Time Irreversibility in Quantum Mechanical Systems

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Für meinen
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Contents

1 Introduction

The question of time irreversibility plays a prominent role in classical physics, where at the end of the 19th century Ludwig Boltzmann gave some explanation for this phenomena. He dealt with the well known problem, that the microscopic laws of mechanics are time reversible, but on a macroscopic level we observe time irreversible processes. Boltzmann explained this phenomena by describing large systems (like gases) in statistical terms and basically telling us that some states of the system have a much higher probability than other states, which leads to time irreversible behaviour.

Already in the early days of quantum mechanics the problem of time irreversibility was attacked, see for example [53]. In 1955 Leon Van Hove [65] gave a derivation of a dissipative master equation based on perturbation theoretical arguments. He discusses at length the relation between the irreversible transport equation and the reversibility of the Schrödinger equation. A more recent treatment of this approach was given by Fischetti in [31] and [32]. He treats electron transport in small semiconductors by using the Pauli master equation and gives also a fine overview over the history of this approach and the problems connected with it.

An alternative approach to dissipation lies in considering quantum mechanical systems coupled to a reservoir, which usually leads to kinetic equations instead of master equations. This approach goes back to Feynman [28] and will be the basis for this work, which is organized as follows:

In Section 1.1 we will revise the problem of time irreversibility in classical physics, by giving an outline of the derivation of the Boltzmann equation and which mathematical assumptions lead to dissipation. We will also shortly comment on the Fokker-Planck equation. In Section 1.2 we will introduce the theory of open quantum systems in general, which is essential for the two special models discussed in the main part of the thesis.

The model treated in Chapter 2 was given by Caldeira and Leggett in [8] and is perhaps the easiest possible model of a system plus reservoir type, where the small system is coupled linearly to the reservoir. Our treatment here largely follows [12]. The limiting procedure of [8] to obtain a Fokker Planck equation is made mathematically rigorous, and after giving some criticism on the mechanism leading to dissipativity in the original approach, two different possible ways are given to obtain diffusion under physically more acceptable conditions. Still there remains the assumption, that the system is coupled linearly to the reservoir, which seems to be not at all possible to justify.

We then study in Chapter 3, following [33], a physically more relevant model without the linear coupling assumption. It describes an electron coupled to a phonon bath described in the formalism of second quantization. By the procedure of tracing out the phonon bath and by asymptotic analysis with respect to a small coupling parameter we obtain a very complicated scattering term which has the so called property of memory, a well known feature in this context (see [17]). We show how our obtained equation, which is still time reversible, is related to the Barker-Ferry equation in the case of a linear potential. Finally we give some scaling limits leading again to Fokker-Planck-like equations.

1.1 Classical Mechanics

First we want to sketch how time irreversibility is treated classically. Conceptually a many particle system is approximately described by a kinetic equation which gives the dynamics of a single-particle density. The complicated interaction with the surrounding and/or other particles is taken into account by collision terms, effective potentials, etc. We just want to give 2 typical examples of time irreversible kinetic equations.

1.1.1 The Boltzmann Equation

In classical mechanics the problem of time irreversibility was first solved by Ludwig Boltzmann in 1872. Clearly the laws of classical mechanics are time reversible, but in nature we observe phenomena which are definitely time irreversible. Boltzmann could give an explanation of this by his famous H–theorem.

We just want to outline the mathematical key ingredients. First of all, the description for a system with a large number of particles is stated in statistical terms. For example to describe a gas in normal conditions the function $P^{(1)}(t,x,\xi)$ gives the probability density of finding one fixed particle at time t at a certain point (x,ξ) of the six-dimensional phase space associated with the position and velocity of the particle. In the simplest model for the molecules of the gas we just might think of the particles as perfectly elastic spheres. To evaluate the effects of collisions on the time evolution of $P^{(1)}$ we have to know the probability of finding another molecule with its center exactly one diameter from the center of the first molecule. Thus in order to write the evolution equation of $P^{(1)}$ one would need $P^{(2)}(t, x_1, x_2, \xi_1, \xi_2)$ which gives the probability density of finding at time t the i - th molecule at x_i with velocity ξ_i, $i = 1, 2$.

