H}t/\hbar)\hat{X}(0)|0\rangle \\ &= \sum_{n=0}^{\infty}|\langle 0|\hat{X}(0)|n\rangle|^2\exp\left(i\frac{(E_0-E_n)t}{\hbar}\right) \\ &= \frac{\hbar}{2m}\sum_{n=1}^{2N}\frac{\tilde{c}_n^2}{\bar{\omega}_n}\exp(-i\bar{\omega}_n t)\ , \end{aligned} \tag{3.77}$$

where we used the relations $\hat{q}_i = \sqrt{\hbar/2m\bar{\omega}_i}(\hat{a}_i^\dagger + \hat{a}_i)$ to calculate the transition strength between the ground state $|0_1 0_2 \dots 0_{2N}\rangle = |0\rangle$ and excited states $|n_1 n_2 \dots n_{2N}\rangle = |n\rangle$. Taking then the Fourier transform of $S(t)$ leads to

$$\tilde{S}(\omega) = \sum_{n=0}^{\infty} |\langle 0|\hat{X}(0)|n\rangle|^2 \delta(\omega - \bar{\omega}_n) = \frac{\hbar}{2m} \sum_{n=1}^{2N} \frac{\tilde{c}_n^2}{\bar{\omega}_n} \delta(\omega - \bar{\omega}_n) \ . \tag{3.78}$$

Although $\tilde{S}(\omega)$ is a quantum mechanical object, we will show now that it is possible to relate it to the dynamics of a purely classical damped harmonic oscillator. To this end we consider the time evolution of the collective coordinate X under the Hamiltonian H with the following initial conditions:

$$\dot{X}(0) = \frac{P_0}{m}, \quad X(0) = 0, \qquad d_i = 0, \ \dot{d}_i(0) = 0, \ \forall i > 1. \tag{3.79}$$

As has been explained in the previous section, the dynamical evolution of $X(t)$ with such boundary conditions is governed by equation (3.60) for the classical damped oscillator. On the other hand, we can express this solution in the diagonalizing coordinates q as follows. The time evolution of $q_n(t)$ is given by

$$q_n = A_n \sin(\bar{\omega}_n t) \ . \tag{3.80}$$

where the constants A_n are fixed by the initial conditions (3.79):

$$\dot{q}_n(0) = A_n \bar{\omega}_n = \frac{P_0}{m} \tilde{c}_n^*. \tag{3.81}$$

Accordingly, for the time evolution of $X(t)$ we obtain

$$X(t) = \sum_{n=1}^{2N} \tilde{c}_n q_n(t) = \frac{P_0}{m} \sum_{n=1}^{2N} \frac{|\tilde{c}_n|^2}{\bar{\omega}_n} \sin(\omega_n t). \tag{3.82}$$

Comparing equations (3.82) and (3.78), we see that the classical quantity $X(t)$ and the imaginary part of $S(t)$ are related via

$$S_1(t) := \mathrm{Im}S(t) = -\frac{\hbar}{2m} \sum_{n=1}^{2N} \frac{|\tilde{c}_n|^2}{\bar{\omega}_n} \sin(\bar{\omega}_n t) = -\frac{\hbar}{2P_0} X(t). \tag{3.83}$$

Taking the Fourier transform of $S_1(t)$ yields

$$\tilde{S}_1(\omega) = \frac{i\hbar}{2m} \sum_{n=1}^{2N} \frac{|\tilde{c}_n|^2}{2\bar{\omega}_n} (\delta(\omega - \bar{\omega}_n) - \delta(\omega + \bar{\omega}_n)) = -\frac{i\hbar}{P_0} \mathrm{Im}\tilde{X}^+(\omega) \tag{3.84}$$

where $\tilde{X}^+(\omega)$ is given by the right-hand side of equation (3.65) via $\tilde{X}(\omega) = \tilde{X}^+(\omega) + \tilde{X}^-(\omega)$. This can be seen by taking the Fourier transform of $X(t)$

$$\tilde{X}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ \exp(i\omega t) X(t) \tag{3.85}$$

from which follows that

$$\tilde{X}^{+}(\omega) = \frac{1}{2\pi}\int_{0}^{\infty} dt\ \exp(i\omega t)X(t) \tag{3.86}$$

and

$$\begin{aligned}\tilde{X}^{-}(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{0} dt\ \exp(i\omega t)X(t) = \frac{1}{2\pi}\int_{\infty}^{0}(-dt)\ \exp(-i\omega t)X(-t)\\ &= -\frac{1}{2\pi}\int_{0}^{\infty} dt\ \exp(-i\omega t)X(t) = -(\tilde{X}^{+}(\omega))^{*},\end{aligned} \tag{3.87}$$

where we used that $X(t) = -X(-t)$. Thus we have

$$\tilde{X}(\omega) = \tilde{X}^{+}(\omega) - (\tilde{X}^{+}(\omega))^{*} = 2i\ \mathrm{Im}\tilde{X}^{+}(\omega),$$

from which we conclude that

$$S_1(t) = -\frac{\hbar}{2P_0}X(t) \Rightarrow \tilde{S}_1(\omega) = -\frac{\hbar}{2P_0}\tilde{X}(\omega) = -\frac{i\hbar}{P_0}\mathrm{Im}\tilde{X}^{+}(\omega), \tag{3.88}$$

which is precisely relation (3.84). Furthermore, comparing the expression (3.84) with (3.78) we recognize the connection

$$\tilde{S}(\omega) = 2i\Theta(\omega)\tilde{S}_1(\omega) = \frac{2\hbar}{P_0}\Theta(\omega)\mathrm{Im}\tilde{X}^{+}(\omega), \tag{3.89}$$

where $\Theta(\omega)$ denotes the Heaviside step function. This can be also written explicitly as

$$\tilde{S}(\omega) = \frac{\hbar}{\pi m}\Theta(\omega)\mathrm{Im}\left(\frac{1}{\Omega_0^2 - \omega^2 - i\omega\tilde{\gamma}(\omega)}\right). \tag{3.90}$$

It is worth noticing that this expression for $\tilde{S}(\omega)$ can also be derived using the fluctuation-dissipation theorem. Suppose at a certain moment a weak time dependent perturbation $\delta\hat{H} = \hat{X}\ F_{\mathrm{ext}}(t)$ is added to the Hamiltonian (4.1). Under this external perturbation the system will be driven away from the ground state. Considering the linear response of the system to $\delta\hat{H}$, it follows (see e.g., [39]) that the averaged displacement of the collective coordinate is given by

$$\langle\hat{X}(t)\rangle = \int_{-\infty}^{\infty} dt'\,\chi(t-t')F_{\mathrm{ext}}(t'), \tag{3.91}$$

where the integration kernel is given by $\hbar\chi(t) = -2\Theta(t)\mathrm{Im}\langle 0|\hat{X}(t)\hat{X}(0)|0\rangle = -2\Theta(t)S_1(t)$. On the other hand, from the previous section we know that for any force $F_{\mathrm{ext}}(t)$ (not necessary weak) the evolution of $\langle\hat{X}(t)\rangle$ is described by the equation:

$$\frac{d^2\langle\hat{X}(t)\rangle}{dt^2} + \Omega_0^2\langle\hat{X}(t)\rangle + \int_0^t ds\ \gamma(t-s)\frac{d\langle\hat{X}(s)\rangle}{ds} = \frac{F_{\mathrm{ext}}(t)}{m}. \tag{3.92}$$

Taking the Fourier transform from both sides of this expression and comparing the result with the Fourier transformed equation (3.91) leads then to (3.90).

From equation (3.90) we clearly see that the information on the distribution of the transition strengths is stored in the damping kernel $\gamma(t)$ of the purely classical equation for the time evolution of the collective mode. One should note, however, that $\tilde{S}(\omega)$ is not a smooth function but a sum of distributions with wildly fluctuating strength. It is easy to see, for instance, that most of the states are actually not coupled at all to the ground state through the operator $\hat{X}$. Thus, in order to see a structural emergence of collective excitations, we need to consider a smoothened version of the spectral function $\tilde{S}(\omega)$ where the average is taken over some interval $[\omega - \Delta\omega/2, \omega + \Delta\omega/2]$, such that $\Delta\omega \gg \delta\bar{\omega}$, with $\delta\bar{\omega} := |\bar{\omega}_{n+1} - \bar{\omega}_n|$ being the difference between two adjacent frequencies. We can define such a smoothened spectral function as the convolution

$$\tilde{S}_1^{(\varepsilon)}(\omega) := \frac{1}{\pi}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{\varepsilon\tilde{S}_1(\tilde{\omega})}{(\omega-\tilde{\omega})^2+\varepsilon^2}\ , \tag{3.93}$$

where the parameter ε satisfies $\Omega_0 \gg \varepsilon \gg \delta\bar{\omega}$. Using then the dynamical equation (3.60) one obtains

$$\tilde{S}^{(\varepsilon)}(\omega) = \frac{\hbar}{m\pi}\theta(\omega)\mathrm{Im}\left(\frac{1}{\Omega_0^2 - (\omega - i\varepsilon)^2 - i(\omega - i\varepsilon)\tilde{\gamma}_\varepsilon(\omega)}\right)\ , \tag{3.94}$$

where $\tilde{\gamma}_\varepsilon(\omega)$ is the smoothened damping kernel

$$\tilde{\gamma}_\varepsilon(\omega) = \int_0^\infty \exp\left((i\omega - \epsilon)\,t\right)\ \gamma(t)\ dt. \tag{3.95}$$

In the case when the spectral density σ obeys the Ohmic law, $\tilde{\gamma}_\varepsilon(\omega) = \gamma_0$ is constant and we find for the averaged $\tilde{S}(\omega)$ the expression

$$\tilde{S}^{(\varepsilon)}(\omega) \approx \frac{\hbar}{m\pi}\theta(\omega)\left(\frac{\omega\gamma_0}{(\Omega_0^2-\omega^2)^2 + (\omega\gamma_0)^2}\right)\ . \tag{3.96}$$

Here we choose the parameter ε to be small compared to γ_0. In the case of an underdamped oscillator $\Omega_0 > \gamma_0/2$, the above expression can be conveniently represented through the parameters of the corresponding classical evolution of the collective coordinate described by equation (3.60). Hence we have

$$X(t) = \frac{P}{m\bar{\Omega}_0} \exp(-\bar{\gamma}_0 t) \sin(\bar{\Omega}_0 t), \quad \bar{\Omega}_0 = \sqrt{\Omega_0^2 - \frac{\gamma_0^2}{4}}, \quad \bar{\gamma}_0 = \gamma_0/2 \ . \tag{3.97}$$

With the parameters $\bar{\Omega}_0, \bar{\gamma}_0$ equation (3.96) takes the form

$$\tilde{S}(\omega) = \theta(\omega) \ \frac{\hbar\bar{\gamma}_0}{2\pi m\bar{\Omega}_0} \left(\frac{1}{(\omega - \bar{\Omega}_0)^2 + \bar{\gamma}_0^2} - \frac{1}{(\omega + \bar{\Omega}_0)^2 + \bar{\gamma}_0^2} \right) \ , \tag{3.98}$$

where we dropped the index ε. In a strongly underdamped regime $\Omega_0 \gg \gamma_0/2$ the transition strength distribution (3.98) has a maximum at the frequency $\omega \approx \Omega_0 \approx \bar{\Omega}_0$ of the collective motion, and the width of the distribution is controlled by γ_0, see fig. (3.1). On the other hand, in the overdamped regime $\Omega_0 < \gamma_0/2$ the maximum is shifted away from Ω_0 and the distribution becomes very broad i.e., there are no pronounced collective excitations.

3.4.2 Transition strengths for general couplings

We notice that the function $\tilde{S}(\omega)$, derived in the previous section, has only one maximum at a frequency near Ω_0. Translating this into the energy domain one concludes that the collective excitations show up only for the first energy level $E_1 = E_0 + \Omega_0\hbar$ of the damped harmonic oscillator, rather than for all energies $E_n = E_0 + n\Omega_0\hbar$. This is directly connected with the choice of the coupling $A(\hat{X})$ and the linear nature of our model, since in a harmonic oscillator the transitions induced by $\hat{X}$ only happen between neighboring states. Let us show that for a more general choice of the coupling $A(\hat{X})$ other collective excitations show up at energies E_n, $n > 1$ of the collective oscillator mode. For the sake of simplicity of exposition we will first consider the case $A(\hat{X}) = \hat{X}^2$ and then comment on the general case. We thus consider the time correlator

$$S^{(2)}(t) := \langle 0|\hat{X}^2(t)\hat{X}^2(0)|0\rangle - \langle 0|\hat{X}^2(0)|0\rangle^2, \tag{3.99}$$

whose Fourier transform keeps information about the transition strengths induced by the operator $\hat{X}^2$,

$$\begin{aligned} \tilde{S}^{(2)}(\omega) &:= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ e^{i\omega t} S^{(2)}(t) \\ &= \sum_{m\neq 0}^{2N} |\langle 0|\hat{X}^2|m\rangle|^2 \delta\left(\omega - \frac{E_m - E_0}{\hbar}\right) \ . \end{aligned} \tag{3.100}$$

It is easy to show that this quantity can be expressed in terms of $\tilde{S}(\omega)$. Indeed, separating the collective mode into annihilation and creation parts,

$$\hat{X}(t) = \hat{X}^+(t) + \hat{X}^-(t), \qquad \hat{X}^+(t)|0\rangle = 0 \ , \quad \langle 0|\hat{X}^-(t) = 0 \ , \tag{3.101}$$

and using their commutation relation leads to

$$S^{(2)}(t) = \langle 0|\hat{X}^2(t)\hat{X}^2(0)|0\rangle - \langle 0|\hat{X}^2(0)|0\rangle^2 = 2S^2(t) \ . \tag{3.102}$$

This immediately implies

$$\tilde{S}^{(2)}(\omega) = \frac{1}{\pi}\int\limits_{-\infty}^{\infty} dt \, \exp(i\omega t) S^2(t) = 2\int\limits_{-\infty}^{\infty} \tilde{S}(\omega')\tilde{S}(\omega-\omega')d\omega'. \tag{3.103}$$

Using then equation (3.89), we obtain

$$\tilde{S}^{(2)}(\omega) = -8\int\limits_{0}^{\omega} \tilde{S}_1(\omega')\tilde{S}_1(\omega-\omega')d\omega'. \tag{3.104}$$

If σ obeys an Ohmic law and if we are in the underdamped regime, the last expression takes the form

$$\begin{aligned}\tilde{S}^{(2)}(\omega) \ &= \ 2\left(\frac{\hbar\bar{\gamma}}{2\pi m\bar{\Omega}_0}\right)^2 \int\limits_{0}^{\omega}\left(\frac{1}{(\omega'+\bar{\Omega}_0)^2+\bar{\gamma}_0^2} - \frac{1}{(\omega'-\bar{\Omega}_0)^2+\bar{\gamma}_0^2}\right) \\ &\left(\frac{1}{(\omega-\omega'+\bar{\Omega}_0)^2+\bar{\gamma}_0^2} - \frac{1}{(\omega-\omega'-\bar{\Omega}_0)^2+\bar{\gamma}_0^2}\right) d\omega'. \end{aligned} \tag{3.105}$$

The function $\tilde{S}^{(2)}(\omega)$ is depicted in figure (3.1). For $\Omega_0 \gg 2\gamma_0$ (i.e., strongly underdamped regime) one can clearly see a spike in the vicinity of the oscillator frequency $2\Omega_0$ with the width of the spike being twice the width of $\tilde{S}(\omega)$ for the same parameters γ_0, Ω_0.

It is straightforward to generalize the above discussion to generic observables of the form $A(\hat{X})$ using the Taylor expansion

$$A(\hat{X}) = \sum_{n=0}^{\infty} \alpha_n \hat{X}^n. \tag{3.106}$$

After substituting this into the definition of the time correlator, and applying Wick's theorem to the products of $X(t)$ we obtain

$$S_A(t) = \langle 0|A(\hat{X}(t))A(\hat{X})|0\rangle = \sum_{n=0}^{\infty} \beta_n S^n(t), \tag{3.107}$$

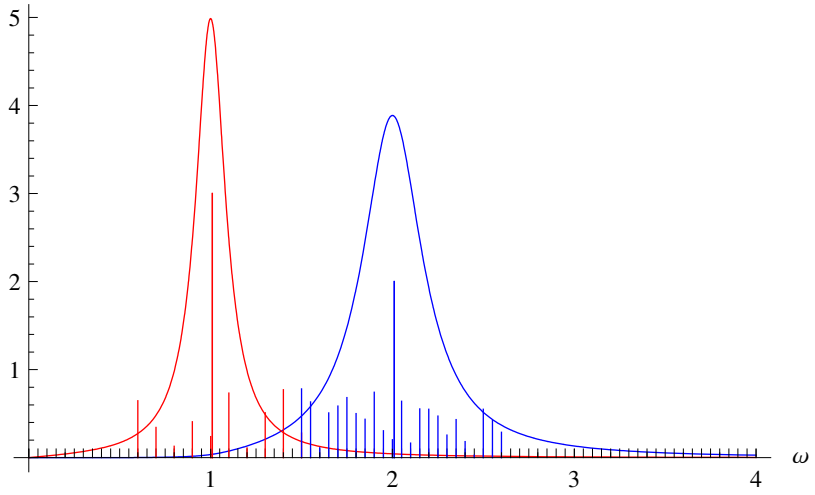

Figure 3.1: The dimensionless functions $\left(\pi m\bar{\Omega}_0^2/\hbar\right)\tilde{S}(\omega)$, $\left(\pi m\bar{\Omega}_0^{3/2}/\hbar\sqrt{2}\right)^2\tilde{S}^{(2)}(\omega)$ are plotted on the left-hand side (red) and the right-hand side (blue) for the parameters $\bar{\Omega}_0 = 1$, $\bar{\gamma}_0 = 0.1$. The spikes at the bottom of the figure schematically depict the states which are coupled to the ground state through the operator $\hat{X}$ and $\hat{X}^2$, respectively.

where β_n are some coefficients having dimension of inverse length in power $2n$. Taking now the Fourier transform from both sides of this expression we obtain for the spectral function

$$\tilde{S}_A(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{it\omega} S_A(t) = \sum_{n=0}^{\infty}\beta_n \underbrace{\tilde{S}(\omega) * \tilde{S}(\omega) * \cdots * \tilde{S}(\omega)}_{n \text{ times}}\,, \qquad (3.108)$$

where the symbol $*$ stands for the convolution. It is quickly seen that, in the underdamped regime, the n-th term of the sum (3.108) has a maximum at the vicinity of $n\Omega_0$ with a width given by $n\gamma$.

3.4.3 Generic collective coordinate

It is worth noticing that in our model any linear combination of x_i, $\bar{x}_i$, that is,

$$Y = \sum_{i=1}^{N}\left(C_i x_i^{(1)} + \bar{C}_i x_i^{(2)}\right), \qquad (3.109)$$

can, in principle be used as a collective coordinate in the same way as X. Specifically, for any such choice of Y we can map the model to Caldeira-Leggett form by applying the arguments of section 3.1. Furthermore, the

connection between the dynamics of Y and the corresponding transition strength is given again by (3.90), (3.108), where the collective frequency Ω_0 and the damping kernel $\tilde{\gamma}(\omega)$ are determined by the choice of the constants $C_i, \bar{C}_i$. Clearly, not every choice of Y would be appropriate for the definition of the collective coordinate. If, for instance, the resulting dynamics of $Y(t)$ becomes overdamped, no visible spike can be observed in the corresponding transition strength. On the other hand, it seems that there is no "unique" choice for the collective coordinate based on the requirement of "minimal friction". Since our system is integrable, we can take Y to be one of the normal coordinates completely decoupled from the rest $2N-1$ degrees of freedom. This would lead to a "collective" motion without friction at all. Let us emphasize, that such a pathological choice of the collective coordinate would be impossible for non-integrable systems. It would be of interest to investigate whether for non-integrable systems a dynamical criterion for the collective coordinate based on "minimal friction" principle is possible.

We now consider a more general (non-linear) choice of a collective coordinate $\tilde{Y}(\{x_i, \bar{x}_i\})$. To leading order in $\hbar$ the correlator

$$\langle 0|\hat{\tilde{Y}}(t)\hat{\tilde{Y}}(0)|0\rangle = \langle 0|\hat{Y}(t)\hat{Y}(0)|0\rangle + O(\hbar^2) \tag{3.110}$$

is determined by the linearization

$$Y(\{x_i, \bar{x}_i\}) = \sum_{i=1}^{N} \left(x_i \left.\frac{\partial \tilde{Y}}{\partial x_i}\right|_{\{x_i=\bar{x}_i=0\}} + \bar{x}_i \left.\frac{\partial \tilde{Y}}{\partial \bar{x}_i}\right|_{\{x_i=\bar{x}_i=0\}} \right) \tag{3.111}$$

of $\tilde{Y}$, where we assumed that $\tilde{Y}(\{x_i, \bar{x}_i\})|_{\{x_i=\bar{x}_i=0\}} = 0$. Using then the previous line of arguing, the leading order of the transition strengths for $\hat{\tilde{Y}}$ can be connected with the classical dynamics of the linearization of $Y(t)$.

Finally, we note that in a typical physical situation the choice of a collective coordinate is crucially dictated by the method of probing the system. In the case of two oppositely charged particle clouds subjected to an electromagnetic external potential, the transitions from the ground state to a higher energy state are induced by the dipole moment operator. From this perspective the choice of the collective coordinate as the difference of the center masses of two "clouds" seems to be the natural one.

Chapter 4

Non-integrable case

In this chapter we extend our previously integrable model into the non-integrable domain. In Sec. 4.1 we derive a perturbative expression for the imaginary part of $S(t)$. We test the perturbative expression in the case of the Caldeira-Leggett model in Sec. 4.2. In Sec. 4.3 we discuss the straightforward application of the obtained perturbative expression for $S_1(t)$ to the non-integrable case.

We already emphasized that collective motion, *i.e.*, coherent motion of the particles in phase space, is a fundamental feature of many–body systems and it emerges out of the incoherent, single–particle motion whenever favored by energy and kinematic conditions. Due to the quantum–classical correspondence principle, the collective dynamics on the classical level should be reflected in the spectral properties of the corresponding quantum many–body system. Hence, the spectrum of a many–body system comprises states of single–particle and of collective character, mixed forms with a partial degree of collectivity exist as well. The details strongly depend on how the system is probed as we demonstrated in the previous chapter for the integrable case.

We mention here again the Giant Dipole Resonance in heavier nuclei as an example that served as an inspiration for our model. As we already laid out in the prelude the cross section of electric dipole radiation and the spectral density of the excitations show at a certain energy a huge peak whose spreading width is orders of magnitudes larger than the mean level spacing. It can be understood in terms of the following picture: the neutrons are confined to one sphere, the protons to another one. There is no or very little relative motion of the nucleons inside these spheres. The two spheres, however, move against each other, resulting in an enormous response function. The difference between the center–of–mass coordinates of the two spheres is the proper collective coordinate.

We explained that it is a demanding challenge to understand the emergence of collective motion and its interplay with the incoherent single–

particle motion. The vast majority of studies in this context relies on effective models whose justification is often mainly phenomenological or even on the level of hand waving if the system in question is too complex. Better understanding of these issues is called for. In the present chapters, we have three goals: (i) We want to address the interplay between collective and single–particle motion from first principles in the framework of a tractable, yet sufficiently general and complex (non-integrable) model. (ii) We aim at doing this analytically in such a way that we identify the collective coordinate, but always keep full control over the single–particle degrees of freedom. (iii) We wish to deliver the important insight that the spectral density of the collective excitations is directly related to classical motion.

We begin with setting up our model which considerably generalizes the integrable model which we studied previously. In one dimension, two chains $a = 1, 2$ of N interacting particles each with positions $x_i^{(a)},\ i = 1, \ldots, N$ and momenta $p_i^{(a)},\ i = 1, \ldots, N$ are coupled to one another. The total Hamiltonian reads

$$H = H_0 + \lambda H_1 \ . \tag{4.1}$$

Here, $H_0 = H_0^{(1)} + H_0^{(2)} + H_0^{(12)}$ is the integrable part considered in chapter (3.1.1). The first two terms

$$\begin{aligned} H_0^{(a)} &= \frac{1}{2m}\left(\mathbf{p}^{(a)}, \mathbf{p}^{(a)}\right) + \left(\mathbf{x}^{(a)}, W\ \mathbf{x}^{(a)}\right) \\ &= \frac{1}{2m}\sum_{i=1}^{N}\left(p_i^{(a)}\right)^2 + \sum_{i,j=1}^{N} x_i^{(a)} W_{ij} x_j^{(a)} \end{aligned} \tag{4.2}$$

model the two chains $a = 1, 2$ before they are coupled. The interaction within each chain is harmonic and described by the matrix W which we assume equal in both chains. We are mainly interested in self-bound systems such as nuclei, where unlike Bose–Einstein condensates, no external confining potential is needed. When we treated the integrable case we also imposed conditions on the matrix W which ensured that the interaction is invariant under translations and the system is bounded. We then coupled the two chains by an interaction which depended on the differences between their coordinates,

$$H_0^{(12)} = \sum_{i,j=1}^{N} K_{ij}\left(x_i^{(1)} - x_j^{(2)}\right)^2 \ . \tag{4.3}$$

For every choice of the coupling matrix K, the Hamiltonian H_0 is translation invariant. Clearly, the model is up to now integrable.

We generalize the model by adding the translation invariant term λH_1 which breaks integrability,

$$H_1 = \sum_{i,j=1}^{N} f(x_i^{(1)} - x_j^{(2)}) \ , \tag{4.4}$$

where f is an arbitrary, positive analytical function. We introduce the parameter λ, because we aim at a perturbative discussion.

To quantize our model, we replace coordinates and momenta by operators $\hat{x}_i^{(a)}$ and $\hat{p}_i^{(a)}$. Importantly, we make this step on the level of the *original* particle degrees of freedom. Motivated by the above mentioned Giant Dipole Resonance, we aim at studying collective excitations and the associated spectral density. We expect that it shows a pronounced peak, which we wish to understand in (semi-)classical terms. Naturally, the collective coordinate X is the difference between the mass centers of the two chains, and it is convenient to rescale it with a factor $\sqrt{N/2}$,

$$X = \frac{1}{\sqrt{2N}} \left(\sum_{i=1}^{N} x_i^{(1)} - \sum_{i=1}^{N} x_i^{(2)} \right) \tag{4.5}$$

and accordingly for the collective operator $\hat{X}$. To probe the existence of quantum collective states in the excitation spectrum, we investigate the correlator

$$S(t) = \langle \Phi_0 | \hat{X}(t) \hat{X}(0) | \Phi_0 \rangle \ , \tag{4.6}$$

where $|\Phi_0\rangle$ is the ground state of the total Hamiltonian $\hat{H}$. Here, $\hat{X}(t)$ is the Heisenberg picture of the operator $\hat{X}$ with the time evolution governed by the total Hamiltonian $\hat{H}$. The Fourier transform of the correlator (4.6),

$$\tilde{S}(\omega) = \sum_{\mu=0}^{\infty} |\langle \Phi_0 | \hat{X} | \Phi_\mu \rangle|^2 \delta \left(\omega - \frac{E_\mu - E_0}{\hbar} \right) \ , \tag{4.7}$$

is the desired spectral density of the collective excitations. It measures the strength of the transitions between the ground and the excited states $|\Phi_\mu\rangle$ of the whole system and can be interpreted as the response of the system that is excited by the transition operator $\hat{X}$. Following the terminology in many–body physics, we say that there is a collective quantum state for an energy $E_{\rm col} = E_0 + \hbar\omega$ if $\tilde{S}(\omega)$ (smoothened over some energy interval) has a pronounced spike at the corresponding frequency ω.

4.1 Perturbation theory

In order to extract information regarding the non-integrable case, that we can not solve exactly we have to take refuge in perturbation theory. Our goal is to obtain a perturbative expression for the correlator $\langle \Phi_0 | \hat{X}_I(t) \hat{X}_I(0) | \Phi_0 \rangle$. In perturbation theory one deals with problems of the form

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1, \tag{4.8}$$

where $\hat{H}_0$ denotes the unperturbed Hamiltonian and $\hat{H}_1$ the perturbation part. Following the philosophy of perturbation theory [41] we want to express the Eigenvalues

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \tag{4.9}$$

and Eigenstates

$$|u_n\rangle = |u_n^0\rangle + \lambda|u_n^1\rangle + \lambda^2|u_n^2\rangle + \dots \tag{4.10}$$

of the perturbed problem $\hat{H}|u_n\rangle = E_n|u_n\rangle$ in terms of the unperturbed problem $\hat{H}_0|u_n^0\rangle = E_n^0|u_n^0\rangle$. The states $|u_n^i\rangle$ are given by perturbation theory. For the first corrections we get

$$|u_n^1\rangle = \sum_k a_{kn}^1|u_k^0\rangle, \quad a_{kn}^1 = \langle u_k^0|u_n^1\rangle = \frac{\langle u_k^0|\hat{H}_1|u_n^0\rangle}{E_n^0 - E_k^0}, \quad a_{nn}^1 = 0. \tag{4.11}$$

For the second we obtain

$$|u_n^2\rangle = \sum_k a_{kn}^2|u_k^0\rangle, \tag{4.12}$$

with

$$a_{kn}^2 = \sum_{k'\neq n} = \frac{\langle u_k^0|\hat{H}_1|u_{k'}^0\rangle\langle u_{k'}^0|\hat{H}_1|u_n^0\rangle}{(E_n^0 - E_k^0)(E_n^0 - E_{k'}^0)} - \frac{\langle u_k^0|\hat{H}_1|u_n^0\rangle\langle u_n^0|\hat{H}_1|u_n^0\rangle}{(E_n^0 - E_k^0)^2}, \ \forall k \neq n \tag{4.13}$$

and

$$a_{nn}^2 = -\frac{1}{2}\sum_{k'\neq n} \frac{|\langle u_{k'}^0|\hat{H}_1|u_n^0\rangle|^2}{(E_n^0 - E_{k'}^0)^2}. \tag{4.14}$$

In our context the correlator $\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle$ plays the central role of identifying the collective dynamics. Thus we start the perturbative investigation of this quantity by sandwiching the operator $\hat{X}(t)\hat{X}(0)$ with the expanded vacuum states

$$|\Phi_0\rangle \approx |u_0^0\rangle + \lambda|u_0^1\rangle + \lambda^2|u_0^2\rangle = |u_0^0\rangle + \lambda\sum_{k\neq 0} a_{k0}^1|u_k^0\rangle + \lambda^2\sum_{k=0} a_{k0}^2|u_k^0\rangle \tag{4.15}$$

and its dual

$$\langle\Phi_0| \approx \langle u_0^0| + \lambda\langle u_0^1 + \lambda^2\langle u_0^2| = \langle u_0^0| + \lambda\sum_{k\neq 0}(a_{k0}^1)^*\langle u_k^0| + \lambda^2\sum_{k=0}(a_{k0}^2)^*\langle u_k^0| \tag{4.16}$$

up to second order. From this we obtain

$$\begin{aligned}\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle \approx &\left(\langle u_0^0| + \lambda\sum_{k\neq 0}(a_{k0}^1)^*\langle u_k^0| + \lambda^2\sum_{k=0}(a_{k0}^2)^*\langle u_k^0|\right) \\ &\times \left(\hat{X}(t)\hat{X}(0)\right)\left(|u_0^0\rangle + \lambda\sum_{k\neq 0} a_{k0}^1|u_k^0\rangle + \lambda^2\sum_{k=0} a_{k0}^2|u_k^0\rangle\right).\end{aligned} \tag{4.17}$$

After multiplication this transforms into

$$\begin{aligned}\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle \approx \langle u_0^0|\hat{X}(t)\hat{X}(0)|u_0^0\rangle + \lambda\sum_{l\neq 0} a_{l0}^1\langle u_0^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle \\ + \lambda\sum_{k\neq 0}(a_{k0}^1)^*\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_0^0\rangle + \lambda^2\sum_{l=0} a_{l0}^2\langle u_0^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle \\ + \lambda^2\sum_{k=0}(a_{k0}^2)^*\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_0^0\rangle + \lambda^2\sum_{k,l\neq 0} a_{l0}^1(a_{k0}^1)^*\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle,\end{aligned} \tag{4.18}$$

where the operator for the collective degree is propagated in the Heisenberg picture via

$$\hat{X}(t) = \exp\left(\frac{i\hat{H}t}{\hbar}\right)\hat{X}(0)\exp\left(\frac{-i\hat{H}t}{\hbar}\right), \tag{4.19}$$

where $\hat{H} = \hat{H}_0 + \lambda\hat{H}_1$ is the full (perturbed) Hamiltonian. It is worth mentioning that up to this point we have only expanded the correlator in terms of the states (perturbing the ground state $|0\rangle$). We have not yet taken into account the corrections that arise from the time propagation of the operator $\hat{X}(0)$. Since we are interested in perturbation theory up to second order of λ it is clear by looking at the expansion of the time propagator

$$\exp\left(\frac{i\hat{H}t}{\hbar}\right) \approx \mathbb{1} + \frac{it}{\hbar}\left(\hat{H}_0 + \lambda\hat{H}_1\right) + \frac{1}{2\hbar^2}(it(\hat{H}_0 + \lambda\hat{H}_1))^2, \tag{4.20}$$

that we have to anticipate further corrections to the correlator

$$\langle\Phi_0|\hat{X}_I(t)\hat{X}_I(0)|\Phi_0\rangle. \tag{4.21}$$

To calculate the contributions that result from terms of the form

$$\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle \tag{4.22}$$

we switch to the interaction picture. Thus these correlators take the following form

$$\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle = \langle u_k^0|\hat{U}^\dagger(t,0)\hat{X}_I(t)\hat{U}(t,0)\hat{X}(0)|u_l^0\rangle, \tag{4.23}$$

where

$$\hat{U}(t,0) = \hat{T}\exp\left(-\frac{i}{\hbar}\int_0^t dt'\hat{H}_I(t')\right), \tag{4.24}$$

is the time ordered evolution operator in the interaction picture and

$$\hat{U}^\dagger(t,0) = \hat{T}\exp\left(\frac{i}{\hbar}\int_0^t dt'\hat{H}_I^\dagger(t')\right), \tag{4.25}$$

its adjoint. The new Operators

$$\hat{X}_I(t) = \exp\left(\frac{i}{\hbar}\hat{H}_0 t\right)\hat{X}(0)\exp\left(-\frac{i}{\hbar}\hat{H}_0 t\right), \tag{4.26}$$

and

$$\hat{H}_I(t') = \lambda\ \exp\left(\frac{i}{\hbar}\hat{H}_0 t'\right)\hat{H}_1(0)\exp\left(-\frac{i}{\hbar}\hat{H}_0 t'\right), \tag{4.27}$$

are the time evolved operators for the collective coordinate and the perturbation part of the Hamiltonian in the interaction picture. It is important to mention that we propagate these only with the unperturbed Hamiltonian $\hat{H}_0$. If we expand $\hat{U}(t,0), \hat{U}^\dagger(t,0)$ in λ we get

$$\begin{aligned}\langle u_k^0|\hat{U}^\dagger(t,0)\hat{X}_I(t)\hat{U}(t,0)\hat{X}(0)|u_l^0\rangle = \langle u_k^0|\ \Bigg(\mathbb{1} + \frac{i\lambda}{\hbar}\int_0^t dt_1'\hat{H}_I^\dagger(t_1) \\ + \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_1'\ \hat{T}^\dagger\left(\hat{H}_I(t_1)\hat{H}_I(t_2)\right)\Bigg)\hat{X}_I(t)\Bigg(\mathbb{1} - \frac{i\lambda}{\hbar}\int_0^t dt_1'\hat{H}_I(t_1) \\ + \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_1'\ \hat{T}\left(\hat{H}_I(t_1)\hat{H}_I(t_2)\right)\Bigg)\hat{X}_I(0)|u_l^0\rangle. \end{aligned}\tag{4.28}$$

Keeping track of the order of operators leads us then to

$$\begin{aligned}\langle u_k^0|\hat{U}^\dagger(t,0)\hat{X}_I(t)\hat{U}(t,0)\hat{X}(0)|u_l^0\rangle = \langle u_k^0|\Bigg(\hat{X}_I(t)\hat{X}_I(0) \\ - \frac{i\lambda}{\hbar}\int_0^t dt_2'\ \hat{X}_I(t)\hat{H}_I^\dagger(t_2)\hat{X}_I(0) \\ + \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_2 dt_2'\ \hat{X}_I(t)\hat{T}(\hat{H}_I(t_2)\hat{H}_I(t_2'))\hat{X}(0) \\ + \frac{i\lambda}{\hbar}\int_0^t dt_1'\ \hat{H}_I^\dagger(t_1)\hat{X}_I(t)\hat{X}_I(0) \\ - \left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_1 dt_2\ (\hat{H}_I^\dagger(t_1)\hat{X}_I(t)\hat{H}_I(t_2))\hat{X}(0) \\ + \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_1'\ \hat{T}^\dagger(\hat{H}_I(t_1)\hat{H}_I(t_1'))\hat{X}_I(t)\hat{X}(0)\Bigg)|u_l^0\rangle. \end{aligned}\tag{4.29}$$

Since $\hat{H}_I(t) = \hat{H}_I^\dagger(t)$ is hermitian we can simplify this further to

$$\begin{aligned}\langle u_k^0|\hat{U}^\dagger(t,0)\hat{X}_I(t)\hat{U}(t,0)\hat{X}(0)|u_l^0\rangle &= \langle u_k^0|\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle \\ &\quad + \frac{i\lambda}{\hbar}\int_0^t dt_1 \langle u_k^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle \\ &\quad \underbrace{+\left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\hat{X}_I(t)\hat{T}\big(\hat{H}_I(t_2),\hat{H}_I(t_1)\big)\hat{X}_I(0)|u_l^0\rangle}_{I} \\ &\quad \underbrace{+\left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\hat{T}^\dagger\big(\hat{H}_I(t_2)\hat{H}_I(t_1)\big)\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle}_{II} \\ &\quad \underbrace{-\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\hat{H}_I(t_1)\big)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)|u_l^0\rangle}_{III}, \quad (4.30)\end{aligned}$$

where the symbol [,] denotes the commutator. Using the definition of the time ordering the terms I, II, III become

$$\begin{aligned}I = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\hat{X}_I(t)\big(&\hat{H}_I(t_2)\hat{H}_I(t_1)\ \Theta(t_2-t_1) \\ &+ \hat{H}_I(t_1)\hat{H}_I(t_2)\ \Theta(t_1-t_2)\big)\hat{X}_I(0)|u_l^0\rangle \quad (4.31)\end{aligned}$$

$$\begin{aligned}II &= \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\big(\hat{H}_I(t_2)\hat{H}_I(t_1)\ \Theta(t_2-t_1) \\ &\qquad + \hat{H}_I(t_1)\hat{H}_I(t_2)\ \Theta(t_1-t_2)\big)^\dagger\ \hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle \\ &= \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\big(\hat{H}_I(t_2)\hat{H}_I(t_1)^\dagger\ \Theta(t_2-t_1) \\ &\qquad + (\hat{H}_I(t_1)\hat{H}_I(t_2))^\dagger\ \Theta(t_1-t_2)\big)\ \hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle \\ &= \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2\int_0^t dt_1 dt_2\ \langle u_k^0|\big(\hat{H}_I(t_1)\hat{H}_I(t_2)\ \Theta(t_2-t_1) \\ &\qquad + (\hat{H}_I(t_2)\hat{H}_I(t_1))\ \Theta(t_1-t_2)\big)\ \hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle \quad (4.32)\end{aligned}$$

$$
\begin{aligned}
III &= -\left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \frac{1}{2}\ \big(\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)\big) \\
&\qquad + \frac{1}{2}\ \big(\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)\big)|u_l^0\rangle \\
&= -\left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \Big(\frac{1}{2}\big(\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)\big) \\
&\quad \big(\Theta(t_2-t_1)+\Theta(t_1-t_2)\big)\Big) + \Big(\frac{1}{2}\big(\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)\big) \\
&\quad \big(\Theta(t_2-t_1)+\Theta(t_1-t_2)\big)\Big)|u_l^0\rangle. \qquad (4.33)
\end{aligned}
$$