Neglecting external forces we have

$$\frac{\partial P^{(1)}}{\partial t} + \xi_1 \cdot \nabla_{x_1} P^{(1)} = G - L \, , \tag{1.1}$$

with the gain term

$$G = (N-1)\sigma^2 \int_{\mathbb{R}^3_{\xi_2}} \int_{B^+} P^{(2)}(t, x_1, x_1 + \sigma n, \xi_1, \xi_2) |(\xi_2 - \xi_1) \cdot n| \, dn \, d\xi_2 \, , \tag{1.2}$$

and the loss term

$$L = (N-1)\sigma^2 \int_{\mathbb{R}^3_{\xi_2}} \int_{B^-} P^{(2)}(t, x_1, x_1 + \sigma n, \xi_1, \xi_2) |(\xi_2 - \xi_1) \cdot n| \, dn \, d\xi_2 \, , \tag{1.3}$$

where N is the number of molecules with diameter σ, $n \in B$ the unit sphere, B^+ is the hemisphere corresponding to $(\xi_2 - \xi_1) \cdot n > 0$ and $B^- = B \setminus B^+$.

We can rewrite G by using the fact that the probability density $P^{(2)}$ is continuous at a collision, i.e.

$$P^{(2)}(t, x_1, x_2, \xi_1, \xi_2) = P^{(2)}(t, x_1, x_2, \xi_1 - n(n \cdot V), \xi_2 + n(n \cdot V)) \, , \tag{1.4}$$

where we have written $V = \xi_2 - \xi_1$ and n is such that $x_2 - x_1 = \sigma n$. Using the notation $\xi_1' = \xi_1 - n(n \cdot V)$, $\xi_2' = \xi_2 + n(n \cdot V)$ we obtain

$$G = (N-1)\sigma^2 \int_{\mathbb{R}^3_{\xi_2}} \int_{B^-} P^{(2)}(t, x_1, x_1 - \sigma n, \xi_1', \xi_2') |(\xi_2 - \xi_1) \cdot n| \, dn \, d\xi_2 \, , \tag{1.5}$$

where we have changed n into $-n$.

The crucial step to obtain a time irreversible evolution equation is the so called Boltzmann – Grad limit, with $N \to \infty, \sigma \to 0$ and $N\sigma^2$ finite. But to obtain a closed equation, Boltzmann had to make a very special assumption, namely the assumption of molecular chaos: The collision between two preselected particles is a rather rare event, thus two particles that are to collide can be thought of to be two randomly chosen particles:

$$P^{(2)}(t, x_1, x_2, \xi_1, \xi_2) = P^{(1)}(t, x_1, \xi_1) P^{(1)}(t, x_2, \xi_2) \tag{1.6}$$

for $(\xi_2 - \xi_1) \cdot n < 0$.

Note that this recipe can be applied for the loss term and the gain term in the form (1.5), but not for (1.2). This is exactly the point where time irreversibility enters in the classical case. The chaos assumption (1.6) is valid just for particles which are about to collide, but not everywhere.

Applying the Boltzmann – Grad limit we obtain the Boltzmann equation

$$
\begin{aligned}
&\frac{\partial P^{(1)}}{\partial t} + \xi_1 \cdot \nabla_{x_1} P^{(1)} \\
&= N \int_{\mathbb{R}^3_{\xi_2}} \int_{B^-} \left[P^{(1)}(t, x_1, \xi_1') P^{(1)}(t, x_2, \xi_2') - P^{(1)}(t, x_1, \xi_1) P^{(1)}(t, x_2, \xi_2) \right] \\
&\times B(\theta, |\xi_2 - \xi_1|) d(\theta, \phi) \, d\xi_2 \; ,
\end{aligned}
\tag{1.7}
$$

where θ is the angle between n and V, and ϕ is the other angle which together with θ identifies the unit vector n. In the case of hard spheres the function $B(\theta, |\xi_2 - \xi_1|)$ specifying the interaction law between the molecules looks like $B(\theta, |\xi_2 - \xi_1|) = \cos\theta \sin\theta |\xi_2 - \xi_1|$.