Adding I, II, III together we obtain

$$
\begin{aligned}
I{+}II{+}III = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \Big(& \underbrace{\hat{X}_I(t)\hat{H}_I(t_2)\hat{H}_I(t_1)\hat{X}_I(0)\Theta(t_2-t_1)}_{a} \\
+ \underbrace{\hat{X}_I(t)\hat{H}_I(t_1)\hat{H}_I(t_2)\hat{X}_I(0)\Theta(t_1-t_2)}_{b} & + \underbrace{\hat{H}_I(t_1)\hat{H}_I(t_2)\hat{X}_I(t)\hat{X}_I(0)\Theta(t_2-t_1)}_{c} \\
+ \underbrace{\hat{H}_I(t_2)\hat{H}_I(t_1)\hat{X}_I(t)\hat{X}_I(0)\Theta(t_1-t_2)}_{d} & - \underbrace{\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_1)\hat{X}_I(0)\Theta(t_2-t_1)}_{c'} \\
- \underbrace{\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)\Theta(t_1-t_2)}_{b'} & - \underbrace{\hat{H}_I(t_2)\hat{X}_I(t)\hat{H}_I(t_1)\hat{X}_I(0)\Theta(t_1-t_2)}_{d'} \\
& - \underbrace{\hat{H}_I(t_2)\hat{X}_I(t)\hat{H}_I(t_1)\hat{X}_I(0)\Theta(t_2-t_1)}_{a'} \Big)|u_l^0\rangle, \qquad (4.34)
\end{aligned}
$$

where we used that

$$
\begin{aligned}
\hat{H}_I(t_1)\hat{X}_I(t)\hat{H}_I(t_2)\hat{X}_I(0)(\Theta(t_2{-}t_1){+}\Theta(t_1{-}t_2)) &= \hat{H}_I(t_2)\hat{X}_I(t)\hat{H}_I(t_1)\hat{X}_I(0) \\
(\Theta(t_1-t_2)+\Theta(t_2-t_1)). \qquad (4.35)
\end{aligned}
$$

Adding together a, a', b, b', c, c' and d, d' separately we obtain

$$
\begin{aligned}
I{+}II{+}III = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \Big(& \big[\hat{X}_I(t), \hat{H}_I(t_2)\big]\hat{H}_I(t_1)\hat{X}_I(0)\Theta(t_2{-}t_1) \\
& + \hat{H}_I(t_1)\big[\hat{H}_I(t_2), \hat{X}_I(t)\big]\hat{X}_I(0)\Theta(t_2-t_1) \\
& + \hat{H}_I(t_2)\big[\hat{H}_I(t_1), \hat{X}_I(t)\big]\hat{X}_I(0)\Theta(t_1-t_2) \\
& + \big[\hat{X}_I(t), \hat{H}_I(t_1)\big]\hat{H}_I(t_2)\hat{X}_I(0)\Theta(t_1-t_2)\Big)|u_l^0\rangle. \qquad (4.36)
\end{aligned}
$$

This can be rewritten as

$$I + II + III = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \Bigg(\Big(\big[\hat{X}_I(t), \hat{H}_I(t_2)\big] \hat{H}_I(t_1) \hat{X}_I(0) - \hat{H}_I(t_1) \big[\hat{X}_I(t), \hat{H}_I(t_2)\big] \hat{X}_I(0) \Big) \ \Theta(t_2 - t_1) + \Big(\hat{H}_I(t_2) \big[\hat{H}_I(t_1), \hat{X}_I(t)\big] \hat{X}_I(0)\big) \big[\hat{H}_I(t_2), \hat{X}_I(t)\big] \hat{H}_I(t_1) \hat{X}_I(0) \Big) \ \Theta(t_1 - t_2) \Bigg) |u_l^0\rangle \quad (4.37)$$

and further simplified to

$$I + II + III = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \Bigg(\Big[\big[\hat{X}_I(t), \hat{H}_I(t_2)\big], \hat{H}_I(t_1) \Big] \hat{X}_I(0) \ \Theta(t_2 - t_1) + \Big[\hat{H}_I(t_2), \big[\hat{H}_I(t_1), \hat{X}_I(t)\big] \Big] \hat{X}_I(0) \ \Theta(t_1 - t_2) \Bigg) |u_l^0\rangle. \quad (4.38)$$

Since $\big[\hat{H}_I(t_2), \big[\hat{H}_I(t_1), \hat{X}_I(t)\big]\big] = \big[\big[\hat{X}_I(t), \hat{H}_I(t_1)\big], \hat{H}_I(t_2)\big]$ we recognize the definition for the time ordering operator and obtain

$$I+II+III = \left(\frac{i\lambda}{\sqrt{2}\hbar}\right)^2 \int_0^t dt_1 dt_2 \ \langle u_k^0| \hat{T} \Big(\big[\big[\hat{X}_I(t), \hat{H}_I(t_2)\big], \hat{H}_I(t_1)\big] \Big) \hat{X}(0) |u_l^0\rangle. \quad (4.39)$$

Using the symmetry of the time ordering

$$\begin{aligned} \int_0^t dt_2 \int_0^{t_2} dt_1 \hat{H}(t_2)\hat{H}(t_1) &= \int_0^t du_1 \int_{u_1}^t du_2 \hat{H}(u_2)\hat{H}(u_1) \\ &= \frac{1}{2} \int_0^t dt_2 dt_1 \big(\hat{H}(t_2)\hat{H}(t_1)\Theta(t_2 - t_1) \\ &\qquad + \hat{H}(t_1)\hat{H}(t_2)\Theta(t_1 - t_2) \big), \end{aligned} \quad (4.40)$$

we obtain for the sum

$$I + II + III = \left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt_2 \int_0^{t_2} dt_1 \ \langle u_k^0| \Big[\big[\hat{X}_I(t), \hat{H}_I(t_2)\big], \hat{H}_I(t_1) \Big] \hat{X}(0) |u_l^0\rangle. \quad (4.41)$$

Thus we have to second order perturbation theory $\mathcal{O}(\lambda^2)$ for the correlator $\langle u_k^0 | \hat{X}(t)\hat{X}(0) | u_l^0 \rangle$ the following expression

$$\langle u_k^0|\hat{X}(t)\hat{X}(0)|u_l^0\rangle \approx \langle u_k^0|\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle + \left(\frac{i\lambda}{\hbar}\right)\int_0^t dt_1\ \langle u_k^0|\big[\hat{H}_I(t_2),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle + \left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_k^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_l^0\rangle. \quad (4.42)$$

We therefore obtained a general expression that is valid for all states $|u_l^0\rangle, |u_k^0\rangle$. Plugging this expression into (4.18) while choosing the appropriate states we obtain the expression for the vacuum to vacuum correlator

$$\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle \approx \underbrace{\langle u_0^0|\hat{X}_I(t)\hat{X}_I(0)|u_0^0\rangle}_{1} + \underbrace{\left(\frac{i\lambda}{\hbar}\right)\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle}_{2} + \underbrace{\lambda\sum_{l\neq 0} a_{l0}^1\ \langle u_0^0|\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle}_{3} + \underbrace{\lambda\sum_{k\neq 0}(a_{l0}^1)^*\ \langle u_k^0|\hat{X}_I(t)\hat{X}_I(0)|u_0^0\rangle}_{4} + \underbrace{\lambda^2\sum_{l\neq 0} a_{l0}^2\ \langle u_0^0|\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle}_{5} + \underbrace{\lambda^2\sum_{k\neq 0}(a_{k0}^2)^*\ \langle u_k^0|\hat{X}_I(t)\hat{X}_I(0)|u_0^0\rangle}_{6} + \underbrace{\lambda^2\sum_{k,l\neq 0} a_{l0}^1\ (a_{k0}^1)^*\ \langle u_k^0|\hat{X}_I(t)\hat{X}_I(0)|u_l^0\rangle}_{7} + \underbrace{\left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle}_{8} + \underbrace{\left(\frac{i\lambda^2}{\hbar}\right)\sum_{k\neq 0}(a_{k0}^1)^*\int_0^t dt_1\ \langle u_k^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle}_{9} + \underbrace{\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_0^0\rangle}_{10}. \quad (4.43)$$

In order to simplify this expression we remind again of expression (4.18), which was the full correlator (propagated with the full Hamiltonian) up to second order perturbation theory. Furthermore we pose here a restriction on the generality of the considered expression. We require the unperturbed System to be time reversal invariant. This ensures that the coefficients $a_{kl} = a_{lk}$ are symmetric. Furthermore we require that the unperturbed Hamiltonian will deliver linear Heisenberg equations of motion ensuring the commutator $[\hat{X}_I(t), \hat{X}_I(0)]$ to be a $\mathbb{C}$-number. Since the full correlator $S(t) = \langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle$ is a complex number we have

$$2i\ \mathrm{Im}S(t) \quad = \quad \langle\Phi_0|[\hat{X}(t), \hat{X}(0)]|\Phi_0\rangle. \tag{4.44}$$

The same relation holds for $\mathrm{Im}\langle\Phi_0|\hat{X}_I(t)\hat{X}_I(0)|\Phi_0\rangle$. If we now write (4.18) propagated with the unperturbed Hamiltonian $\hat{H}_0$ we get

$$\begin{aligned}\langle\Phi_0|\hat{X}_I(t)\hat{X}_I(0)|\Phi_0\rangle &= \langle u_0^0|\hat{X}_I(t)\hat{X}_I(0)|u_0^0\rangle \\ &+ \text{ terms of structure } \big(\langle u_l^0|\hat{X}_I(t)\hat{X}_I(0)|u_k^0\rangle\big).\end{aligned} \tag{4.45}$$

We now consider

$$\begin{aligned}\mathrm{Im}\langle\Phi_0|\hat{X}_I(t)\hat{X}_I(0)|\Phi_0\rangle &= \frac{1}{2i}\ \langle\Phi_0|[\hat{X}_I(t), \hat{X}_I(0)]|\Phi_0\rangle \\ &= \frac{1}{2i}\ \langle u_0^0|[\hat{X}_I(t), \hat{X}_I(0)]|u_0^0\rangle + \text{ terms.}\end{aligned} \tag{4.46}$$

If as we mentioned above the commutator

$$[\hat{X}_I(t), \hat{X}_I(0)] = c \in \mathbb{C} \Rightarrow (c/2i)\ \underbrace{\langle\Phi_0|\Phi_0\rangle}_{1} = (c/2i)\ \underbrace{\langle u_0^0|u_0^0\rangle}_{1} + \text{terms.} \tag{4.47}$$

From this we can conclude that only the first term contributes and all other disappear if we take the imaginary part. Thus if we take the imaginary part in (4.43) we see that $\mathrm{Im}(3, 4, 5, 6, 7) = 0$ because these terms originate from $\langle u_0^0|[\hat{X}_I(t), \hat{X}_I(0)]|u_0^0\rangle$. Therefore we obtain for the imaginary part of the

correlator

$$
\begin{aligned}
S_1(t) &= \mathrm{Im}\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle = \frac{1}{2i}\langle\Phi_0|[\hat{X}(t),\hat{X}(0)]|\Phi_0\rangle \\
&\approx \frac{1}{2i}\langle u_0^0|[\hat{X}_I(t),\hat{X}_I(0)]|u_0^0\rangle + \mathrm{Im}\Big(\Big(\frac{i\lambda}{\hbar}\Big)\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle\Big) \\
&\quad + \underbrace{\mathrm{Im}\Big(\Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle\Big)}_{\alpha} \\
&\quad + \underbrace{\mathrm{Im}\Big(\Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{k\neq 0} (a_{k0}^1)^*\int_0^t dt_1\ \langle u_k^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle\Big)}_{\beta} \\
&\quad + \mathrm{Im}\Big(\Big(\frac{i\lambda}{\hbar}\Big)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_0^0\rangle\Big) \qquad (4.48)
\end{aligned}
$$

We simplify the sum $\alpha+\beta$

$$
\begin{aligned}
\alpha+\beta &= \Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle \\
&\quad + \Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{k\neq 0}(a_{k0}^1)^*\int_0^t dt_1\ \langle u_k^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle \\
&= \Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_l^0\rangle \\
&\quad + \Big(\frac{i\lambda^2}{\hbar}\Big)\sum_{k\neq 0}(a_{k0}^1)^*\int_0^t dt_1 \\
&\qquad\qquad \Big(\langle u_0^0|\hat{X}_I^\dagger(0)\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]^\dagger|u_k^0\rangle\Big)^*. \qquad (4.49)
\end{aligned}
$$

Since $\big(\langle u_0^0|\hat{X}_I^\dagger(0)\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]^\dagger|u_k^0\rangle\big)^* = \big(\langle u_0^0|\hat{X}_I(0)\big[\hat{X}_I(t),\hat{H}_I(t_1)\big]|u_k^0\rangle\big)^*$,

we obtain for the sum

$$\begin{aligned}
\alpha+\beta &= \left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a^1_{l0}\int_0^t dt_1\ \langle u^0_0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u^0_l\rangle \\
&\quad -\left(\frac{i\lambda^2}{\hbar}\right)\Big(\sum_{k\neq 0} a^1_{k0}\int_0^t dt_1\ \langle u^0_k|\hat{X}_I(0)\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]|u^0_0\rangle\Big)^* \\
&= \left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a^1_{l0}\int_0^t dt_1\ \langle u^0_0|\big[\underbrace{\hat{H}_I(t_1),\hat{X}_I(t)}_{\hat{A}}\big]\underbrace{\hat{X}_I(0)}_{\hat{B}}|u^0_l\rangle \\
&\quad +\Big(\left(\frac{i\lambda^2}{\hbar}\right)\sum_{k\neq 0} a^1_{k0}\int_0^t dt_1 \\
&\qquad\qquad \langle u^0_0|\underbrace{\hat{X}_I(0)}_{\hat{B}}\big[\underbrace{\hat{H}_I(t_1),\hat{X}_I(t)}_{\hat{A}}\big]|u^0_k\rangle\Big)^*. \qquad (4.50)
\end{aligned}$$

Using now the relations

$$\begin{aligned}
(i\langle 0|\hat{A}\hat{B}|l\rangle)+(i\langle 0|\hat{A}\hat{B}|l\rangle)^* &= (i\langle 0|\hat{A}\hat{B}|l\rangle)+(i\langle 0|[\hat{A},\hat{B}]|l\rangle+i\langle 0|\hat{A}\hat{B}|l\rangle)^* \\
&= \underbrace{(i\langle 0|\hat{A}\hat{B}|l\rangle)}_{z}+\underbrace{(i\langle 0|\hat{A}\hat{B}|l\rangle)^*}_{z^*} \\
&\quad +(i\langle 0|[\hat{B},\hat{A}]|l\rangle)^* \qquad (4.51)
\end{aligned}$$

and the well-known fact that $\mathrm{Im}\ z+\mathrm{Im}\ z^*=0$ we get

$$\mathrm{Im}\big((i\langle 0|\hat{A}\hat{B}|l\rangle)+(i\langle 0|\hat{A}\hat{B}|l\rangle)^*\big)=\mathrm{Im}(i\langle 0|[\hat{B},\hat{A}]|l\rangle)^*. \qquad (4.52)$$

Putting everything together we obtain for the imaginary part of $\alpha+\beta$ in (4.48)

$$\begin{aligned}
\mathrm{Im}(\alpha+\beta) &= \mathrm{Im}\Big(\left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a^1_{l0}\int_0^t dt_1\ \langle u^0_0|\big[\hat{X}_I(0),\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\big]|u^0_l\rangle\Big)^* \\
&= \mathrm{Im}\Big(\left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a^1_{l0}\int_0^t dt_1 \\
&\qquad\qquad \langle u^0_0|\big[\big[\hat{H}_I(t_1),\hat{X}_I(t)\big],\hat{X}_I(0)\big]|u^0_l\rangle\Big). \qquad (4.53)
\end{aligned}$$

Thus we finally obtain

$$
\begin{aligned}
S_1(t) &= \mathrm{Im}\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle = \frac{1}{2i}\langle\Phi_0|[\hat{X}(t)\hat{X}(0)]|\Phi_0\rangle \\
&\approx \frac{1}{2i}\langle u_0^0|[\hat{X}_I(t),\hat{X}_I(0)]|u_0^0\rangle + \mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle\Bigg) \\
&\quad + \mathrm{Im}\Bigg(\left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\big[\hat{H}_I(t_1),\hat{X}_I(t)\big],\hat{X}_I(0)\big]|u_l^0\rangle\Bigg) \\
&\quad + \mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_0^0\rangle\Bigg).
\end{aligned}
\tag{4.54}
$$

This expression is generally valid up to second order perturbation theory and does not depend on the particular form of $\hat{H}_0$ and $\hat{H}_I$. The only restrictions we forced upon the model was that the commutator $[\hat{X}(t),\hat{X}(0)]$ is a $\mathbb{C}$-number and that the coefficients a_{kl}^1 are symmetric, which implies time reversal invariance of the model.

4.2 Comparison with the integrable case

We are now in a position where we can attack with the help of (4.54) the extraction of information regarding collective motion. More explicitly we are interested in the recognition of spreading in this perturbative framework when the Hamiltonian is not integrable anymore. The immediate problem with an expression like (4.54) is that it is not obvious which parts contain the information regarding spreading. It is therefore helpful to test this approach with a known model. Such a testing ground is provided by the Caldeira-Leggett model (see Appendix B) . In this particular case we know what to expect and this is of decisive support for the recognition of the spreading in a perturbative framework. Thus the first term in (4.54) becomes

$$
\begin{aligned}
\frac{1}{2i}\langle u_0^0|[\hat{X}_I(t),\hat{X}_I(0)]|u_0^0\rangle &= \frac{1}{2i}\langle 0_E|\langle 0_S|[\hat{X}_I(t),\hat{X}_I(0)]|0_S\rangle|0_E\rangle \\
&= \frac{1}{2i}\langle 0_S|[\hat{X}_I(t),\hat{X}_I(0)]|0_S\rangle,
\end{aligned}
\tag{4.55}
$$

where $|0_S\rangle, |0_E\rangle$ describe the ground state of the system

$$
\hat{H}_S = \frac{\hat{P}^2}{2M} + \frac{M\Omega}{2}\hat{X}^2 \tag{4.56}
$$

and the environment

$$
\hat{H}_E = \sum_k \left(\frac{\hat{p}_k^2}{2m} + \frac{m\omega_k^2\hat{q}_k^2}{2}\right) \tag{4.57}
$$

respectively. With this the commutator becomes

$$[\hat{X}_I(t), \hat{X}_I(0)] = \left[\exp\left(\frac{i}{\hbar}\hat{H}_S t\right)\hat{X}(0)\exp\left(-\frac{i}{\hbar}\hat{H}_S t\right), \hat{X}_I(0)\right], \tag{4.58}$$

where the time propagation is given by

$$\hat{X}(t) = \hat{X}(0)\cos(\Omega t) + \frac{\hat{P}(0)}{M\Omega}\sin(\Omega t). \tag{4.59}$$

Using this we obtain

$$\frac{1}{2i}\langle 0_S|[\hat{X}_I(t), \hat{X}_I(0)]|0_S\rangle = -\frac{\hbar}{2M\Omega}\sin(\Omega t). \tag{4.60}$$

For the term

$$\mathrm{Im}\left(\left(\frac{i\lambda}{\hbar}\right) \int_0^t dt_1 \ \langle u_0^0|\big[\hat{H}_I(t_1), \hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle \right) \tag{4.61}$$

we need to calculate the commutator

$$\big[\hat{H}_I(t_1), \hat{X}_I(t)\big] = \sum_i c_i \hat{q}_i(t_1)[\hat{X}(t_1), \hat{X}(t)], \tag{4.62}$$

where we used that

$$\hat{H}_I(t_1) = \exp\left(\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t_1\right)\hat{H}_1(0)\exp\left(-\frac{i}{\hbar}(\hat{H}_S + \hat{H}_E)t_1\right) \tag{4.63}$$

and

$$\hat{X}_I(t) = \exp\left(\frac{i}{\hbar}\hat{H}_S t\right)\hat{X}(0)\exp\left(-\frac{i}{\hbar}\hat{H}_S t\right) \tag{4.64}$$

with

$$\hat{H}_1 = \hat{X}\sum_k c_k \hat{q}_k. \tag{4.65}$$

Using (4.60) we obtain for (4.61)

$$\mathrm{Im}\left(\left(\frac{\lambda}{M\Omega}\right) \int_0^t dt_1 \ \sin(\Omega(t_1 - t))\langle 0_S|\hat{X}(0)|0_S\rangle \right) = 0 \tag{4.66}$$

since for the harmonic oscillator we have $\langle 0_S|\hat{X}(0)|0_S\rangle = 0$. A similar argument can be pushed forward for the term

$$\mathrm{Im}\left(\left(\frac{i\lambda^2}{\hbar}\right) \sum_{l\neq 0} a_{l0}^1 \int_0^t dt_1 \ \langle u_0^0|\big[\big[\hat{H}_I(t_1), \hat{X}_I(t)\big], \hat{X}_I(0)\big]|u_l^0\rangle \right). \tag{4.67}$$