Now mathematically the time irreversibility of (1.7) is expressed by the famous H–theorem. From now on we use the more usual notation $f(t, x, \xi)$ instead of $P^{(1)}(t, x_1, \xi_1)$ for the probability density. Then the Boltzmann equation reads

$$
\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f = Q(f, f) \; , \tag{1.8}
$$

with the collision term $Q(f, f)$ (for more details see [13]). Multiplying both sides of this equation by $\log f$ and integrating with respect to ξ, we obtain

$$
\frac{\partial \mathcal{H}}{\partial t} + \nabla_x \cdot J = S \; , \tag{1.9}
$$

where

$$
\begin{aligned}
\mathcal{H} &= \textstyle\int f \log f d\xi \; , \\
J &= \textstyle\int \xi f \log f d\xi \; , \\
S &= \textstyle\int \log f Q(f, f) d\xi \; .
\end{aligned}
$$

For the Boltzmann equation the inequality $S \leq 0$ holds ([13]), with equality $S = 0$ iff f is a Maxwellian. Therefore for space homogeneous solutions we arrive at the H–theorem:

$$
\frac{\partial \mathcal{H}}{\partial t} \leq 0 \; , \tag{1.10}
$$

i.e. $\mathcal{H}$ is a decreasing quantity unless f is a Maxwellian. In the general case the situation ia a little bit more complicated due to boundary conditions in space. We can define $H = \int_\Omega \mathcal{H} dx$ where Ω is the space domain occupied by the gas. So the inequality

$$\frac{\partial H}{\partial t} \leq \int_{\partial\Omega} J \cdot n \, d\sigma \tag{1.11}$$

holds, where n is the inward normal and $d\sigma$ the surface element. If we assume for example that Ω is a compact domain with specular reflection then the boundary term disappears (cf. [13]) and we obtain

$$\frac{dH}{dt} \leq 0 \, . \tag{1.12}$$

Boltzmann's H–theorem shows the basic feature of irreversibility of his equality, the quantities $\mathcal{H}$ (in the space homogeneous case) and H (in the cases with suitable boundary conditions) always decrease in time and up to the sign they have physically the meaning of entropy.

1.1.2 The Fokker-Planck Equation

The nonlinear Boltzmann equation is the archetypical example of a kinetic equation, which approximately describes dynamical processes of many-body systems. It is the special case for describing an interacting particle system in the low density limit. An alternative approach is to look at models consisting of a small system coupled to a reservoir. For an excellent review discussing system + reservoir models and interacting particle systems with all sorts of Markovian limits leading to different kinetic equations see [62].

In view of our quantum mechanical results we just want to mention the linear Fokker-Planck equation

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f = \gamma x \cdot \nabla_x f + D \Delta_x f \ , \tag{1.13}$$

γ and D being some physical constants. Fokker-Planck equations were first derived in the context of Brownian motion of particles, but today they are applied in incredibly many different situations in various disciplines such as physics, chemistry or electrical ingeneering. Of course due to its linear character the Fokker-Planck equation is much easier to handle than the nonlinear Boltzmann equation, still it has similar features of entropy and equilibrium solutions. For an extensive treatment of derivations and analytical properties of Fokker-Planck equations see [59].

To describe transport phenomena one usually considers a free test-particle subject to a collision mechanism. In these models the collisions are provided by impurities (Lorenz gas) or by a system of many noninteracting particles (Rayleigh gas or phonon models) and one focuses only on the dynamics of the test-particle. The goal is to derive an equation for the reduced phase space distribution from the Hamiltonian dynamics with many degrees of freedom. A scaling limit is necessary to eliminate the details of the single collisions and to keep only their cumulative long-time effects. The effect of a single collision is weakened. In the case of a heavy test-particle ([24]) the scaling limit leads to the Fokker-Planck equation, which can be obtained in a two step limit as well: first one obtains a linear Boltzmann equation via a low density limit, then a Fokker-Planck equation from a mass rescaling (see [62]).

1.2 Quantum Mechanics

For quite a while it has been a dream of physicist to derive something like a Quantum Boltzmann equation, but although there has been a considerable amount of research on this topic (see e.g. [41]), this is still an open problem. In the recent literature there are suggestions of how a nonlinear Quantum Boltzmann term might look like (see e.g. [23]), but up to our knowledge a derivation starting from microscopic principles like in Section 1.1.1 is still missing.

So we are not going to treat the quantum mechanical many particle system case, but only models of the form Particle + Reservoir. Besides perturbation theoretical arguments the concept of open quantum systems forms the basic approach to obtain diffusion for quantum mechanical systems.

1.2.1 Open Quantum Systems

Thermodynamics distinguishes all systems on the basis of interaction with their surroundings into

1. isolated systems, which can exchange neither energy nor matter with their surroundings,

2. closed systems, which can exchange all the energy in the form of heat and

3. open systems, which may exchange both matter and energy.

The theory of open systems plays an increasing role, not only in physics, but also in chemistry, biology, even in social sciences and others. This is closely related to the wide range of applications of the Fokker–Planck equation (for the concept of synergetics see [59] and the literature given there). There are attempts to view biological and chemical phenomena as features of open systems in the sense of physics, we just want to mention the dissipative structures of Prigogine [55], the Gaia hypothesis by James Lovelock and Lynn Margulis or the ultraweak bioluminiscence discovered by Fritz Popp [54]. Like in laser physics, these are examples of open systems far from equilibrium, whereas we are going to concentrate on open systems close to thermal equilibrium.

The notion of open systems in quantum mechanics has a slightly different definition than in thermodynamics, because it is not so clear how to distinguish between matter and energy. Actually it depends very much on the formalism, if we think in terms of exchange of energy (first quantization) or in terms of particles (second quantization). Furthermore the total number of particles involved might change. The usual approach is to look at a quantum mechanical system consisting of a small system (the 'open' system) coupled to a large system (the reservoir), which is actually that large, that it is basically not influenced by the behaviour of the small system.

For describing the open system A we use a complete microscopic description of the composite system $A+R$, where R is some reservoir, in our case close to thermal equilibrium. The composite system is isolated and therefore it may be described in any quantum mechanical formalism. The Hamiltonian of $A+R$ typically looks like

$$H = H_A + H_R + H_I \ , \tag{1.14}$$

where H_A is the free Hamiltonian for the test-particle, H_R is the free Hamiltonian for the reservoir, and H_I is the interaction Hamiltonian. Now the detailed state of the reservoir R is of no relevance and therefore we want to eliminate the coordinates of R, which might be done by taking the trace with respect to the variables of the reservoir. Still, just applying this recipe usually does not lead to time irreversibility but to a time reversible equation with a memory term. (For a very general outline of this process see [17]).

Like in classical statistical mechanics one has to consider in some sense an infinite system to obtain the macroscopic property of time irreversibility. The process of passing to an infinite reservoir leads to the quantum theory of collective phenomena, treated extensively in [60]. This non-trivial generalization of traditional quantum mechanics is assumed to be able to give rise to several physically relevant structures, that do not occur in the quantum theory of finite systems.

2 The model of Caldeira and Leggett

As a first model of the form (1.14) we want to study the following Hamiltonian given by Caldeira and Leggett in [8]:

$$\begin{aligned} H_{CL} &= \left(-\frac{\hbar^2}{2M}\Delta_x + V(x)\right) \\ &\quad + \sum_{j=1}^{N\Omega}\left(-\frac{\hbar^2}{2}\Delta_{R_j} + \frac{1}{2}\omega_j^2|R_j|^2\right) + \frac{1}{\sqrt{N}}\left(\sum_{j=1}^{N\Omega} C_j R_j\right)\cdot x\ . \end{aligned} \tag{2.1}$$