We notice that for the commutator under the integral we obtain

$$\begin{aligned}\big[\big[\hat{H}_I(t_1),\hat{X}_I(t)\big],\hat{X}_I(0)\big] &= \big[\sum_i c_i\hat{q}_i(t_1)\underbrace{\big[\hat{X}(t_1),\hat{X}(t)\big]}_{-\frac{i\hbar}{M\Omega}\sin(\Omega(t_1-t))},\hat{X}(0)\big] \quad (4.68)\\ &= -\frac{i\hbar}{M\Omega}\sin(\Omega(t_1-t))\sum_i c_i\big[\hat{q}_i(t_1),\hat{X}(0)\big]\\ &= 0, \quad (4.69)\end{aligned}$$

because $\hat{q}_i(t_1)$ and $\hat{X}(0)$ commute with each other. We thus see that (4.67) disappears as well. At this point we turn to the last term in (4.54)

$$\mathrm{Im}\bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_0^0\rangle\bigg), \quad (4.70)$$

which we need to evaluate the interaction term $\hat{H}_1=\hat{X}\sum_k c_k\hat{q}_k$. This gives

$$\begin{aligned}&\mathrm{Im}\bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{X}(t_2)\sum_k c_k\hat{q}_k(t_2)\big],\\ &\qquad\qquad \hat{X}(t_1)\sum_k c_k\hat{q}_k(t_1)\Big]\hat{X}(0)|u_0^0\rangle\bigg)\\ &=\mathrm{Im}\bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\sum_k c_k\hat{q}_k(t_2)\big[\hat{X}(t),\hat{X}(t_2)\big],\\ &\qquad\qquad \hat{X}(t_1)\sum_k c_k\hat{q}_k(t_1)\Big]\hat{X}(0)|u_0^0\rangle\bigg), \quad (4.71)\end{aligned}$$

where we use the previous result for the commutator

$$\big[\hat{X}(t),\hat{X}(t_2)\big]=-\frac{i\hbar}{M\Omega}\sin(\Omega(t-t_2)) \quad (4.72)$$

and obtain

$$\begin{aligned}&\mathrm{Im}\bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \frac{(-i\hbar)}{M\Omega}\sin(\Omega(t-t_2))\\ &\qquad\langle u_0^0|\bigg(\big[\sum_k c_k\hat{q}_k(t_2),\hat{X}(t_1)\big]\sum_k c_k\hat{q}_k(t_1)\\ &\qquad+\hat{X}(t_1)\big[\sum_k c_k\hat{q}_k(t_2),\sum_k c_k\hat{q}_k(t_1)\big]\bigg)\hat{X}(0)|u_0^0\rangle\bigg). \quad (4.73)\end{aligned}$$

In the upper expression we also used that $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$. Since $[\hat{q}_k(t_2), \hat{X}(t_1)] = 0$ this reduces to

$$\mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt_2 \int_0^{t_2} dt_1 \; \frac{(-i\hbar)}{M\Omega} \sin(\Omega(t-t_2)) \sum_k c_k^2 \; \langle u_0^0 | \hat{X}(t_1) \big[\hat{q}_k(t_2), \hat{q}_k(t_1)\big] \hat{X}(0) | u_0^0 \rangle \Bigg). \quad (4.74)$$

Inserting

$$\big[\hat{q}_k(t_2), \hat{q}_k(t_1)\big] = -\frac{i\hbar}{m\omega_k} \sin(\omega_k(t_2 - t_1)) \quad (4.75)$$

and

$$\langle 0_S | \hat{X}(t_1) \hat{X}(0) | 0_S \rangle = \frac{\hbar}{2M\Omega} \exp(-i\Omega t_1) \quad (4.76)$$

leads then to

$$\mathrm{Im}\Bigg(\frac{1}{2} \left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2 \hbar}{m\omega_k} \int_0^t dt_2 \int_0^{t_2} dt_1 \; \sin(\omega_k(t_2 - t_1)) \sin(\Omega(t - t_2)) \exp(-i\Omega t_1) \Bigg). \quad (4.77)$$

After performing the time integrations we obtain

$$\begin{aligned} \mathrm{Im}\Bigg(-\frac{1}{8} \left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2 \hbar}{m\omega_k} \Bigg(& -\frac{2\omega_k}{\Omega(\Omega^2 - \omega_k^2)} \sin(\Omega t) \\ & + \frac{2}{(\Omega^2 - \omega_k^2)} \sin(\omega_k t) + \frac{2\omega_k}{(\Omega^2 - \omega_k^2)} \; t \cos(\Omega t) \\ & + \left(\frac{1}{(\Omega + \omega_k)^2} + \frac{1}{(\Omega - \omega_k)^2} \right) \sin(\omega_k t) \\ & + \left(\frac{1}{(\Omega + \omega_k)^2} - \frac{1}{(\Omega - \omega_k)^2} \right) \sin(\Omega t) \Bigg), \end{aligned} \quad (4.78)$$

which after taking the imaginary part provides us with

$$-\frac{1}{8} \left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2 \hbar}{m\omega_k} \Bigg(\frac{4\Omega^2}{(\Omega^2 - \omega_k^2)^2} \sin(\omega_k t) + \frac{2\omega_k^3 - 6\Omega^2 \omega_k}{\Omega(\Omega^2 - \omega_k^2)^2} \; \sin(\Omega t) + \frac{2\omega_k}{(\Omega^2 - \omega_k^2)} \; t \cos(\Omega t) \Bigg). \quad (4.79)$$

Putting (4.60) and (4.79) together we obtain for the imaginary part of the correlation function for the Caldeira-Leggett Hamiltonian up to $\mathcal{O}(\lambda^2)$

$$S_1(t) \approx \frac{1}{2i}\langle u_0^0|[\hat{X}_I(t),\hat{X}_I(0)]|u_0^0\rangle + \mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt_2 \int_0^{t_2} dt_1 \ \langle u_0^0| \Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big] \hat{X}(0)|u_0^0\rangle \Bigg), \quad (4.80)$$

which explicitly takes the form

$$S_1(t) \approx -\frac{\hbar}{2M\Omega}\sin(\Omega t) - \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\Bigg(\frac{4\Omega^2}{(\Omega^2-\omega_k^2)^2}\sin(\omega_k t) + \frac{2\omega_k^3 - 6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\ \sin(\Omega t) + \frac{2\omega_k}{(\Omega^2-\omega_k^2)}\ t\cos(\Omega t)\Bigg). \quad (4.81)$$

In this expression it is still not easy to extract the information regarding the spreading. The first term describes the free particle oscillating. The spreading has to be extracted from the other terms. For a more detailed investigation of this issue we switch to the frequency domain. From (4.81) we obtain

$$\tilde{S}(\omega) = \frac{\hbar}{2M\Omega}\delta(\Omega-\omega) + \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_n \frac{\hbar c_n^2}{m\omega_n}\Bigg(\left(\frac{2\omega_n^3 - 6\Omega^2\omega_n}{\Omega(\Omega^2-\omega_n^2)^2}\right)\delta(\Omega-\omega) - \frac{2\omega_n}{(\Omega^2-\omega_n^2)}\frac{\partial}{\partial\omega}\delta(\Omega-\omega)\Bigg) + \frac{\lambda^2}{2M^2}\sum_n \frac{\hbar c_n^2}{m\omega_n}\frac{\delta(\omega_n-\omega)}{(\Omega^2-\omega_n^2)^2}, \quad (4.82)$$

where we put the explicit calculation into Appendix C. In order to recognize the physical meaning of the different terms in (4.82) we re-derive the expression from a different point of view since it can also be obtained from

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\big((\Omega^2-\gamma(0)) - (\omega+i\epsilon)^2 - i(\omega+i\epsilon)\tilde{\gamma}(\omega+i\epsilon)\big)^{-1}, \quad (4.83)$$

as demonstrated in Appendix D. Here

$$\tilde{\gamma}(\omega+i\epsilon) = \int_0^\infty \gamma(s)\exp(i(\omega+i\epsilon)s)ds \quad (4.84)$$

encodes the information regarding the damping kernel and $\gamma(s)$ is given by

$$\gamma(s) = \frac{2}{M}\int_0^\infty d\omega \frac{\sigma(\omega)}{\omega}\cos(\omega s), \quad (4.85)$$

where the spectral density

$$\sigma(\omega) = \sum_n \frac{c_n^2}{2m\omega_n}\delta(\omega - \omega_n). \tag{4.86}$$

was taken into account. From this it follows that

$$\gamma(0) = \frac{1}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}. \tag{4.87}$$

which is of singular nature when performing a continuum limit for the frequencies as required in the Caldeira-Leggett case. From the calculation in Appendix D it can thus be seen that the last term in (4.82) encodes the information connected with $\tilde{\gamma}(\omega + i\epsilon)$ which in turn is the Fourier transform of

$$-\frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\frac{4\Omega^2}{(\Omega^2 - \omega_k^2)^2}\sin(\omega_k t) \tag{4.88}$$

in expression (4.81). The second and third term in (4.82) are connected with $\gamma(0)$. The first term just corresponds to free oscillation. In order to reproduce (perturbatively) the results of quantum Brownian motion (a kernel without memory) one has to perform an averaging along the lines of Caldeira-Leggett [30], where our spectral $\sigma(\omega)$ density takes the form

$$\sigma(\omega) = \frac{M\gamma\omega}{\pi}, \tag{4.89}$$

with $\tilde{\gamma}(\omega + i\epsilon) = \gamma$ being a damping constant which also originates from the above spectral density. We will not demonstrate the details of the exact averaging procedure since it was our task to connect the different terms of the perturbation series (4.82) with the spreading and dynamics encoding quantity $\tilde{\gamma}(\omega + i\epsilon)$ in a perturbative framework of the Caldeira-Leggett model. The reason for this was to test our developed formalism for a well understood model in order to apply it to a non-integrable setup with a noninteracting system as starting point for the perturbative expansion.

4.3 Beyond the integrable case

In order to investigate collective motion in a bound system using our perturbative expression

$$\begin{aligned} S_1(t) &= \mathrm{Im}\langle\Phi_0|\hat{X}(t)\hat{X}(0)|\Phi_0\rangle = \frac{1}{2i}\langle\Phi_0|[\hat{X}(t)\hat{X}(0)]|\Phi_0\rangle \\ &\approx \frac{1}{2i}\langle u_0^0|[\hat{X}_I(t),\hat{X}_I(0)]|u_0^0\rangle + \mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)\int_0^t dt_1\ \langle u_0^0|\big[\hat{H}_I(t_1),\hat{X}_I(t)\big]\hat{X}_I(0)|u_0^0\rangle\Bigg) \\ &\quad + \mathrm{Im}\Bigg(\left(\frac{i\lambda^2}{\hbar}\right)\sum_{l\neq 0} a_{l0}^1\int_0^t dt_1\ \langle u_0^0|\big[\big[\hat{H}_I(t_1),\hat{X}_I(t)\big],\hat{X}_I(0)\big]|u_l^0\rangle\Bigg) \\ &\quad + \mathrm{Im}\Bigg(\left(\frac{i\lambda}{\hbar}\right)^2\int_0^t dt_2\int_0^{t_2} dt_1\ \langle u_0^0|\Big[\big[\hat{X}_I(t),\hat{H}_I(t_2)\big],\hat{H}_I(t_1)\Big]\hat{X}(0)|u_0^0\rangle\Bigg). \end{aligned} \tag{4.90}$$

we also have to chose an appropriate interaction that is still sufficiently complicated and describes a bounded system. We already specified the system to be

$$H = H_0 + \lambda H_1, \tag{4.91}$$

where $H_0 = H_0^{(1)} + H_0^{(2)} + H_0^{(12)}$ is the integrable Hamiltonian with (4.2) and (4.3). One can chose an interaction of the form

$$H_1 = \sum_n a_n\ f^n(\{x_i^{(1)}\},\{x_j^{(2)}\}) \tag{4.92}$$

which is a polynomial with coefficients a_n. This interaction makes the system non-integrable. In order to investigate the contributions in our perturbation series of such an interaction it is necessary to bring it into a form that reflects the coupling of the Collective coordinate with the remaining degrees of freedom. For this to happen the center of mass coordinates of the two clouds have to decouple from the other degrees of freedom. Therefore we chose a translational invariant potential

$$f^n(\{x_i^{(1)}\},\{x_j^{(2)}\}) = \sum_{ij}(x_i^{(1)} - x_j^{(2)})^n. \tag{4.93}$$

With this property we can cast

$$H_1 = \sum_{ijn} a_n\ (x_i^{(1)} - x_j^{(2)})^n \tag{4.94}$$

into the form

$$H_1 = \sum_n X^n F_n\left(\{d_i^{(1)}\},\{d_i^{(2)}\}\right), \tag{4.95}$$

where X is the collective coordinate and $F_n(\{d_i^{(1)}\}, \{d_i^{(2)}\})$ are polynomials of the single particle degrees of freedom of $H_0^{(1)}$ and $H_0^{(2)}$ respectively which decouple from X^n. While it is possible to perform such a transformation it will result in a much more complicated expression for the Interaction term $\hat{H}_1$ to be inserted into (4.90) than in the case of Caldeira-Leggett that we analyzed previously. This means that the already elaborate evaluation of (4.90) in the Caldeira-Leggett case will be much more complicated for the interaction (4.92) and only be feasible with further approximations. Fortunately, while in principle possible to follow this path it turns out that there is a much more illuminating approach for the general coherent physical picture. Instead of performing a perturbative analysis up to second order in λ with the mapped Hamiltonian (4.95) it turns out that we only have to study perturbations up to linear order to extract corrections of the spreading in a non-integrable setup if we introduce a renormalization of $\hat{H}_0$. This will be presented in the next chapter.

Chapter 5

Perturbation theory to linear order

We derived a general expression for the correlator $S(t)$ which is valid up to second order perturbation theory for a very general class of Hamiltonians. In order to expand our investigation from the integrable into the non-integrable regime we will have to chose an appropriate starting point for the perturbative analysis. For the investigation of collective dynamics in quantum many-body systems in our perturbative framework there are two approaches which are quite natural. The first choice is to start from the Hamiltonian H, map it to generalized Caldeira-Leggett-form (i.e. coupling of collective coordinate with remaining degrees of freedom) and start to evaluate the correlator perturbatively. This approach contains immediate complications on a technical level (the calculations become very extensive). These calculations even dwarf the level of complexity that our example with the integrable Caldeira-Leggett model had in stock for us, where the analysis of $S(t)$ was already rather elaborate. But as we already mentioned it is sufficient to go only up to linear order perturbation theory and therefore to avoid problems that arise from mapping the non-integrable H_1 to Caldeira-Leggett form altogether.

It will become evident that we can avoid all technical complications in such an approach and get a much clearer picture of what is going on on a physical level if we perform a renormalization of H_0. Furthermore in such a framework we obtain a beautiful connection to classical physics. Here we specify the form of the interaction. In order to obtain a bounded model we chose the interaction

$$H_1 = \sum_{i,j=1}^{N} f(x_i^{(1)} - x_i^{(2)}), \tag{5.1}$$

with f being a positive and even analytical function of the form

$$f(x) = \sum_{n=2}^{\infty} f_n x^{2n} \ . \tag{5.2}$$

To leading order λ in perturbation theory, we obtain the following expression for the correlator

$$\begin{aligned} S(t) \approx & \langle 0|\hat{X}_I(t)\hat{X}_I(0)|0\rangle \\ & + \lambda \sum_{l\neq 0} \left(a^1_{l0} \langle 0|\hat{X}_I(t)\hat{X}_I(0)|l\rangle + (a^1_{l0})^* \langle l|\hat{X}_I(t)\hat{X}_I(0)|0\rangle \right) \\ & + \frac{i\lambda}{\hbar} \int_0^t dt_1 \langle 0|[H_{1I}(t_1), \hat{X}_I(t)]\hat{X}_I(0)|0\rangle + \mathcal{O}(\lambda^2) \ , \end{aligned} \tag{5.3}$$

where the sum runs over the eigenstates $|l\rangle$ of $\hat{H}_0$, and where $|0\rangle$ is the ground state of $\hat{H}_0$. The coefficients $a^1_{l0} = \langle l|\hat{H}_1|0\rangle/(E_0 - E_l)$ turn out to be real due to time reversal invariance. The sum in Eq. (5.3) arises from the correction to the ground state while the last term results from the perturbation of the Hamiltonian. The collective operator $\hat{X}_I$ and the non–integrable part $\hat{H}_{1I}$ of the Hamiltonian, whose time evolution is governed by the integrable Hamiltonian $\hat{H}_0$ appear in the interaction picture. For any operator $\hat{F}$, we have

$$\hat{F}_I(t) = \exp\left(\frac{i}{\hbar}\hat{H}_0 t\right) \hat{F} \exp\left(-\frac{i}{\hbar}\hat{H}_0 t\right) \ . \tag{5.4}$$

We consider the imaginary part of the correlator, $\mathrm{Im}S(t) = S_1(t)$. We notice again that, by virtue of Eq. (4.7), the Fourier transforms of $S(t)$ and $S_1(t)$ are connected through

$$\tilde{S}(\omega) = 2i\Theta(\omega)\tilde{S}_1(\omega) \ , \tag{5.5}$$

where $\Theta(\omega)$ denotes the Heaviside step function. Since $\mathrm{Im}\langle 0|\hat{X}_I(t)\hat{X}_I(0)|l\rangle$ vanishes for $l \neq 0$, the imaginary part of the correlator simplifies, and we find

$$\begin{aligned} S_1(t) \approx & \ \mathrm{Im}\langle 0|\hat{X}_I(t)\hat{X}_I(0)|0\rangle \\ & + \frac{\lambda}{2\hbar} \int_0^t dt_1 \langle 0| \left[[\hat{H}_{1I}(t_1), \hat{X}_I(t)], \hat{X}_I(0) \right] |0\rangle + \mathcal{O}(\lambda^2) \ . \end{aligned} \tag{5.6}$$

At this point, we may use our previous results from the integrable setup. The first term of Eq. (5.6) was evaluated by mapping H_0 into the form of a Caldeira–Leggett–like model, in which X can be viewed as the coordinate

of a "big" particle in a harmonic potential which is coupled to a "bath" of harmonic oscillators. The interpretation of the "bath", however, differs significantly form the standard Caldeira–Leggett situation [30]. In our case, the "bath" is not external, it is part of the system and formed by the internal degrees of freedom. The resulting expression for the spectral function $\tilde{S}(\omega)$ in that case was

$$\tilde{S}(\omega) \approx \frac{\hbar}{\pi m}\Theta(\omega)\ \mathrm{Im}\ \frac{1}{\Omega_0^2 - \omega^2 - i\omega\tilde{\gamma}(\omega)}\ , \tag{5.7}$$

where $\tilde{\gamma}$ formally coincides with the classical "damping" kernel, but here it describes the spreading of the collective excitation over the spectrum. We repeat once more that there is not an energy loss or any kind of dissipation in our system. The resonance frequency $\bar{\Omega}_0$ is the fundamental oscillator frequency of the corresponding classical problem. To illustrate this result, we mention that, when the collective degree of freedom X interacts with an ohmic "bath" (see Ref. [39]), the spreading kernel $\tilde{\gamma}(\omega) = \gamma_0$ is a constant and $\tilde{S}(\omega)$ has a Lorentzian shape with the width γ_0 at the position of the classical oscillator frequency $\bar{\Omega}_0 = \sqrt{\Omega_0^2 - (\gamma_0/2)^2}$.

Next we consider the crucial second term on the right hand side of Eq. (5.6). As we mentioned a naive continuation of the approach that was used in the integrable case quickly becomes cumbersome. Luckily, there is much better way of tackling this term which eventually leads to a new insight to our problem. The second term is easily seen to be of the form $\frac{\lambda}{2\hbar}\int_0^t dt_1\chi(t_1,t)$, with the kernel $\chi(t_1,t)$ given by

$$\chi(t_1,t) = \sum_{ij}\langle 0|\left[[f(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1)), \hat{X}(t)], \hat{X}(0)\right]|0\rangle\ . \tag{5.8}$$

The harmonic form of $\hat{H}_0$ means that $\hat{X}$ and $\hat{x}_i^{(1),(2)}$can be decomposed into a sum of eigenmodes $\hat{X} = \sum_j a_j\hat{c}_j$ and $\hat{x}_i = \sum_j b_{ji}\hat{c}_j$ we find the identity

$$[(\hat{x}_i^{(1)}(0) - \hat{x}_j^{(2)}(0))^n, \hat{X}(-t)] = n(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^{n-1}\beta_{ij}(t) \tag{5.9}$$

for the commutator of the n–th powers of differences with the collective operator. Here we used that we have for general operators $\hat{A}, \hat{B}, \hat{C}$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}] \tag{5.10}$$

and for operators $\hat{P}, \hat{Q}$

$$\begin{aligned}
[\hat{P}(t), \hat{Q}^n(0)] &= [\hat{P}(t), \hat{Q}^{n-1}(0)\hat{Q}(0)] \\
&= [\hat{P}(t), \hat{Q}^{n-1}(0)]\hat{Q}(0) + \hat{Q}^{n-1}(0)[\hat{P}(t), \hat{Q}(0)] \\
&= \underbrace{[\hat{P}(t), \mathbb{1}]\hat{Q}^3(0)}_{0} + \underbrace{3\hat{Q}^{n-1}(0)}_{\hat{Q}'(0)}[\hat{P}(t), \hat{Q}(0)],
\end{aligned} \tag{5.11}$$

where we assumed that the operator $\hat{P}(t)$ is a linear function of $\hat{P}(0)$ and $\hat{Q}(0)$.