The first term of (2.1) represents the Hamiltonian of the test-particle with mass M where $x \in \mathbb{R}^d$ denotes the test-particle position in dimension d. The abstract reservoir is a set of finitely many (say $N\Omega$, which is assumed to be integer) independent oscillators written in normal variables $R_j \in \mathbb{R}^d$, having frequencies $\omega_j \in [0,\Omega]$ and masses $m = 1$. Here Ω is the maximum frequency of the oscillators and N is the number of oscillators per unit frequency. The typical case is the uniform frequency distribution: $\omega_j = \frac{j}{N}$ on $[0,\Omega]$. The coupling is linear in x and the R_j's, with coupling coefficients given by the C_j's. The normalization factor $N^{-1/2}$ simply stems from the central limit theorem, since, roughly speaking, the variables R_j's become independent random variables with vanishing expectation in the thermodynamic limit $N \to \infty$ (cf. Section 2.2.3 and Sectionstochint). The operator H acts on the Hilbert space $L^2_x(\mathbb{R}^d) \otimes \left(\bigotimes_{j=1}^{N\Omega} L^2_{R_j}(\mathbb{R}^d)\right)$. The authors of [8] consider only $d = 1$ for simplicity, as we shall do as well, but the method extends to any dimension.

This is perhaps the simplest model of an open quantum system, due to the linear coupling assumption. We want to treat it here just as an abstract model, without referring to special physical situations. For some criticism of the model itself in physical terms see the beginning of Chapter 3.

Caldeira and Legett used the Feynman path integral formalism, which is particularly powerful when H_R is quadratic and the interaction is linear in the reservoir variables. In this case the partial trace Tr_R leads to explicit Gaussian integrals in the reservoir variables, but in general it is not Gaussian in the test-particle variables. However, if the total Hamiltonian is quadratic, in particular if the coupling is linear in the test-particle variables, then the full evolution is given by a Gaussian integral, which, in principle, is explicit. The difficulty stems from the large (infinite) number of variables. The idea of how to treat this problem was first developped by Feynman, Hibbs, and Vernon [28], [29]. They integrated out the reservoir variables, i.e. they computed the time evolution of the wave function of the test-particle itself, given by $Tr_R\{\exp(it\hbar^{-1}(H_A + H_R + H_I))\}$, where Tr_R is the partial trace on the Hilbert space of the reservoir and $\hbar = h/2\pi$, where h is the Planck constant.

Caldeira-Leggett also assume that the reservoir is initially in thermal equilibrium at inverse temperature β, i.e. the initial density matrix of the system $A+R$ is given by

$$\rho^0 = \rho_A^0 \otimes \exp\left(-\beta H_R\right) , \tag{2.2}$$

where ρ_A^0 is the initial state of the test-particle. Finally, they choose the coupling coefficients,

$$C_j := \lambda\omega_j \tag{2.3}$$

with some $\lambda > 0$.

Remarks:

- Instead of uniformly spaced oscillator frequencies $\omega_j = \frac{j}{N}$, it is sufficient to assume that the frequency distribution $\varrho_N(\omega)d\omega = \frac{1}{N}\sum_{j=1}^{N\Omega}\delta(\omega-\omega_j)d\omega$ tends, in the thermodynamic limit ($N \to \infty$), to a uniform distribution $\varrho(\omega)d\omega$ on $[0,\Omega]$ with density, say, c, i.e.

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N\Omega}h(\omega_j) = \int_0^\infty h(\omega)\varrho(\omega)d\omega = c\int_0^\Omega h(\omega)d\omega, \quad \forall h \in C[0,\Omega] \tag{2.4}$$

  with $\varrho(\omega)$ being c times the characteristic function of $[0,\Omega]$. Without loss of generality $c = 1$ can be assumed because changing c to 1 is equivalent to changing $\lambda \to \sqrt{c}\lambda$.

- In fact, the physically relevant quantity is the spectral density of the bath, i.e. the measure

$$J_N(\omega)d\omega = \frac{C^2(\omega)}{\omega}\varrho_N(\omega)d\omega = \frac{1}{N}\sum_{j=1}^{N\Omega}\frac{C_j^2}{\omega_j}\delta(\omega-\omega_j) \tag{2.5}$$

  (see (3.23) in [8], apart from constants), which in the case of [8] converges to the measure $\lambda^2\omega \cdot 1(\omega \leq \Omega)d\omega$ in the limit $N \to \infty$ (here $1(\cdot)$ is the characteristic function). The original model can be considered for any spectral density, but our analysis shows that the assumption $J(\omega) \sim \omega$ is needed for the Caldeira-Leggett derivation. However, in Section 2.4 we present a model where this assumption is not needed to derive a modified Fokker-Planck equation. For a different model in Section 2.5 we show that the diffusion mechanism is robust with respect to the spectral density; derivation of the Laplacian term in the Fokker-Planck equation does not require uniform frequency distribution. However, in that model the friction term would be time-delayed if ϱ is not uniform.

- We chose N to denote the number of oscillators per unit frequency instead of the total number of oscillators. Since $N \to \infty$ limit will be taken first, mathematically it is equivalent to letting the total number of oscillators go to infinity. However, in case of the only physical model discussed here (in Section 3), this choice of N will have a physical meaning: it will be the the size of the harmonic crystal measured on the lengthscale of the confining potential.

Now the main steps of [8] are the following:

• *First*, using that $H_I + H_R$ is quadratic and relying on Feynman path integrals, Caldeira and Leggett explicitly compute the evolution of the test-particle after tracing out the reservoir variables. The evolution equation of the test-particle involves a diffusive forcing term and a memory term (friction), the latter being non-local in time (see (2.8) below, as well as (2.25)). These terms translate the effect of the evolution of the reservoir on the test-particle. It is very standard in this context that integrating out the reservoir variables gives rise to a non-Markovian evolution for the test-particle, despite that the evolution of the full system is Markovian (cf. also (3.21)).

• *Second*, they perform the thermodynamical limit where the number of oscillators (per unit frequency) in (2.1) becomes infinite ($N \to \infty$).

• *Third*, they consider the semiclassical limit $\hbar \to 0$, they perform the limit $\Omega \to \infty$, i.e. the frequency range becomes infinite (removing ultraviolet cutoff), and they let the inverse temperature β go to zero.

These last two limits allow them to eliminate all the non-Markovian effects. Caldeira and Leggett state the Fokker Planck equation

$$\partial_t w + v \cdot \nabla_x w - \nabla_x V_{eff}(x) \cdot \nabla_v w = \gamma \nabla_v (vw) + \sigma \Delta_v w \tag{2.6}$$

for the particle's Wigner distribution $w = w(t, x, v)$, which can be interpreted as a phase space (quasi)density, as a result of their asymptotic procedures. The friction coefficient γ is given as $\gamma = \sigma\beta/M$, which is the well-known Einstein's relation between friction, diffusivity and inverse temperature.

This type of equation is also known under the name of "Quantum Brownian motion", or "Quantum Langevin equation", and received a large interest in the context of interaction between light and matter (see, e.g. [16]).

The paper by Caldeira and Leggett raises several questions which have to be addressed. The most serious is that the limiting equation (2.6) is not of Lindblad form (see [1], [21], [48]), which is a generic condition for quantum systems to preserve the complete positivity of the density operator along the evolution. Recall that the true quantum evolution preserves this property. This shortcoming is closely related to the fact, that the equation itself contains β (as the ratio of γ and σ), while $\beta \to 0$ limit was actually used along its derivation. This is not just a mathematical inconsistency. Either the friction term should be negligible compared to the diffusion term in (2.6) if $\beta \to 0$ limit is really taken; or there should be an extra term in the equation if β is thought of as a small but nonzero number. In the latter case this extra term should restore the Lindblad form of the equation, and it is not clear why this term could be considered negligible compared to the friction.

The confusion probably comes from the unspecified order of limits, which is the second important question and the paper [8] is admittedly vague about it (see comments after (3.33) in [8]). In fact, in several cases [8] uses "asymptotic regimes" without taking rigorous limits. The Caldeira-Leggett system relaxes to equilibrium under very mild conditions without any further limits (apart from $N \to \infty$). However, the precise equation which governs this relaxation depends on the physical parameters of the system. In particular, only in some limiting regimes it is true that the limiting equation is a differential equation (i.e. time-delayed memory terms vanish). Furthermore, to obtain a Fokker-Planck type equation, especially a Laplacian term (Δ_v), requires further restrictions which are implicitly assumed in various steps of the Caldeira-Leggett derivation. We will demonstrate in particular, that the Δ_v term in (2.6) is due to the special choice of the coupling constants $C_k \sim \omega_k$ (or, equivalently, to $J(\omega) \sim \omega$) *and* to the fact that the cutoff frequency Ω goes to infinity. In physical systems finite Ω is more realistic, but then the resulting equation contains a modified (cutoff) Laplacian, and the system will not be described by a diffusive equation for short times. Although apparently Caldeira-Leggett are not interested in short times (see their remark below (3.35) in [8]) they do not formulate this concept rigorously. The scaling limit, we introduce in Sections 2.4 and 2.5 will be the precise mathematical tool for this.