Labeling $\hat{P}(t) = \hat{X}(t)$ and $\hat{Q}(0) = (\hat{x}_i^{(1)}(0) - \hat{x}_j^{(2)}(0))$ we define

$$[(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})(t_1), \hat{X}(t_2)] = \beta_{ij}(t_1 - t_2)\mathbf{1}, \tag{5.12}$$

where $\beta_{ij}(t_1 - t_2)$ is a function. This can be seen because we can write the commutator in normal coordinates $\hat{c}_k$ of the harmonic oscillator with

$$\hat{X}(t_2) = \sum_k^{2N} a_k \hat{c}_k(t_2) \tag{5.13}$$

and

$$\hat{x}_i^{(1)}(t_1) = \sum_k^{2N} b_{ik}\hat{c}_k(t_1),\ \hat{x}_j^{(2)}(t_1) = \sum_k^{2N} \gamma_{jk}\hat{c}_k(t_1). \tag{5.14}$$

With this we can write the commutator (5.12) as

$$\begin{aligned}\sum_k (b_{ik}a_k)\ [\hat{c}_k(t_1), \hat{c}_k(t_2)] - (\gamma_{jk}a_k)\ [\hat{c}_k(t_1), \hat{c}_k(t_2)] \\ = \sum_k (b_{ik}a_k - \gamma_{jk}a_k)[\hat{c}_k(t_1), \hat{c}_k(t_2)] = \beta_{ij}(t_1 - t_2)\end{aligned} \tag{5.15}$$

because the commutator $[\hat{c}_k(t_1), \hat{c}_k(t_2)]$ is a $\mathbb{C}$-number for the case of a harmonic oscillator. Hence we demonstrated that for all n the commutator in (5.9) can be reduced to the operator $(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^{n-1}$ multiplied with the function $\beta_{ij}(t)$ which is defined by $[(\hat{x}_i^{(1)} - \hat{x}_j^{(2)}), \hat{X}(-t)] = \beta_{ij}(t)\mathbf{1}$. We notice that the commutator in the latter expression is proportional to the unit operator $\mathbf{1}$. Applying this formula twice yields

$$\begin{aligned}\sum_{i,j} \langle 0| \left[[f(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1)), \hat{X}(t)], \hat{X}(0)\right] |0\rangle \\ = \sum_{i,j} \langle 0| \left[\big(f'(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))\beta_{ij}(t_1 - t)\big), \hat{X}(0)\right] |0\rangle \\ = \sum_{i,j} \beta_{ij}(t_1 - t)\ \langle 0| \left[\big(f'(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))\big), \hat{X}(0)\right] |0\rangle \\ = \sum_{i,j} \beta_{ij}(t_1 - t)\ \beta_{ij}(t_1)\ \langle 0|\big(f''(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))\big)|0\rangle.\end{aligned} \tag{5.16}$$

Hence we obtain

$$\chi(t_1, t) = \sum_{i,j} \beta_{ij}(t_1 - t)\beta_{ij}(t_1)C_{ij}(0)\ , \tag{5.17}$$

where the elements of the matrix C are given by the ground state expectation values involving the second derivative of the arbitrary function f defining the non–integrable part of the interaction in Eq. (5.2)

$$C_{ij} = \langle 0|f''(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})|0\rangle \ . \tag{5.18}$$

The matrix is time independent because for an operator $\hat{A}$ we have

$$\begin{aligned} \langle 0|\hat{A}(t)|0\rangle &= \langle 0| \exp\left(\frac{i\hat{H}_0 t}{\hbar}\right) \hat{A}(0) \exp\left(-\frac{i\hat{H}_0 t}{\hbar}\right)|0\rangle \\ &= \langle 0|\hat{A}(0)|0\rangle. \end{aligned} \tag{5.19}$$

For the linear term of the perturbation expansion we get

$$\frac{\lambda}{2\hbar}\int_0^t dt_1 \sum_{i,j}\ C_{ij}\ \beta_{ij}(t_1 - t)\beta_{ij}(t_1)\ . \tag{5.20}$$

We emphasize that this result is not due to an expansion of the function $f(x)$, it applies in leading order λ to all functions of the form (5.2).

We arrive at the important insight anticipated above: precisely the same equation for the kernel $\chi(t_1, t)$ follows when using the harmonic Hamiltonian

$$\hat{H}_0^{\mathrm{R}} = \hat{H}_0 + \frac{\lambda}{2}\sum_{i,j=1}^{N} C_{ij}(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2\ . \tag{5.21}$$

We demonstrate this explicitly by inserting the harmonic part into our expression for the first order perturbation correction $\frac{\lambda}{2\hbar}\int_0^t dt_1\ \chi(t_1, t)$

$$\begin{aligned} &\frac{\lambda}{2\hbar}\sum_{i,j}\langle 0|\Big[\Big[\frac{1}{2}\int_0^t dt_1\ C_{ij}\ (\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))^2, \hat{X}(t)\Big], \hat{X}(0)\Big]|0\rangle \\ &\quad = \frac{\lambda}{2\hbar}\sum_{i,j}\ \frac{1}{2}\int_0^t dt_1\ C_{ij}\ \langle 0|\big[\big[(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))^2, \hat{X}(t)\big], \hat{X}(0)\big]|0\rangle \\ &\quad = \frac{\lambda}{2\hbar}\sum_{i,j}\int_0^t dt_1\ C_{ij}\ \langle 0|\big[(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1))\beta_{ij}(t_1 - t), \hat{X}(0)\big]|0\rangle \\ &\quad = \frac{\lambda}{2\hbar}\sum_{i,j}\int_0^t dt_1\ C_{ij}\ \beta_{ij}(t_1 - t)\ \langle 0|\big[(\hat{x}_i^{(1)}(t_1) - \hat{x}_j^{(2)}(t_1)), \hat{X}(0)\big]|0\rangle \\ &\quad = \frac{\lambda}{2\hbar}\sum_{i,j}\int_0^t dt_1\ C_{ij}\ \beta_{ij}(t_1 - t)\beta_{ij}(t_1), \end{aligned} \tag{5.22}$$

which has the same form as (5.20). In other words, the effect of a general, non–integrable perturbation can, to leading order λ, be fully accounted for by a proper renormalization of the integrable Hamiltonian $\hat{H}_0$. Since the renormalized $\hat{H}_0^{\mathrm{R}}$ is harmonic, the spectral function $\tilde{S}(\omega)$ is given by Eq. (5.7), where the renormalized oscillation frequency Ω_0^{R} and the spreading kernel γ^{R} depend on the constant matrix elements C_{ij}.

The C_{ij} themselves depend on the parameters of the integrable Hamiltonian $\hat{H}_0$. We therefore have to derive an explicit expression for them. Introducing the Fourier transform of the function f'' we get

$$\begin{aligned}
C_{ij} = \langle 0|f''(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})|0\rangle &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \tilde{f}''(k) \langle 0| \exp\left(ik(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})\right)|0\rangle \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \tilde{f}''(k) \exp\left(- \frac{k^2}{2} \langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle \right) \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx f''(x) \int_{-\infty}^{\infty} dk \exp\left(ikx - \frac{k^2}{2} \langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle \right) \\
= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \frac{f''(x)}{\sqrt{\langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle}} \exp\left(- \frac{x^2}{2\langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle} \right) \\
= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du \; f''(\sqrt{\langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle}\; u) \exp\left(- \frac{u^2}{2} \right), \quad (5.23)
\end{aligned}$$

where we have used the relation $\langle \exp(-iqx) \rangle = \exp(-q^2 \langle x^2 \rangle / 2)$. The next step is to express the quantity $\alpha_{ij} := \langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})|0\rangle$ in terms of the original interaction matrices $W, \hat{K}, K$ of the unperturbed model. In order to achieve that we express our quantity in the set of coordinates that separated the center of mass coordinates and the relative coordinates

$$x_i^{(1)} = \frac{1}{\sqrt{2}} \left(\frac{x_i^{(1)} - x_i^{(2)}}{\sqrt{2}} + \frac{x_i^{(1)} + x_i^{(2)}}{\sqrt{2}} \right) = \frac{c_i^{(1)} + c_i^{(2)}}{\sqrt{2}} \quad (5.24)$$

and

$$x_j^{(2)} = \frac{1}{\sqrt{2}} \left(\frac{x_j^{(1)} + x_j^{(2)}}{\sqrt{2}} - \left(\frac{x_j^{(1)} - x_j^{(2)}}{\sqrt{2}} \right) \right) = \frac{c_j^{(2)} - c_j^{(1)}}{\sqrt{2}}. \quad (5.25)$$

Substituting these expressions into α_{ij} we get

$$\begin{aligned}
\alpha_{ij} &= \langle 0|(\hat{x}_i^{(1)} - \hat{x}_j^{(2)})^2|0\rangle = \langle 0|\left(\frac{\hat{c}_i^{(1)} + \hat{c}_i^{(2)}}{\sqrt{2}} - \frac{\hat{c}_j^{(2)} - \hat{c}_j^{(1)}}{\sqrt{2}}\right)^2|0\rangle \\
&= \langle 0|\frac{1}{2}(\hat{c}_i^{(1)} + \hat{c}_i^{(2)})^2 + \frac{1}{2}(\hat{c}_j^{(2)} + \hat{c}_j^{(1)})^2 \\
&\qquad -(\hat{c}_i^{(1)} + \hat{c}_i^{(2)})(\hat{c}_j^{(2)} + \hat{c}_j^{(1)})|0\rangle \\
&= \langle 0^{(1)}|\langle 0^{(2)}|\ \frac{1}{2}(\hat{c}_i^{(1)} + \hat{c}_i^{(2)})^2 + \frac{1}{2}(\hat{c}_j^{(2)} + \hat{c}_j^{(1)})^2 \\
&\qquad -(\hat{c}_i^{(1)} + \hat{c}_i^{(2)})(\hat{c}_j^{(2)} + \hat{c}_j^{(1)})|0^{(2)}\rangle|0^{(1)}\rangle \\
&= \langle 0^{(1)}|\frac{1}{2}\big((\hat{c}_i^{(1)})^2 + (\hat{c}_j^{(1)})^2\big)|0^{(1)}\rangle + \langle 0^{(2)}|\frac{1}{2}\big((\hat{c}_i^{(2)})^2 + (\hat{c}_j^{(2)})^2\big)|0^{(2)}\rangle \\
&\qquad -\langle 0^{(1)}|\langle 0^{(2)}|\{\hat{c}_i^{(1)}\hat{c}_j^{(2)}, \hat{c}_i^{(2)}\hat{c}_j^{(1)}\}|0^{(2)}\rangle|0^{(1)}\rangle\ , \qquad (5.26)
\end{aligned}$$

where $|0^{(1)}\rangle$ and $|0^{(2)}\rangle$ denote the vacuum states of the subsystems with the coordinates $\{c_i^{(1)}\}$ and $\{c_i^{(2)}\}$ respectively. In order to evaluate the expression (5.26) we switch to coordinates that diagonalize the Hamiltonians of these subsystems $H_{c^{(1)}}(\{c_i^{(1)}\})$ and $H_{c^{(2)}}(\{c_i^{(2)}\})$ ($H_0 = H_{c^{(1)}}(\{c_i^{(1)}\}) + H_{c^{(2)}}(\{c_i^{(2)}\})$) with the transformations

$$y_i^{(1)} = \sum_j^N B_{ij}^{(1)} c_j^{(1)} \Leftrightarrow c_i^{(1)} = \sum_j^N B_{ij}^{(1)T} y_j^{(1)}, \qquad (5.27)$$

$$y_i^{(2)} = \sum_j^N B_{ij}^{(2)} c_j^{(2)} \Leftrightarrow c_i^{(2)} = \sum_j^N B_{ij}^{(2)T} y_j^{(2)}. \qquad (5.28)$$

In this basis it is very simple to evaluate the terms in (5.26). The mixed terms

$$\begin{aligned}
\langle 0^{(1)}|\langle 0^{(2)}|\hat{c}_i^{(1)}\hat{c}_j^{(2)}|0^{(2)}\rangle|0^{(1)}\rangle &= \langle 0^{(1)}|\hat{c}_i^{(1)}|0^{(1)}\rangle\langle 0^{(2)}|\hat{c}_j^{(2)}|0^{(2)}\rangle \\
&= \sum_l B_{il}^{(1)}\langle 0^{(1)}|\hat{y}_i^{(1)}|0^{(1)}\rangle \sum_k B_{ik}^{(2)}\langle 0^{(2)}|\hat{y}_j^{(2)}|0^{(2)}\rangle = 0 \qquad (5.29)
\end{aligned}$$

disappear since we are dealing with harmonic oscillators. Therefore α_{ij} takes the form

$$\begin{aligned}
\alpha_{ij} = \langle 0|(x_i^{(1)} - x_j^{(2)})^2|0\rangle = \frac{1}{2}\Big(&\langle 0^{(1)}|\big((\hat{c}_i^{(1)})^2 + (\hat{c}_j^{(1)})^2\big)|0^{(1)}\rangle \\
&+ \langle 0^{(2)}|\big((\hat{c}_i^{(2)})^2 + (\hat{c}_j^{(2)})^2\big)|0^{(2)}\rangle\Big). \qquad (5.30)
\end{aligned}$$

Since

$$\begin{aligned}\langle 0^{(1)}|(\hat{c}_i^{(1)})^2|0^{(1)}\rangle &= \sum_{jk}^{N} B_{ij}^{(1)T} B_{ik}^{(1)T} \langle 0^{(1)}|\hat{y}_j^{(1)}\hat{y}_k^{(1)}|0^{(1)}\rangle \\ &= \sum_{jk}^{N} B_{ij}^{(1)T} B_{ik}^{(1)T} \left(\frac{\hbar}{2m\omega_j^{(1)}}\right) \delta_{jk} = \sum_{j}^{N} B_{ij}^{(1)T} B_{ij}^{(1)T} \left(\frac{\hbar}{2m\omega_j^{(1)}}\right) \\ &= \sum_{j}^{N} B_{ij}^{(1)T} B_{ji}^{(1)} \left(\frac{\hbar}{2m\omega_j^{(1)}}\right) = [B^{(1)T} D^{(1)} B^{(1)}]_{ii}, \quad (5.31)\end{aligned}$$

with $D^{(1)} = \left\{\frac{\hbar}{2m\omega_j^{(1)}}\right\}\mathbb{1}$. Furthermore we obtain

$$\langle 0^{(1)}|(\hat{c}_j^{(1)})^2|0^{(1)}\rangle = [B^{(1)T} D^{(1)} B^{(1)}]_{jj} \quad (5.32)$$

and therefore

$$\langle 0^{(1)}|\left(\left(\hat{c}_i^{(1)}\right)^2 + \left(\hat{c}_j^{(1)}\right)^2\right)|0^{(1)}\rangle = [B^{(1)T} D^{(1)} B^{(1)}]_{ii} + [B^{(1)T} D^{(1)} B^{(1)}]_{jj}. \quad (5.33)$$

Using the same argument we get similar expressions for

$$\langle 0^{(2)}|\left(\left(\hat{c}_i^{(2)}\right)^2 + \left(\hat{c}_j^{(2)}\right)^2\right)|0^{(2)}\rangle = [B^{(2)T} D^{(2)} B^{(2)}]_{ii} + [B^{(2)T} D^{(2)} B^{(2)}]_{jj} \quad (5.34)$$

with $D^{(2)} = \left\{\frac{\hbar}{2m\omega_j^{(2)}}\right\}\mathbb{1}$. Putting all these terms together we obtain for α_{ij}

$$\begin{aligned}\alpha_{ij} = \frac{1}{2}\Bigg(&\underbrace{[B^{(1)T} D^{(1)} B^{(1)}]_{ii} + [B^{(2)T} D^{(2)} B^{(2)}]_{ii}}_{\Gamma_{ii}} \\ &+ \underbrace{[B^{(1)T} D^{(1)} B^{(1)}]_{jj} + [B^{(2)T} D^{(2)} B^{(2)}]_{jj}}_{\Gamma_{jj}}\Bigg), \quad (5.35)\end{aligned}$$

where Γ_{ii}, Γ_{jj} are the matrices that we have to connect to the interaction matrices $K_{ij}, \hat{K}_{ij}, W_{ij}$. In order to do that we consider the potential $V(x^{(1)}, x^{(2)})$ (the kinetic part is trivial) of the unperturbed Hamiltonian H_0

$$V_0 = \underbrace{\sum_{ij} W_{ij}\ \left(x_i^{(1)} x_j^{(1)} + x_i^{(2)} x_j^{(2)}\right)}_{I} + \underbrace{\sum_{ij} K_{ij}\ \left(x_i^{(1)} - x_j^{(2)}\right)^2}_{II}. \quad (5.36)$$

To evaluate this expression we need the following relations

$$x_i^{(1)} x_j^{(1)} = \frac{1}{2}\left(c_i^{(1)} + c_i^{(2)}\right)\left(c_j^{(1)} + c_j^{(2)}\right) = \frac{1}{2}\ \left(\hat{c}_i^{(1)} c_j^{(1)} + c_i^{(1)} c_j^{(2)} + c_i^{(2)} c_j^{(1)} + c_i^{(2)} c_i^{(2)}\right) \quad (5.37)$$

$$x_i^{(2)}x_j^{(2)} = \frac{1}{2}\big(c_i^{(2)} - c_i^{(1)}\big)\big(\hat{c}_j^{(2)} - \hat{c}_j^{(1)}\big) = \frac{1}{2}\,\big(c_i^{(2)}c_j^{(2)} - c_i^{(2)}c_j^{(1)} - c_i^{(1)}c_j^{(2)} + c_i^{(1)}c_i^{(1)}\big) \tag{5.38}$$

$$x_i^{(1)}x_j^{(2)} = \frac{1}{2}\big(c_i^{(1)} + c_i^{(2)}\big)\big(c_j^{(2)} - c_j^{(1)}\big) = \frac{1}{2}\,\big(c_i^{(1)}c_j^{(2)} - c_i^{(1)}c_j^{(1)} + c_i^{(2)}c_j^{(2)} - c_i^{(2)}c_j^{(1)}\big) \tag{5.39}$$

Putting (5.37) and (5.38) into (I) gives us

$$\sum_{ij} W_{ij}\,\big(x_i^{(1)}x_j^{(1)} + x_i^{(2)}x_j^{(2)}\big) = \sum_{ij} W_{ij}\,\big(c_i^{(1)}c_j^{(1)} + c_i^{(2)}c_j^{(2)}\big). \tag{5.40}$$

The second term (II) can be rewritten as

$$\sum_{ij} K_{ij}\,\big(x_i^{(1)} - x_j^{(2)}\big)^2 = \underbrace{\sum_{ij} K_{ij}\,\big(\big(x_i^{(1)}\big)^2 + \big(x_j^{(2)}\big)^2\big)}_{(a)} - \underbrace{2\sum_{ij} K_{ij}\,x_i^{(1)}x_j^{(2)}}_{(b)}. \tag{5.41}$$

The evaluation of the term (a) gives,

$$\begin{aligned}
(a) &= \sum_{ijk} K_{ij}\,\big(\delta_{ik}\,x_i^{(1)}x_k^{(1)} + \delta_{ik}\,x_i^{(2)}x_k^{(2)}\big) \\
&= \sum_{ik} \underbrace{\delta_{ik}\,\sum_j K_{ij}}_{\hat{K}_{ik}}\,\big(x_i^{(1)}x_k^{(1)} + x_i^{(2)}x_k^{(2)}\big) \\
&= \sum_{ij} \hat{K}_{ij}\big(x_i^{(1)}x_j^{(1)} + x_i^{(2)}x_j^{(2)}\big) \\
&= \sum_{ij} \hat{K}_{ij}\big(c_i^{(1)}c_j^{(1)} + c_i^{(2)}c_j^{(2)}\big),
\end{aligned} \tag{5.42}$$

where we used (5.37) and (5.38) again. The term (b) becomes

$$\begin{aligned}
(b) &= -2\sum_{ij} K_{ij}\; x_i^{(1)} x_j^{(2)} \\
&= -2\sum_{ij} K_{ij}\big(c_i^{(1)} c_j^{(2)} - c_i^{(1)} c_j^{(1)} + c_i^{(2)} c_i^{(2)} - c_i^{(2)} c_j^{(1)}\big) \\
&= 2\sum_{ij} K_{ij}\big(c_i^{(1)} c_j^{(1)} - c_i^{(2)} c_j^{(2)}\big) - 2\sum_{ij} K_{ij}\; c_i^{(1)} c_j^{(2)} \\
&\quad + \underbrace{2\sum_{ij} K_{ij}\; c_i^{(2)} c_j^{(1)}}_{= 2\;\sum_{ij} K_{ji}\; c_j^{(2)} c_i^{(1)} = 2\;\sum_{ij} K_{ij}\; c_i^{(1)} c_j^{(2)}} \\
&= 2\sum_{ij} K_{ij}\big(c_i^{(1)} c_j^{(1)} - c_i^{(2)} c_j^{(2)}\big). \qquad (5.43)
\end{aligned}$$