Finally, from a mathematical point of view, it is desirable to eliminate the non-rigorous steps in the original derivation; especially since the order of limits actually does influence the form of the limiting equation. In addition, the systematic use of the Feynman path integral should be avoided in a rigorous proof, since it is a mathematically undefined concept.

Our main results are Theorem 2.1, 2.2 and 2.3.

2.1 Source of Diffusion in Various Kinetic Models

In order to explain the origin of diffusion (Δ_v) in [8], we have to analyze the effects of the limits introduced there. To avoid Feynman path integrals, we present the basic idea of [8] in the mathematical language we will use in our proofs.

We take the Hamiltonian as in [8] (see (2.1)) with $M = 1$ and specify the choice $V(x) = \frac{1}{2}x^2$ (harmonic oscillator), in the spirit of [18], [2], [36], [64], [16]. We use the fact that, for Gaussian Hamiltonians, the evolution equation for the Wigner transform of the density matrix is a first order linear partial differential equation ([66], [49], [35]), which can be solved by the method of characteristics (see also [64] for a similar observation).

In the quadratic case, we can scale $\hbar$ out of the equation (2.1). Let

$$H := \frac{1}{2}\Big(-\Delta_x + x^2\Big) + \frac{1}{2}\sum_{j=1}^{N\Omega}\Big(-\Delta_{R_j} + \omega_j^2 R_j^2\Big) + \frac{1}{\sqrt{N}}\Big(\sum_{j=1}^{N\Omega} C_j R_j\Big)\cdot x, \qquad (2.7)$$

then $\exp(-it\hbar^{-1}H_{CL})$ and $\exp(-itH)$ are unitarily equivalent under the rescaling of variables $x \to x\hbar^{-1/2}$, $R_j \to R_j\hbar^{-1/2}$, or in other words, we choose units where $\hbar = 1$, $M = 1$.

If $V(x)$ is not quadratic, then it gives rise to a genuine pseudodifferential operator in the Wigner equation and $\hbar$ cannot be scaled out. In the semiclassical limit ($\hbar \to 0$) this term converges to the differential operator $\nabla_x V \cdot \nabla_v w$ in (2.6). This fact is well-known for general semiclassical Wigner equations [49], [50], [37], [51].

We will not prove Theorem 2.1 for a general potential because our main goal is to find the origin of diffusivity which is independent of the confining potential. We restrict ourselves to the most convenient quadratic case.

We also present two different scaling limits starting from (2.7) which allows to follow the dynamics up to long times. However, we believe that not just our result on the original Caldeira-Leggett model (in Section 2.3) can be extended to include general potentials, but also the resonance effect in Sections 2.4 and 2.5.

2.1.1 Diffusion in the Original Model

After integrating out the reservoir variables in the equations for the characteristics, it eventually reduces to the following ODE for the particle's position variable $X(t)$ (see (2.25) for the exact result),

$$X''(t) + X(t) = f(t) + \lambda^2 \int_0^t S(t-s)X(s)\, ds\,. \tag{2.8}$$

Here λ is as in (2.3), S is an explicit function corresponding to the memory effect, and the forcing term f is,

$$f(t) = -\frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N\Omega} \omega_j \left[R_j \cos\omega_j t + P_j \frac{\sin\omega_j t}{\omega_j} \right] , \tag{2.9}$$

where R_j, P_j are the initial position and momentum variables of the oscillators. Let $R_j^* := \sqrt{2\beta}\omega_j R_j$ and $P_j^* := \sqrt{2\beta} P_j$ be their rescaled versions. In the high temperature limit these become standard Gaussian variables since the classical Gibbs distribution is given by,