We employed the symmetry of K_{ji} and the relation (5.39). Putting (a) and (b) together and substituting (I) and (II) into (5.36) leads us therefore to a representation of the potential $V_0 = V^{(1)}(\{c_i^{(1)}\}) + V^{(2)}(\{c_i^{(2)}\})$ that reads

$$V_0 = \sum_{ij} \big(\underbrace{\big(W_{ij} + \hat{K}_{ij} + 2K_{ij}\big)}_{V_{ij}^{(1)}}\; c_i^{(1)} c_j^{(1)} + \underbrace{\big(W_{ij} + \hat{K}_{ij} - 2K_{ij}\big)}_{V_{ij}^{(2)}}\; c_i^{(2)} c_j^{(2)} \big). \qquad (5.44)$$

In this expression we have separated the potential into parts containing only $c_i^{(1)}$ and $c_i^{(2)}$ without mixed terms. In order to establish the connection between the matrices $V^{(1)}$, $V^{(2)}$ and Γ_{ii}, Γ_{jj} we need to diagonalize the matrices $V^{(1)}$, $V^{(2)}$. We will demonstrate this for $V^{(1)}$, the calculation for $V^{(2)}$ will then be analogous. We will introduce the normal coordinates $B\,\mathbf{c} = \mathbf{y} \Leftrightarrow \mathbf{c} = B^T \mathbf{y}$, which leads to

$$\begin{aligned}
V^{(1)} &= \sum_{ij} V_{ij}^{(1)} c_i^{(1)} c_j^{(1)} = \sum_{ij}\sum_{lk} V_{ij}^{(1)} B_{il}^{(1)T} y_l^{(1)} B_{jk}^{(1)T} y_k^{(1)} \\
&= \sum_{ijlk} B_{il}^{(1)T} B_{kj}^{(1)} V_{ij}^{(1)} y_l^{(1)} y_k^{(1)} = \sum_{ijk} B_{ik}^{(1)T} B_{kj}^{(1)} V_{ij}^{(1)} \big(y_k^{(1)}\big)^2 \\
&= \sum_{ijk} B_{ki}^{(1)} V_{ij}^{(1)} B_{jk}^{(1)T} \big(y_k^{(1)}\big)^2 = \sum_{k} \left(\sum_{ij} B_{ki}^{(1)} V_{ij}^{(1)} B_{jk}^{(1)T} \right) \big(y_k^{(1)}\big)^2 \\
&= y^{(1)T} \underbrace{B^{(1)} V^{(1)} B^{(1)T}}_{\text{diagonal}} y^{(1)}, \qquad (5.45)
\end{aligned}$$

from which we can conclude that

$$B^{(1)} V^{(1)} B^{(1)T} = \left\{ \frac{m(\omega_i^{(1)})^2}{2} \right\} \mathbb{1} = \left(\frac{\hbar^2}{8m} \right) (D^{(1)})^{-2}, \qquad (5.46)$$

with

$$D^{(1)} = \left\{ \frac{\hbar}{2m\omega_i^{(1)}} \right\} \mathbb{1}. \tag{5.47}$$

An equivalent relation holds for $V_0^{(2)}$

$$B^{(2)} V^{(2)} B^{(2)T} = \left\{ \frac{m(\omega_i^{(2)})^2}{2} \right\} \mathbb{1} = \left(\frac{\hbar^2}{8m} \right) (D^{(2)})^{-2}, \tag{5.48}$$

with

$$D^{(2)} = \left\{ \frac{\hbar}{2m\omega_i^{(2)}} \right\} \mathbb{1}. \tag{5.49}$$

From these relations we deduce by multiplying $B^{(1),(2)T}$ from the left and $B^{(1),(2)}$ from the right and using orthogonality that

$$V^{(1)} = \frac{\hbar^2}{8m} B^{(1)T} (D^{(1)})^{-2} B^{(1)} \tag{5.50}$$

and

$$V^{(2)} = \frac{\hbar^2}{8m} B^{(2)T} (D^{(2)})^{-2} B^{(2)}. \tag{5.51}$$

This yields

$$B^{(1)T} D^{(1)} B^{(1)} = \left(\frac{8m}{\hbar^2 V^{(1)}} \right)^{1/2} \tag{5.52}$$

and

$$B^{(2)T} D^{(2)} B^{(2)} = \left(\frac{8m}{\hbar^2 V^{(2)}} \right)^{1/2}, \tag{5.53}$$

which can be seen from the following relation

$$\begin{aligned} V^{((1),(2))} &= \frac{\hbar^2}{8m} B^{((1),(2))T} \left(D^{((1),(2))} \right)^{-2} B^{((1),(2))} \\ &= \underbrace{\sqrt{\frac{\hbar^2}{8m}} B^{((1),(2))T} \left(D^{((1),(2))} \right)^{-1} B^{((1),(2))}}_{\Theta^{((1),(2))}} \\ &\qquad \times \underbrace{\sqrt{\frac{\hbar^2}{8m}} B^{((1),(2))T} \left(D^{((1),(2))} \right)^{-1} B^{((1),(2))}}_{\Theta^{((1),(2))}} \\ &= (\Theta^{((1),(2))})^2, \end{aligned} \tag{5.54}$$

where we used that $B^{((1),(2))}$ are orthogonal matrices with $B^{((1),(2))T} = (B^{((1),(2))})^{-1}$. From this we deduce that

$$\begin{aligned} (V^{((1),(2))})^{1/2} &= \Theta^{((1),(2))} \\ &= \sqrt{\frac{\hbar^2}{8m}}\, B^{((1),(2))T} \left(D^{((1),(2))} \right)^{-1} B^{((1),(2))}. \end{aligned} \tag{5.55}$$

Applying $B^{((1),(2))}$ from the left and $B^{((1),(2))T}$ from the right gives us

$$B^{((1),(2))}\left(\frac{8m}{\hbar^2}V^{((1),(2))}\right)^{1/2}B^{((1),(2))T} = \left(D^{((1),(2))}\right)^{-1}. \tag{5.56}$$

Furthermore taking the inverse provides us with

$$\begin{aligned} D^{((1),(2))} &= \left(B^{((1),(2))}\left(\frac{8m}{\hbar^2}V^{((1),(2))}\right)^{1/2}B^{((1),(2))T}\right)^{-1} \\ &= B^{((1),(2))}\left(\frac{8m}{\hbar^2}V^{((1),(2))}\right)^{-1/2}B^{((1),(2))T}, \end{aligned} \tag{5.57}$$

where we used orthogonality and the relation $(AB)^{-1} = B^{-1}A^{-1}$ which is valid for general matrices. Multiplying (5.57) from the left with $B^{((1),(2))T}$ and from the right with $B^{((1),(2))}$ leads us then to

$$\left(\frac{\hbar^2}{8m}V^{((1),(2))}\right)^{-1/2} = B^{((1),(2))T}D^{((1),(2))}B^{((1),(2))}, \tag{5.58}$$

which are the relations (5.52) and (5.53). We thus connected the matrices $V^{((1),(2))}$ with the matrices $B^{((1),(2))T}D^{((1),(2))}B^{((1),(2))}$ and can therefore represent the quantity α_{ij} using the matrices $V^{((1),(2))}$. This means that (5.35) transforms into

$$\begin{aligned} \alpha_{ij} &= \frac{\sqrt{2m}}{\hbar}\left(\left(\frac{1}{W+\hat{K}+2K}\right)^{1/2}_{ii} + \left(\frac{1}{W+\hat{K}-2K}\right)^{1/2}_{ii}\right. \\ &\quad \left. + \left(\frac{1}{W+\hat{K}+2K}\right)^{1/2}_{jj} + \left(\frac{1}{W+\hat{K}-2K}\right)^{1/2}_{jj}\right). \end{aligned} \tag{5.59}$$

After this rather technical discussion, it is worthwhile to recapitulate quickly what we did up to this point in the present section. Starting from the definition (5.18), we derived

$$C_{ij} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f''(x\sqrt{\alpha_{ij}})\exp\left(-\frac{x^2}{2}\right)dx\ , \tag{5.60}$$

where the quantities $\alpha_{ij} = \langle 0|(x_i^{(1)} - x_j^{(2)})^2|0\rangle$ can be related to the parameters of $\hat{H}_0$. They are given by $\alpha_{ij} = (\Gamma_{ii} + \Gamma_{jj})/4$, where Γ_{kk} is the k-th diagonal element of the matrix

$$\Gamma = \frac{\hbar}{\sqrt{2m}}\left(\left(\frac{1}{W+\hat{K}-2K}\right)^{1/2} + \left(\frac{1}{W+\hat{K}+2K}\right)^{1/2}\right)\ , \tag{5.61}$$

and $\hat{K}$ is a diagonal matrix whose elements read $\hat{K}_{ij} = \delta_{ij} \sum_l K_{il}$. The coefficients C_{ij} depend on $\hbar$ since they result from sandwiching the function f with the ground states of the integrable Hamiltonian.

If we restrict ourselves to leading order $\hbar$, only the first term of the expansion (5.2) enters. In such a semi-classical regime Eq. (5.60) simplifies and we have $C_{ij} = 3f_2(\Gamma_{ii} + \Gamma_{jj})$.

Since H_0^{R} is harmonic, the spectral function $\tilde{S}(\omega)$ can now be calculated using Eq. (5.7). The renormalized oscillator frequency Ω_0^{R} and the renormalized spreading kernel γ^{R} are determined by the renormalized coupling constants $K_{ij}^{\mathrm{R}} = K_{ij} + \lambda C_{ij}/2$ and by W_{ij}. The spreading kernel can be expressed through the spectral density function $\sigma^{\mathrm{R}}(\omega)$ [39],

$$\gamma^{\mathrm{R}}(t) = \frac{2}{m} \int_0^\infty \frac{\sigma^{\mathrm{R}}(\omega)}{\omega} \cos(\omega t) d\omega \ . \tag{5.62}$$

Employing our previous results from the integrable case, we express the spectral density function through the parameters of the harmonic Hamiltonian. This yields

$$\sigma^{\mathrm{R}}(\omega) = -\frac{1}{2\pi m\omega} \mathrm{Im}\, \mathbf{k}^T \frac{\mathbb{1}}{(\omega + i\epsilon)\mathbb{1} - (2K_r/m)^{1/2}} \mathbf{k}, \tag{5.63}$$

where K_r and $\mathbf{k}$ are obtained from the matrix $\tilde{K}^{\mathrm{R}} = A^T(W + \hat{K}^{\mathrm{R}} + 2K^{\mathrm{R}})A$, with A being a discrete $N \times N$ cosine transform, that we introduced in the integrable set up. More precisely, K_r is the $(N-1)\times(N-1)$ matrix obtained from $\tilde{K}^{\mathrm{R}}$ by deleting the first row and the first column while the vector $\mathbf{k}$ is the first column (excluding the first element) of $\tilde{K}^{\mathrm{R}}$. The renormalized oscillator frequency turns out to be

$$\Omega_0^{\mathrm{R}} = \sqrt{2\tilde{K}_{11}^{\mathrm{R}}/m + \gamma^{\mathrm{R}}(0)} \ . \tag{5.64}$$

It is important to notice that the spreading kernel (5.62), the oscillator frequency (5.64) and therefore the spectral density $\tilde{S}(\omega)$ are fully determined by the *classical* dynamics of the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. In particular, using our previous results, the equation for the classical time evolution of the collective coordinate reads

$$\frac{d^2X(t)}{dt^2} + (\Omega_0^{\mathrm{R}})^2 X(t) + \int_0^t \gamma^{\mathrm{R}}(t-s) \frac{dX(s)}{ds} ds = F(t) \ , \tag{5.65}$$

with $F(t)$ being a force term. A homogeneous differential equation holds for the expectation value $\langle \hat{X} \rangle(t)$ if the initial state of the system is properly chosen

$$\frac{d^2\langle X\rangle(t)}{dt^2} + (\Omega_0^{\mathrm{R}})^2 \langle X\rangle(t) + \int_0^t \gamma^{\mathrm{R}}(t-s) \frac{d\langle X\rangle(s)}{ds} ds = 0. \tag{5.66}$$

Equation (5.66) describes a damped, *i.e.* in our case spread, harmonic oscillator whose spreading kernel $\gamma^{\mathrm{R}}(t)$ and oscillator frequency Ω_0^{R} are given by Eqs. (5.62) and (5.64), respectively. Importantly, the solution of Eq. (5.66) also determines, for properly chosen initial conditions, the spectral density of the collective excitations. We notice, however, that $\hat{H}_0^{\mathrm{R}}$ itself contains quantum corrections which depend on $\hbar$. Put differently, $\hat{H}_0^{\mathrm{R}}$ is identified as the proper effective Hamiltonian whose classical dynamics — rather than the classical dynamics of the original, total Hamiltonian $\hat{H}$ — determines the spectrum of collective excitations in leading order λ. We also notice that higher order terms in the perturbative treatment of $S(t)$ come with higher powers of $\hbar$. Indeed, it is straightforward to see that in the case of $f(x) = f_2 x^4$ the n–th term of the perturbative expansion scales as $(\hbar\lambda)^n$. In this sense the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$ provides the first semi-classical correction to the spectrum of the collective modes.

We briefly discuss the conditions for the validity of our perturbative approach. The approximation (5.3) can be used if the following conditions are satisfied, see Ref. [42]. First, the gap between the ground state and the first excited state of $\hat{H}_0$ must be sufficiently large, i.e., $\lambda|\langle 0|\hat{H}_1|0\rangle| \ll \hbar\omega_{\min}$, where $\omega_{\min}$ is the minimal oscillator frequency of the classical system given by the lowest eigenvalue of the matrix $W + \hat{K} + 2K$. Second, the time t of propagation must be bounded by $\lambda|\langle 0|\hat{H}_1|0\rangle|t/\hbar \ll 1$. As we are interested in time scales of order $t \sim \Omega_0^{-1}$, the first condition implies the second one. Under these conditions the spectral characteristics such as energy and spreading width of the collective excitations are close to their values for the unperturbed Hamiltonian $\hat{H}_0$. We notice, however, that such a "small" perturbation λH_1 might be quite large on the scale of the mean level spacing which is of the order $\hbar^N$. This means that the local distribution of the energy levels of the Hamiltonian H might be essentially different from the energy level distribution of the integrable Hamiltonian H_0.

Chapter 6

Summary

In the first part (chapter 3) we studied collective behavior in an integrable model consisting of two coupled chains of harmonic oscillators. We chose the rescaled difference of the center of mass modes of the chains as a collective coordinate X, and mapped our system onto a model of Caldeira-Leggett-type. The resemblance with the well-known Caldeira-Leggett model provided an intuitive physical picture of the energy exchange between the collective coordinate and the remaining degrees of freedom playing the role of the internal bath. As a result, the dynamics of the collective mode is described by the spread harmonic oscillator equation. We then related this dynamical equation to the problem of the existence of collective quantum excitations in the spectrum of the corresponding quantum Hamiltonian. These collective excitations are probed through the transition strengths induced by observables $A(\hat{X})$, depending on the collective coordinate. As we showed, for the dynamically underdamped regime the spikes in the distribution of the transition strengths appear precisely at the energies $E_n = E_0 + n\hbar\Omega_0$ (E_0 = ground state energy) of the quantized collective harmonic oscillator, while the width of the spikes is controlled by the spreading coefficient γ_0 of the corresponding dynamical problem. It is worth mentioning that based on fluctuation-dissipation type of arguments we can extend the present approach to any Hamiltonian system with quadratic interactions.

One of the important features of the integrable model is the freedom of choice for the collective coordinate. Note that our definition of X in a technical sense was somewhat arbitrary. In principle, we could take any linear combination Y as a collective coordinate, and implement the same type of mapping procedure (as in the case of X) onto the model of Caldeira-Leggett-type. We would get then precisely the same equation of motion for $Y(t)$, but with a different collective frequency Ω_0 and spreading kernel $\gamma(t)$. Not every choice for Y would be, of course, appropriate in order to regard it as a collective coordinate. If, for instance, the resulting dynamics becomes overdamped, no clear spikes will be visible at the corresponding

spectral function. On the other hand, it seems that there exists no "unique" choice for the collective coordinate. This means the parameters Ω_0, γ_0 are not intrinsic properties of the considered integrable model but are rather affected by the definition of the collective coordinate. In real experiments the choice of the collective coordinate is dictated by the way the system of interest is probed. For example, in the case of the GDR the photon-induced reaction causes the separation of centers of mass and charge in the nucleus that leads to a dipole moment coupling. This interaction between photons and the nucleus implies that the difference of centers of masses of protons and neutrons serves as a natural choice for the collective degree of freedom.

Beside the fundamental aspects just mentioned, there is further motivation for our study: Statistical analysis of the spectra indicates that collective motion is typically regular while the incoherent single–particle motion yields spectral statistics described by random matrices, see Refs. [22, 23, 24]. This coexistence of both regular and chaotic dynamics in the same system is a truly intriguing dynamical aspect of many–body systems [29]. The regularity of collective motion implies that the recent arguments [43] strongly supporting the Bohigas–Giannoni–Schmit conjecture for single–particle systems do not carry over in a straightforward manner to many–body systems. In short, this conjecture states that the spectral statistics of the single–particle system is of random–matrix type if the corresponding classical system is chaotic. Our study is thus needed when addressing the role of collectivity in quantum chaos.

An important step towards the resolution of this question is the perturbative approach that we undertook in the second part (chapter 4 and chapter 5) of the thesis. There we recognized that the quantum-classical relation can even be pushed beyond the limits of the integrable model as long as one studies perturbation theory to linear order in the expansion parameter λ. In such a framework the equation for the time evolution of the collective coordinate is still determined by a classical equation

$$\frac{d^2X(t)}{dt^2} + (\Omega_0^{\mathrm{R}})^2 X(t) + \int_0^t \gamma^{\mathrm{R}}(t-s)\frac{dX(s)}{ds}ds = F(t) \ , \tag{6.1}$$

with the renormalized dynamical quantities that are determined by the *classical* dynamics of a renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. We obtain a homogeneous equation for the quantum mechanical expectation value $\langle\hat{X}\rangle(t)$ if we choose the initial state properly

$$\frac{d^2\langle X\rangle(t)}{dt^2} + (\Omega_0^{\mathrm{R}})^2 \langle X\rangle(t) + \int_0^t \gamma^{\mathrm{R}}(t-s)\frac{d\langle X\rangle(s)}{ds}ds = 0 \ . \tag{6.2}$$

This means that the spreading kernel $\gamma^{\mathrm{R}}(t)$, the oscillator frequency Ω_0^{R} and the spectral function $\tilde{S}(\omega)$ are determined by the *classical* dynamics

of the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$. Thus we obtain a description for a damped, *i.e.* in our case spread, harmonic oscillator with renormalized spreading kernel $\gamma^{\mathrm{R}}(t)$ and oscillator frequency Ω_0^{R}. In addition the solution of Eq. (6.2) determines the spectral density of the collective excitations if we chose the initial conditions properly.

Because $\hat{H}_0^{\mathrm{R}}$ itself contains quantum corrections which depend on $\hbar$, we can identify it as an effective Hamiltonian whose classical dynamics determines the spectrum of collective excitations in leading order λ. Furthermore, higher order terms in the perturbative treatment of $S(t)$ come with higher powers of $\hbar$. From that perspective it is therefore legitimate to say that the renormalized Hamiltonian $\hat{H}_0^{\mathrm{R}}$ provides the first semi-classical correction to the spectrum of the collective modes.

In conclusion, we studied, in the framework of a simple model, the emergence of collectivity from first principles. We did not start from an effective model, we rather derived an effective description and still kept full control over the original degrees of freedom. In doing so, we related the expectation value of the collective operator and the spectral density of the collective excitations to a purely *classical* equation. We consider that to be important, as it can be viewed as a justification of the routinely used strategy in many–body physics, where effective models are set up classically and are then quantized (*e.g.* the liquid drop model in nuclear physics). In that sense the above "semi-classical" connection between the classical dynamics of a collective mode and collective excitations of the corresponding quantum problem can be extended to a more general class of non-integrable systems. We think that our detailed study of the emergence of collective motion in a (relatively simple) many body model establishes a solid basis for further research that aims to shed light on the interplay between chaos and regularity in quantum many body systems. Our approach contains the possibility to see both phenomena (integrable and non-integrable dynamics) in the set-up of a relatively simple model.

Appendix A

Feynman-Vernon theory

The Caldeira-Leggett model is is a prominent integrable model that allows to study phenomenologically the physics of an open quantum system. It is fully analytically solvable and therefore serves as a useful testing ground for studies related to damping, spreading and dissipation in a quantum mechanically context. We will give an overview about the major physical aspects of the model and follow the path of A. Caldeira and A. Leggett in their original research paper [30]. Everything we can possibly know about the dynamics of the full quantum system is encoded in the density matrix

$$\rho(t) = \exp\left(-\frac{iHt}{\hbar}\right)\rho(0)\exp\left(\frac{iHt}{\hbar}\right). \tag{A.1}$$

In the coordinate representation this becomes

$$\begin{aligned}\langle x\mathbf{R}|\rho(t)|y\mathbf{Q}\rangle &= \int_{-\infty}^{\infty} dx'dy'd\mathbf{R}'d\mathbf{Q}'\ \langle x\mathbf{R}|\exp\left(-\frac{iHt}{\hbar}\right)|x'\mathbf{R}'\rangle \\ &\quad \langle x'\mathbf{R}'|\rho(0)|y'\mathbf{Q}'\rangle\langle y'\mathbf{Q}'|\exp\left(\frac{iHt}{\hbar}\right)|y\mathbf{Q}\rangle, \end{aligned}\tag{A.2}$$

where $\mathbf{R}, \mathbf{Q}$ represent the vectors with components R_k, Q_k. We rewrite the propagators as path integrals

$$\begin{aligned}\langle x\mathbf{R}|\exp\left(-\frac{iHt}{\hbar}\right)|x'\mathbf{R}'\rangle &= \int_{x(0)=x'}^{x(t)=x}\mathcal{D}x(t')\int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}}\mathcal{D}\mathbf{R}(t')\exp\left(\frac{iS[x,\mathbf{R}]}{\hbar}\right) \\ &= K(x,\mathbf{R},t;x'\mathbf{R}',0) \end{aligned}\tag{A.3}$$

and

$$\begin{aligned}\langle y'\mathbf{Q}'|\exp\left(\frac{iHt}{\hbar}\right)|y\mathbf{Q}\rangle &= \int_{y(0)=y'}^{y(t)=y}\mathcal{D}y(t')\int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{Q}}\mathcal{D}\mathbf{Q}(t')\exp\left(-\frac{iS[y,\mathbf{Q}]}{\hbar}\right) \\ &= K^*(y,\mathbf{Q},t;y'\mathbf{Q}',0). \end{aligned}\tag{A.4}$$

Therefore we obtain for the density matrix in the coordinate basis

$$\langle x\mathbf{R}|\rho(t)|y\mathbf{Q}\rangle = \int_{-\infty}^{\infty} dx'dy'd\mathbf{R}'d\mathbf{Q}'\ K(x,\mathbf{R},t;x'\mathbf{R}',0) \\ K^*(y,\mathbf{Q},t;y'\mathbf{Q}',0)\langle x'\mathbf{R}'|\rho(0)|y'\mathbf{Q}'\rangle. \quad \text{(A.5)}$$

We are particular interested in the dynamics of the coordinate x which is embedded into the environmental degrees of freedom. Hence we have to get rid of the other degrees of freedom by tracing out the environment. This operation provides us with the reduced density matrix of the system

$$\begin{aligned}\tilde{\rho}(x,y,t) &= \int_{-\infty}^{\infty} d\mathbf{R}\ \langle x\mathbf{R}|\rho(t)|y\mathbf{R}\rangle \\ &= \int_{-\infty}^{\infty} dx'dy'd\mathbf{R}'d\mathbf{Q}'d\mathbf{R}\ K(x,\mathbf{R},t;x'\mathbf{R}',0)K^*(y,\mathbf{R},t;y'\mathbf{Q}',0) \\ &\qquad \langle x'\mathbf{R}'|\rho(0)|y'\mathbf{Q}'\rangle, \end{aligned} \quad \text{(A.6)}$$

with

$$\begin{aligned}\langle y'\mathbf{Q}'|\exp\left(\frac{iHt}{\hbar}\right)|y\mathbf{R}\rangle &= \int_{y(0)=y'}^{y(t)=y}\mathcal{D}y(t')\int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}}\mathcal{D}\mathbf{Q}(t')\exp\left(-\frac{iS[y,\mathbf{Q}']}{\hbar}\right) \\ &= K^*(y,\mathbf{R},t;y'\mathbf{Q}',0). \end{aligned} \quad \text{(A.7)}$$

We assume that the systems are initially uncoupled which means for the density matrix that

$$\rho(0) = \rho_S(0)\otimes\rho_R(0)$$

and therefore for the reduced density matrix

$$\begin{aligned}\tilde{\rho}(x,y,t) = \int_{-\infty}^{\infty} dx'dy'd\mathbf{R}'d\mathbf{Q}'d\mathbf{R}\int_{x(0)=x'}^{x(t)=x}\mathcal{D}x(t')\int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}}\mathcal{D}\mathbf{R}(t') \\ \times\int_{y(0)=y'}^{y(t)=y}\mathcal{D}y(t')\int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}}\mathcal{D}\mathbf{Q}(t')\exp\left(\frac{iS[x,\mathbf{R}]}{\hbar}\right) \\ \times\exp\left(-\frac{iS[y,\mathbf{Q}]}{\hbar}\right)\rho_S(x',y',0)\rho_R(\mathbf{R}',\mathbf{Q}',0). \end{aligned} \quad \text{(A.8)}$$

The action is analogous to the Hamiltonian $S = S_S + S_R + S_I = \int_0^t L dt$. With this the reduced density matrix becomes

$$\tilde{\rho}(x,y,t) = \int_{-\infty}^{\infty} dx' dy' J(x,y,t;x',y',0)\rho_S(x',y',0), \tag{A.9}$$

where

$$J(x,y,t;x',y',0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x(t') \int_{y(0)=y'}^{y(t)=y} \mathcal{D}y(t') \exp\left(\frac{i}{\hbar}\Big(S_S[x] - S_S[y]\Big)\right) \times \mathcal{F}[x,y], \tag{A.10}$$

with the influence functional

$$\mathcal{F}[x,y] = \int_{-\infty}^{\infty} d\mathbf{R}' d\mathbf{Q}' d\mathbf{R}\ \rho_R(\mathbf{R}',\mathbf{Q}',0) \int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}} \mathcal{D}\mathbf{Q}(t') \int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}} \mathcal{D}\mathbf{R}(t') \times \exp\left(\frac{i}{\hbar}\Big(S_I[x,\mathbf{R}] - S_I[y,\mathbf{Q}] + S_R[\mathbf{R}] - S_R[\mathbf{Q}]\Big)\right). \tag{A.11}$$

In the case of no interaction between the system and the bath the influence functional becomes

$$\mathcal{F}[x,y] = \int_{-\infty}^{\infty} d\mathbf{R}' d\mathbf{Q}' d\mathbf{R}\ \rho_R(\mathbf{R}',\mathbf{Q}',0) \int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}} \mathcal{D}\mathbf{Q}(t') \int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}} \mathcal{D}\mathbf{R}(t') \times \exp\left(\frac{i}{\hbar}\Big(S_R[\mathbf{R}] - S_R[\mathbf{Q}]\Big)\right), \tag{A.12}$$

which can be recast as

$$\begin{aligned} \mathcal{F}[x,y] &= \int_{-\infty}^{\infty} d\mathbf{R}' d\mathbf{Q}' d\mathbf{R}\ \langle\mathbf{Q}'| \exp\left(\frac{iH_R}{\hbar}\right)|\mathbf{R}\rangle\langle\mathbf{R}| \exp\left(-\frac{iH_R}{\hbar}\right)|\mathbf{R}'\rangle \\ &\quad \times\langle\mathbf{R}'|\rho(0)|\mathbf{Q}'\rangle \\ &= \int_{-\infty}^{\infty} d\mathbf{Q}'\langle\mathbf{Q}'|\rho(0)|\mathbf{Q}'\rangle = \mathrm{Tr}\rho = 1. \end{aligned} \tag{A.13}$$

Thus the expression for $J(x,y,t;x',y',0)$ takes a product structure of two propagators which propagates the system in positive and negative time direction respectively. In the above free case this propagation happens therefore independently but in the case of a non-vanishing interaction the influence

functional couples the two propagators. Any information regarding the impact of the interaction between bath and system on the quantum dynamics of the system is therefore encoded in the influence functional. One has just to evaluate (A.10) in order to obtain the time evolution for the reduced density matrix, which in turn encodes all the necessary information to calculate the physical observables of the system S.

Appendix B

The Caldeira-Leggett model

The formulas that have been provided are valid for a much more general class of Hamiltonians than the integrable Caldeira-Leggett case. Unfortunately only a few models can be solved exactly analytically. Nevertheless the Caldeira-Leggett model serves as an important testing ground for questions ranging from dissipation to decoherence and also served us in our investigation of collective motion in many body systems as an important guideline. We will therefore evaluate the influence functional for the integrable Caldeira-Leggett model still following the path that A. Caldeira and A. Leggett layed out in their paper [30]. After that we will give a short overview of the main physical aspects of the model and their relation to our investigation regarding collective degrees of freedom. The model consists of a System S that interacts with a system R described by the Hamiltonian

$$H = H_S + H_R + H_I, \tag{B.1}$$

with

$$H_S = \frac{P^2}{2M} + V(x) \tag{B.2}$$

$$H_R = \sum_k \frac{p_k^2}{2m} + \sum_k \frac{m\omega_k^2 R_k^2}{2} \tag{B.3}$$

$$H_I = x \sum_k c_k R_k. \tag{B.4}$$

The influence functional for this system is

$$\mathcal{F}[x,y] = \int_{-\infty}^{\infty} d\mathbf{R}' d\mathbf{Q}' d\mathbf{R}\ \rho_R(\mathbf{R}',\mathbf{Q}',0) \times \int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}} \mathcal{D}\mathbf{Q}(t') \exp\left(-\frac{i}{\hbar}\Big(S_R[\mathbf{Q}] + S_I[y,\mathbf{Q}]\Big)\right) \times \int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}} \mathcal{D}\mathbf{R}(t') \exp\left(\frac{i}{\hbar}\Big(S_R[\mathbf{R}] - S_I[x,\mathbf{R}]\Big)\right). \quad \text{(B.5)}$$

for the Caldeira-Leggett model takes the form

$$\mathcal{F}[x,y] = \int_{-\infty}^{\infty} d\mathbf{R}' d\mathbf{Q}' d\mathbf{R}\ \rho_R(\mathbf{R}',\mathbf{Q}',0) \int_{\mathbf{Q}(0)=\mathbf{Q}'}^{\mathbf{Q}(t)=\mathbf{R}} \mathcal{D}\mathbf{Q}(t') \times \exp\left(-\frac{i}{2\hbar}\int_0^t dt \sum_k \Big(m\dot{Q}_k^2 - m\omega_k^2 Q_k^2 - 2yc_kQ_k\Big)\right) \times \int_{\mathbf{R}(0)=\mathbf{R}'}^{\mathbf{R}(t)=\mathbf{R}} \mathcal{D}\mathbf{R}(t') \exp\left(\frac{i}{2\hbar}\int_0^t dt \sum_k \Big(m\dot{R}_k^2 - m\omega_k^2 R_k^2 - 2yc_kR_k\Big)\right). \quad \text{(B.6)}$$

The two path integrals in this expression are of standard form. A system with the classical action

$$S_{\rm cl} = \int_{t_a}^{t_b} \left(\frac{m\dot{q}^2(t)}{2} - \frac{m\omega^2 x^2(t)}{2} + f(t)x\right) dt \quad \text{(B.7)}$$

has the propagator

$$G(x_b,t_b;x_a,t_a) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega(t_b-t_a))}} \exp\left(\frac{im\omega}{2\hbar\sin\omega T}\Big((x_b^2+x_a^2) \times\cos(\omega T) - 2x_ax_b + \frac{2x_b}{m\omega}\int_{t_a}^{t_b} f(t)\sin(\omega(t-t_a))dt + \frac{2x_a}{m\omega}\int_{t_a}^{t_b} f(t)\sin(\omega(t_b-t))dt - \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t} f(t)f(s)\sin(\omega(t_b-t))\sin(\omega(s-t_a))\ dsdt\Big)\right), \quad \text{(B.8)}$$

with $T = (t_b - t_a)$, see Refs. [44, 45, 46].

Thus after performing the path integration we obtain for the influence functional

$$\mathcal{F}[x,y] = \prod_{k=1}^{\infty} \int_{-\infty} dR'_k dQ'_k dR_k \; \rho_R^k(R'_k, Q'_k, 0) \Bigg(\frac{m\omega_k}{2\pi i\hbar |\sin(\omega_k(t_b - t_a))|} \Bigg)$$
$$\times \exp\Bigg(- \frac{im\omega_k}{2\hbar \sin\omega_k t} \Bigg((Q_k'^2 - R_k'^2)\cos(\omega_k t) + 2R_k(R'_k - Q'_k)$$
$$+ \frac{2R_k c_k}{m\omega_k} \int_0^t (x(t') - y(t'))\sin(\omega_k(t'))dt'$$
$$+ \frac{2c_k}{m\omega_k} \int_0^t (R'_k x(t') - Q'_k y(t'))\sin(\omega_k(t - t'))dt'$$
$$+ \frac{2c_k^2}{m^2\omega_k^2} \int_0^t \int_0^\tau (x(\tau)x(s) - y(\tau)y(s))\sin(\omega_k(t-\tau))\sin(\omega_k s)\; ds d\tau \Bigg) \Bigg). \quad \text{(B.9)}$$

Into this we substitute the expression for the density matrix of a system that is in equilibrium at a temperature T

$$\rho_R^k(R'_k, Q'_k, 0) = \sqrt{\frac{m\omega_k}{2\pi\hbar \sinh(\hbar\omega_k/kT)}}$$
$$\times \exp\Bigg(- \frac{m\omega_k}{2\hbar \sinh(\hbar\omega_k/kT)} \Bigg((R_k'^2 + Q_k'^2)\cosh(\hbar\omega_k/kT) - 2R'_k Q'_k \Bigg) \Bigg) \quad \text{(B.10)}$$

and obtain

$$\mathcal{F}[x,y] = \exp\Bigg(-\frac{1}{\hbar} \int_0^t \int_0^\tau (x(\tau) - y(\tau))(\alpha(\tau - s)x(s) - \alpha^*(\tau - s)y(s)) \Bigg) ds d\tau \quad \text{(B.11)}$$

with

$$\alpha(\tau - s) = \sum_k \frac{c_k^2}{2m\omega_k} \Bigg(\exp(-i\omega_k(\tau - s)) + \frac{\exp(i\omega_k(\tau - s))}{\exp(\hbar\omega_k/kT) - 1}$$
$$+ \frac{\exp(-i\omega_k(\tau - s))}{\exp(\hbar\omega_k/kT) - 1} \Bigg). \quad \text{(B.12)}$$

The propagator for the reduced density matrix can then be expressed as

$$J(x,y,t;x',y',0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x(t') \int_{y(0)=y'}^{y(t)=y} \mathcal{D}y(t') \exp\left(\frac{i}{\hbar}\Big(S_S[x] - S_S[y] - \int_0^t \int_0^\tau (x(\tau)-y(\tau))\alpha_I(\tau-s)(x(s)+y(s))d\tau ds\Big)\right) \times \exp\left(-\frac{i}{\hbar}\int_0^t \int_0^\tau (x(\tau)-y(\tau))(x(s)-y(s))\alpha_R(\tau-s)d\tau ds\right), \quad \text{(B.13)}$$

with

$$\alpha_R(\tau-s) = \sum_k \frac{c_k^2}{2m\omega_k} \coth(\hbar\bar{\omega}_k/2KT)\cos(\omega_k(\tau-s)) \quad \text{(B.14)}$$

and

$$\alpha_I(\tau-s) = -\sum_k \frac{c_k^2}{2m\omega_k}\sin(\omega_k(\tau-s)). \quad \text{(B.15)}$$

The investigation of Caldeira and Leggett [30] proceeded with the exploration of the exact conditions that are necessary in order to obtain classical Brownian motion from the Hamiltonian (B.1). This is not a trivial task since the Hamiltonian is integrable and it is not a priori clear how to extract an irreversible process from this. For this it is necessary to consider the high temperature behavior of $\hbar\alpha_R(\tau-s)$ which is given by

$$\hbar\alpha_R(\tau-s) \approx \frac{kT}{m}\sum_k \frac{c_k^2}{\omega_k^2}\cos(\omega_k(\tau-s)) + \mathcal{O}(\hbar^2) \quad \text{(B.16)}$$

and compare it with the correlation of forces

$$\langle F(\tau)F(s)\rangle = 2\eta kT\delta(\tau-s) \quad \text{(B.17)}$$

that one obtains in the classical theory of Brownian motion with a damping constant η. This is necessary because the real part of B.13 corresponds to the density matrix where instead of coupling System S to a bath one excites it by a classical external force $F(\tau)$. This produces the following Kernel of the reduced density matrix

$$J(x,y,t;x',y',0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x(t') \int_{y(0)=y'}^{y(t)=y} \mathcal{D}y(t') \exp\left(\frac{i}{\hbar}\Big(S_S[x] - S_S[y] + \int_0^t (x(\tau)-y(\tau))F(\tau)d\tau\Big)\right), \quad \text{(B.18)}$$

which becomes

$$J(x,y,t;x',y',0) = \int\limits_{x(0)=x'}^{x(t)=x} \mathcal{D}x(t') \int\limits_{y(0)=y'}^{y(t)=y} \mathcal{D}y(t') \exp\left(\frac{i}{\hbar}\Big(S_S[x] - S_S[y]\Big)\right)$$
$$\times \exp\left(-\frac{1}{\hbar^2}\left(\int\limits_0^t \int\limits_0^\tau (x(\tau)-y(\tau))\langle F(\tau)F(s)\rangle (x(s)-y(s))d\tau ds\right)\right), \tag{B.19}$$

if we assume that the external force is Gaussian distributed. This on the other hand is of the same form as (B.13) apart from the extra complex part in its exponent. Thus we obtain

$$\hbar\alpha_R(\tau - s) \approx \frac{kT}{m} \int\limits_o^\infty \sigma_D(\omega)\ \frac{c^2(\omega)}{\omega^2} \cos(\omega_k(\tau - s))d\omega \tag{B.20}$$

if we assume a continuous distribution of oscillators with density $\sigma_D(\omega)$. In order to obtain the classical theory of Brownian motion from the Hamiltonian (B.1) we have to require

$$\sigma_D(\omega)c^2(\omega) = \begin{cases} \frac{2m\eta\omega^2}{\pi}, & \omega < \Omega, \\ \\ 0, & \omega > \Omega, \end{cases} \tag{B.21}$$

with a cutoff Ω. Hence the integral (B.20) gives

$$\hbar\alpha_R(\tau - s) = \frac{2\eta kT}{\pi} \frac{\sin(\Omega(\tau - s))}{(\tau - s)}. \tag{B.22}$$

If we sent the cutoff Ω in this expression to infinity we obtain the correlation of forces for the case of classical Brownian motion

$$\begin{aligned} \lim_{\Omega\to\infty} \hbar\alpha_R(\tau - s) &= \frac{2\eta kT}{\pi} \lim_{\Omega\to\infty} \frac{\sin(\Omega(\tau - s))}{(\tau - s)} \\ &= 2\eta kT\delta(\tau - s) \\ &= \langle F(\tau)F(s)\rangle. \end{aligned} \tag{B.23}$$

We mention that we obtain the classical case of Brownian motion if we introduce a continuum of oscillators which means that the recurrence time of the system becomes infinite and therefore enables the system to loose its energy to the environment. Furthermore it is critical that we consider times that are much longer than the typical time Ω^{-1} in order to obtain (B.17). This means that the important contributions for the Brownian motion stem

from the low-frequency behavior of $\sigma_D(\omega)c^2(\omega)$. We briefly mention here the connection to to our investigation. In chapter 3.3 we investigated the dynamics of the collective coordinate in our system which was mapped to a model of Caldeira-Leggett-type. We obtained the equation of motion for the collective degree of freedom from the Heisenberg equations, where we eliminated the bath-modes. The expectation values for the collective observable $\hat{X}(t)$ where then given by

$$\langle \hat{X}(t) \rangle = \mathrm{Tr}(\hat{\rho}\hat{X}(t)), \tag{B.24}$$

where $\hat{\rho}$ was the full density matrix of the system. The original Caldeira-Leggett approach is basically equivalent since one derives an expression of the time evolution of the reduced density matrix (which can be technically difficult) of the system, with which one calculates then the time evolution of expectation values of observables. This method is particularly powerful in the context of dynamical questions. The situation in our analysis is somewhat different though. We are interest in the quantity

$$\langle 0|\hat{X}(t)\hat{X}(0)|0\rangle = \mathrm{Tr}(\hat{\rho}_0\hat{X}(t)\hat{X}(0)), \tag{B.25}$$

with $\hat{\rho}_0 = |0\rangle\langle 0|$ and its relation between spectral and dynamical properties. As we have demonstrated in this work, the connection with semi-classics is somewhat different to the case of the original Caldeira-Leggett work. For example as demonstrated here previously, in the Caldeira-Leggett-model the classical limit arises from the high energy/high temperature case (density matrix in thermal equilibrium) whereas our correlation function $\langle 0|\hat{X}(t)\hat{X}(0)|0\rangle$ connects low energy states (the ground state) with spectral properties using semi-classics in a more subtle way.

Appendix C

$\tilde{S}(\omega)$ for the Caldeira-Leggett case

We obtained the imaginary part of the correlation function

$$S_1(t) \approx \underbrace{-\frac{\hbar}{2M\Omega}\sin(\Omega t)}_{(I)} - \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\Bigg(\underbrace{\frac{4\Omega^2}{(\Omega^2-\omega_k^2)^2}\sin(\omega_k t)}_{(II)} + \underbrace{\frac{2\omega_k^3 - 6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\ \sin(\Omega t)}_{(III)} + \underbrace{\frac{2\omega_k}{(\Omega^2-\omega_k^2)}\ t\cos(\Omega t)}_{(IV)}\Bigg). \quad \text{(C.1)}$$

which encodes the frequency domain of the correlation function via

$$\tilde{S}(\omega) = 2i\Theta(\omega)\tilde{S}_1(\omega) = \frac{2\hbar}{P_0}\Theta(\omega)\mathrm{Im}\tilde{X}^\dagger(\omega). \quad \text{(C.2)}$$

We know that

$$S_1(t) = -\frac{\hbar}{2P_0}X(t), \quad \text{(C.3)}$$

with the initial conditions $X(0) = X(-\infty)$, $\dot{X}(-\infty) = X(0)$ and $\dot{X}(0) = P_0/M$. With this we get

$$\tilde{X}^\dagger(\omega) = \frac{1}{2\pi}\int_0^\infty X(t)\exp(i\omega t)dt = \frac{1}{2\pi}\int_0^\infty \Big(-\frac{2P_0}{\hbar}\Big)S_1(t)\exp(i\omega t)dt \quad \text{(C.4)}$$

and thus

$$\tilde{S}(\omega) = -\frac{2\Theta(\omega)}{\pi}\mathrm{Im}\Big(\int_0^\infty S_1(t)\exp(i\omega t)dt\Big). \quad \text{(C.5)}$$

We will evaluate the different terms in (C.1). The first term gives

$$\begin{aligned}
\tilde{S}_{(I)}(\omega) &= \frac{2\Theta(\omega)}{\pi}\mathrm{Im}\Big(\int_0^\infty (I)\exp(i\omega t)dt\Big) \\
&= \frac{\hbar\Theta(\omega)}{M\Omega\pi}\mathrm{Im}\Big(\int_0^\infty \sin(\Omega t)\exp(i\omega t)dt\Big) \\
&= \frac{\hbar\theta(\omega)}{M\Omega\pi}\lim_{\epsilon\to 0}\mathrm{Im}\Big(\int_0^\infty \sin(\Omega t)\exp(-\epsilon)\exp(i\omega t)dt\Big) \\
&= \frac{\hbar\Theta(\omega)}{M\Omega\pi}\lim_{\epsilon\to 0}\mathrm{Im}\Big(\frac{1}{2i}\Big(\frac{\exp(i(\Omega+(\omega+i\epsilon))t)}{i(\Omega+(\omega+i\epsilon))}\Big|_0^\infty \\
&\quad + \frac{\exp(-i(\Omega-(\omega+i\epsilon))t)}{i(\Omega-(\omega+i\epsilon))}\Big|_0^\infty\Big)\Big) \\
&= \frac{\hbar\Theta(\omega)}{2M\Omega\pi}\lim_{\epsilon\to 0}\mathrm{Im}\Big(\frac{(\Omega-\omega)+i\epsilon}{(\Omega-\omega)^2+\epsilon^2}+\frac{(\Omega+\omega)-i\epsilon}{(\Omega+\omega)^2+\epsilon^2}\Big) \\
&= \frac{\hbar\Theta(\omega)}{2M\Omega\pi}(\pi\delta(\Omega-\omega))-\pi\delta(\Omega+\omega)) = \frac{\hbar}{2M\Omega}\delta(\Omega-\omega). \qquad \text{(C.6)}
\end{aligned}$$

From the term

$$IV = -\frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2\sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k(\Omega^2-\omega_k^2)}{(\Omega^2-\omega_k^2)^2}\ t\cos(\Omega t)\right) \qquad \text{(C.7)}$$

we obtain

$$\begin{aligned}
\tilde{S}_{(IV)} = 2i\Theta(\omega)\Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2\sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k(\Omega^2-\omega_k^2)}{(\Omega^2-\omega_k^2)}\right) \\
\times\frac{1}{2\pi}\int_{-\infty}^{\infty} t\cos(\Omega t)\exp(i\omega t)dt. \qquad \text{(C.8)}
\end{aligned}$$

This can be reformulated as

$$\begin{aligned}
\tilde{S}_{(IV)} = 2i\Theta(\omega)\Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2\sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k(\Omega^2-\omega_k^2)}{(\Omega^2-\omega_k^2)}\right) \\
\times\frac{1}{2\pi i}\frac{\partial}{\partial\omega}\underbrace{\int_{-\infty}^{\infty}\cos(\Omega t)\exp(i\omega t)dt}_{\frac{1}{2}\int_{-\infty}^{\infty}(\exp(i(\Omega+\omega)t)+\exp(-i(\Omega-\omega)t))dt}, \qquad \text{(C.9)}
\end{aligned}$$

which turns into

$$\tilde{S}_{(IV)}(\omega) = \Theta(\omega)\Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k(\Omega^2-\omega_k^2)}{(\Omega^2-\omega_k^2)}\right) \times\frac{\partial}{\partial\omega}(\delta(\Omega+\omega)+\delta(\Omega-\omega)). \quad \text{(C.10)}$$

Using the step function leads to

$$\tilde{S}_{(IV)}(\omega) = \Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k(\Omega^2-\omega_k^2)}{(\Omega^2-\omega_k^2)}\right) \times\frac{\partial}{\partial\omega}(\delta(\Omega-\omega)). \quad \text{(C.11)}$$

Applying the Fourier transform to the third term

$$-\frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k^3-6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\right)\sin(\Omega t) \quad \text{(C.12)}$$

gives

$$\tilde{S}_{(III)}(\omega) = 2i\Theta(\omega)\Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k^3-6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\right) \times\frac{1}{4\pi i}\int_{-\infty}^{\infty}\big(\exp(i(\Omega+\omega)t)-\exp(-i(\Omega-\omega)t)\big)dt. \quad \text{(C.13)}$$

Performing the integration leads to

$$\tilde{S}_{(III)}(\omega) = 2i\Theta(\omega)\Big(-\frac{1}{8}\Big)\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k^3-6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\right) \times\frac{1}{2i}\big(\delta(\Omega+\omega)-\delta(\Omega-\omega)\big), \quad \text{(C.14)}$$

which reduces to

$$\tilde{S}_{(III)}(\omega) = \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{2\omega_k^3-6\Omega^2\omega_k}{\Omega(\Omega^2-\omega_k^2)^2}\right)\delta(\Omega-\omega). \quad \text{(C.15)}$$

We treat the Fourier transform of (II) in an analogous way and obtain

$$\tilde{S}_{(II)}(\omega) = \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_k \frac{c_k^2\hbar}{m\omega_k}\left(\frac{4\Omega^2}{(\Omega^2-\omega_k^2)^2}\right)\delta(\omega_k-\omega). \quad \text{(C.16)}$$

Putting $\tilde{S}_{(I)}$, $\tilde{S}_{(II)}$, $\tilde{S}_{(III)}$ and $\tilde{S}_{(IV)}$ together we finally obtain

$$\tilde{S}(\omega) = \frac{\hbar}{2M\Omega}\delta(\Omega-\omega) + \frac{1}{8}\left(\frac{\lambda}{M\Omega}\right)^2 \sum_n \frac{\hbar c_n^2}{m\omega_n}\left(\left(\frac{2\omega_n^3-6\Omega^2\omega_n}{\Omega(\Omega^2-\omega_n^2)^2}\right)\delta(\Omega-\omega) - \frac{2\omega_n}{(\Omega^2-\omega_n^2)}\frac{\partial}{\partial\omega}\delta(\Omega-\omega)\right) + \frac{\lambda^2}{2M^2}\sum_n \frac{\hbar c_n^2}{m\omega_n}\frac{\delta(\omega_n-\omega)}{(\Omega^2-\omega_n^2)^2}. \quad \text{(C.17)}$$

Appendix D

Identification of the spreading kernel

We calculate $\tilde{S}(\omega)$ in an alternative way in order to check the correctness of the previous obtained results for the Caldeira-Leggett case. Instead of evaluating perturbatively the correlation function as in Appendix C we use an expansion of

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M} \lim_{\epsilon\to 0} \mathrm{Im}\big((\Omega^2 - \gamma(0)) - (\omega + i\epsilon)^2 - i(\omega + i\epsilon)\tilde{\gamma}(\omega + i\epsilon)\big)^{-1}, \quad \text{(D.1)}$$

where

$$\tilde{\gamma}(\omega + i\epsilon) = \int_0^\infty \gamma(s) \exp(i(\omega + i\epsilon)s) ds. \quad \text{(D.2)}$$

The function $\gamma(s)$ in this expression is given by

$$\gamma(s) = \frac{2}{M} \int_0^\infty d\omega \frac{\sigma(\omega)}{\omega} \cos(\omega s), \quad \text{(D.3)}$$

with the spectral density

$$\sigma(\omega) = \sum_n \frac{c_n^2}{2m\omega_n} \delta(\omega - \omega_n). \quad \text{(D.4)}$$

Together this gives

$$\begin{aligned} \gamma(s) &= \frac{1}{Mm} \sum_n c_n^2 \int_0^\infty d\omega \ \frac{1}{\omega} \frac{1}{\omega_n} \delta(\omega - \omega_n) \cos(\omega s) \\ &= \frac{1}{Mm} \sum_n \frac{c_n^2}{\omega_n^2} \cos(\omega_n s), \end{aligned} \quad \text{(D.5)}$$

from which follows

$$\gamma(0) = \frac{1}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}. \tag{D.6}$$

Thus for (D.2) we obtain

$$\begin{aligned}
\tilde{\gamma}(\omega + i\epsilon) &= \frac{1}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}\int_0^\infty \cos(\omega_n s)\exp(i(\omega + i\epsilon)s)ds \\
&= \frac{1}{2Mm}\sum_n \frac{c_n^2}{\omega_n^2}\left(\frac{\exp(i((\omega+\omega_n)+i\epsilon)s)}{i((\omega+\omega_n)+i\epsilon)}\bigg|_0^\infty\right. \\
&\quad \left. -\frac{\exp(-i((\omega_n-\omega)-i\epsilon)s)}{i((\omega_n-\omega)-i\epsilon)}\bigg|_0^\infty\right) \\
&= \frac{1}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}\frac{i(\omega+i\epsilon)}{(\omega+i\epsilon)^2-\omega_n^2}.
\end{aligned} \tag{D.7}$$

Because the coefficients are $c_n = (\lambda c_n')^2$ we omit the prime and obtain

$$\begin{aligned}
\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(&\left(\Omega^2 - (\omega+i\epsilon)^2\right) - \frac{\lambda^2}{Mm}\sum_n \frac{c_n^2}{\omega_n^2} \\
&+ \frac{\lambda^2}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}\frac{(\omega+i\epsilon)^2}{(\omega+i\epsilon)^2-\omega_n^2}\Bigg)^{-1},
\end{aligned} \tag{D.8}$$

which can be expressed as

$$\begin{aligned}
\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(&\left(\Omega^2 - (\omega+i\epsilon)^2\right) \\
&- \frac{\lambda^2}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}\left(1 - \frac{(\omega+i\epsilon)^2}{(\omega+i\epsilon)^2-\omega_n^2}\right)\Bigg)^{-1}.
\end{aligned} \tag{D.9}$$

Using the familiar approximation

$$(a-x)^{-m} \approx a^{-m}\left(1 + \frac{mx}{a}\right) \tag{D.10}$$

we get

$$\begin{aligned}
\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(&\left(\Omega^2 - (\omega+i\epsilon)^2\right)^{-1} \\
&- \frac{\lambda^2\left(\Omega^2 - (\omega+i\epsilon)^2\right)^{-2}}{Mm}\sum_n \frac{c_n^2}{\omega_n^2}\left(1 - \frac{(\omega+i\epsilon)^2}{(\omega+i\epsilon)^2-\omega_n^2}\right)\Bigg).
\end{aligned} \tag{D.11}$$

This can be simplified to

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1} - \frac{\lambda^2}{Mm}\sum_n c_n^2\Bigg(\frac{1}{(\Omega^2-(\omega+i\epsilon)^2)^2((\omega+i\epsilon)^2-\omega_n^2)}\Bigg)\Bigg), \quad \text{(D.12)}$$

and rewritten as

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1} - \frac{\lambda^2}{Mm}\sum_n c_n^2\Bigg(-\frac{1}{2\Omega}\Bigg)\frac{\partial}{\partial\Omega}\Bigg(\frac{1}{(\Omega^2-(\omega+i\epsilon)^2)((\omega+i\epsilon)^2-\omega_n^2)}\Bigg)\Bigg). \quad \text{(D.13)}$$

We can further condense this expression to

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1} + \frac{\lambda^2}{Mm}\sum_n c_n^2\Bigg(\frac{1}{2\Omega}\Bigg)\frac{\partial}{\partial\Omega}\Bigg(\frac{1}{(\Omega^2-\omega_n^2)}\Bigg(\frac{1}{(\Omega^2-(\omega+i\epsilon)^2)} + \frac{1}{((\omega+i\epsilon)^2-\omega_n^2)}\Bigg)\Bigg)\Bigg), \quad \text{(D.14)}$$

which can be expressed as

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(\big(\Omega^2-\omega+i\epsilon)^2\big)^{-1} + \frac{\lambda^2}{Mm}\sum_n c_n^2\Bigg(\frac{1}{2\Omega}\Bigg) \times\frac{\partial}{\partial\Omega}\Bigg(\frac{1}{(\Omega^2-\omega_n^2)}\Bigg(\frac{1}{2\Omega}\Bigg(\frac{1}{((\Omega-\omega)-i\epsilon)}+\frac{1}{((\Omega+\omega)+i\epsilon))}\Bigg) - \frac{1}{2\omega_n}\Bigg(\frac{1}{((\omega_n-\omega)-i\epsilon)}+\frac{1}{(\omega_n+\omega)+i\epsilon))}\Bigg)\Bigg)\Bigg) \quad \text{(D.15)}$$

and reformulated as

$$\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Bigg(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1} + \frac{\lambda^2}{Mm}\sum_n c_n^2\Bigg(\frac{1}{2\Omega}\Bigg) \times\frac{\partial}{\partial\Omega}\Bigg(\frac{1}{(\Omega^2-\omega_n^2)}\Bigg(\frac{1}{2\Omega}\Bigg(\frac{((\Omega-\omega)+i\epsilon)}{((\Omega-\omega)^2+\epsilon^2)}+\frac{(\Omega+\omega)-i\epsilon))}{((\Omega+\omega)^2+i\epsilon))}\Bigg) - \frac{1}{2\omega_n}\Bigg(\frac{((\omega_n-\omega)+i\epsilon)}{((\omega_n-\omega)^2+\epsilon^2)}+\frac{(\omega_n+\omega)-i\epsilon))}{(\omega_n+\omega)^2+\epsilon^2))}\Bigg)\Bigg)\Bigg). \quad \text{(D.16)}$$

We evaluate the derivative

$$\frac{\partial}{\partial\Omega}\Bigg(\frac{1}{(\Omega^2-\omega_n^2)}\Bigg(\frac{1}{2\Omega}\Bigg(\frac{((\Omega-\omega)+i\epsilon)}{((\Omega-\omega)^2+\epsilon^2)}\Bigg)\Bigg)\Bigg) = \frac{\Omega(\omega_n-\omega+i\epsilon)}{\omega_n(\Omega^2-\omega_n^2)^2((\omega_n-\omega)^2+\epsilon^2)}, \quad \text{(D.17)}$$

where the other terms can be obtained by $\omega \to -\omega$ and $i \to -i$. With this we obtain

$$\begin{aligned}\tilde{S}(\omega) = \frac{\hbar\Theta(\omega)}{\pi M}\lim_{\epsilon\to 0}\mathrm{Im}\Big(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1}\Big) \\ + \lim_{\epsilon\to 0}\Bigg(\frac{\lambda^2\hbar}{\pi M^2 m}\sum_n \frac{c_n^2}{2\Omega}\Bigg(-\frac{1}{(\Omega^2-\omega_n^2)^2}\frac{\epsilon}{((\Omega-\omega)^2+\epsilon^2)} \\ -\frac{1}{(\Omega^2-\omega_n^2)\Omega}\frac{(\Omega-\omega)\epsilon}{((\Omega-\omega)^2+\epsilon^2)^2} - \frac{1}{(\Omega^2-\omega_n^2)2\Omega^2}\frac{\epsilon}{((\Omega-\omega)^2+\epsilon^2)} \\ + \frac{1}{(\Omega^2-\omega_n^2)^2\omega_n}\frac{\Omega\epsilon}{((\omega_n-\omega)^2+\epsilon^2)}\Bigg)\Bigg). \quad \text{(D.18)}\end{aligned}$$

Evaluating the imaginary part of the first term

$$\begin{aligned}\mathrm{Im}\Big(\big(\Omega^2-(\omega+i\epsilon)^2\big)^{-1}\Big) &= \mathrm{Im}\Bigg(\frac{1}{2\Omega}\Bigg(\frac{1}{(\Omega-(\omega+i\epsilon))} \\ &\quad + \frac{1}{(\Omega+(\omega+i\epsilon))}\Bigg) \\ &= \frac{1}{2\Omega}\Bigg(\frac{\epsilon}{(\Omega-\omega)^2+\epsilon^2} \\ &\quad - \frac{\epsilon}{(\Omega+\omega)^2+\epsilon^2}\Bigg) \quad \text{(D.19)}\end{aligned}$$

and using the relations

$$\delta(\Omega-\omega) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{(\Omega-\omega)^2+\epsilon^2} \quad \text{(D.20)}$$

and

$$\frac{\partial}{\partial\omega}\delta(\Omega-\omega) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{2\epsilon(\Omega-\omega)}{((\Omega-\omega)^2+\epsilon^2)^2} \quad \text{(D.21)}$$

then leads to

$$\begin{aligned}\tilde{S}(\omega) = \frac{\hbar}{2M\Omega}\delta(\Omega-\omega) + \frac{1}{8}\Bigg(\frac{\lambda}{M\Omega}\Bigg)^2\sum_n\frac{\hbar c_n^2}{m\omega_n}\Bigg(\Bigg(\frac{2\omega_n^3-6\Omega^2\omega_n}{\Omega(\Omega^2-\omega_n^2)^2}\Bigg)\delta(\Omega-\omega) \\ - \frac{2\omega_n}{(\Omega^2-\omega_n^2)}\frac{\partial}{\partial\omega}\delta(\Omega-\omega)\Bigg) + \frac{\lambda^2}{2M^2}\sum_n\frac{\hbar c_n^2}{m\omega_n}\frac{\delta(\omega_n-\omega)}{(\Omega^2-\omega_n^2)^2}, \quad \text{(D.22)}\end{aligned}$$

which is the previously obtained relation (C.17).

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