$$\prod_j e^{-\beta(P_j^2 + \omega_j^2 R_j^2)} = \prod_j e^{-\frac{1}{2}[(P_j^*)^2 + (R_j^*)^2]} ,$$

and at high temperature the quantum Gibbs distribution converges to the classical one (for the precise formulas, see (2.26)-(2.27)). Hence the choice (2.3) for C_j gives that,

$$f(t) = -\frac{\lambda}{\sqrt{2\beta}} \sum_{j=1}^{N\Omega} \left[\frac{R_j^*}{\sqrt{N}} \cos(\omega_j t) + \frac{P_j^*}{\sqrt{N}} \sin(\omega_j t) \right] , \tag{2.10}$$

and as $\beta \to 0$, R_j^*, P_j^* approach to standard Gaussians.

After integration by parts in the memory term in (2.8) we obtain (see (2.44))

$$X''(t) + X(t) = f(t) + \lambda^2 \Omega X(t) - (M \star X')(t) - xM(t) \tag{2.11}$$

where M is an approximate Dirac delta function $M(t) \sim \lambda^2 \delta_0(t)$ in the limit $\Omega \to \infty$. Here $\star$ stands for convolution. The term $\lambda^2\Omega$ is the frequency shift of the test-particle oscillator. The friction term $M \star X'$ has a main Markovian part $\lambda^2 X'$ and a non-Markovian part which is negligible as $\Omega \to \infty$.

The effect of the limits introduced in [8] are as follows

• The high temperature limit ($\beta \to 0$) plays two roles. First, it makes the rescaled initial data R_j^*, P_j^* standard Gaussians. Second, it forces the full friction term to be negligible compared to the forcing term.

• In the thermodynamic limit ($N \to \infty$) the sum in (2.10) becomes the sum of the real and imaginary parts of the truncated complex white noise,

$$dW^{(\Omega)}(t) := \int_0^\Omega e^{i\omega t} g(d\omega) \ ,$$

where $g(d\omega)$'s are independent centered Gaussian random variables with variance $\mathbf{E}\Big[g(d\omega)^2\Big] = d\omega$ (for precise definition see Section 2.2).

• Removing the ultraviolet cutoff ($\Omega \to \infty$) gives the (complex) white noise,

$$dW(t) = \int_0^\infty e^{i\omega t} g(d\omega) \tag{2.12}$$

for the forcing term. To prevent instability ($\lambda^2\Omega > 1$), we have to take the simultaneous limit $\lambda \to 0$, $\Omega \to \infty$ which may lead to a nonzero constant phase shift $\lambda^2\Omega$.

Our main concern is to identify the origin of the Δ_v (diffusion) term, which will come from the forcing term. Hence this term should not vanish in the limit, which indicates that $\beta \to 0$ and $\lambda \to 0$ limits must be related:

$$\lambda = \lambda_0 \beta^{1/2} \tag{2.13}$$

with some fixed λ_0.

In summary, the solution $X(t)$ to (2.8) converges to the solution of a pure harmonic oscillator with a white noise forcing, i.e. $\theta X(t) + \sigma X'(t) \sim (\eta \star dW)(t)$, where

$\eta(s) = \theta \sin s + \sigma \cos s$ is the harmonic oscillator trajectory (with initial condition $\eta(0) = \sigma$, $\eta'(0) = \theta$). In particular the mean square displacement (both in space and velocity)

$$\mathbf{E}\Big|\theta X(t) + \sigma X'(t)\Big|^2 \sim \mathbf{E}\Big|\Big(\eta \star dW^{(\Omega)}\Big)(t)\Big|^2 = \int_0^\Omega \Big| \int_0^t \eta(t-s) e^{-i\omega s} ds\Big|^2 d\omega \quad (2.14)$$

behaves *quadratically* in t for small t for every finite Ω, hence it is *not* diffusive for short times. The diffusive behavior (linear mean square displacement) is regained only *after* the $\Omega \to \infty$ limit or after long times.

We emphasize that, from this point of view, the v-Laplacian in the CL model immediately stems from the particular asymptotic distribution of the frequencies (uniform from zero to infinity) in the forcing term. In other terms this model demonstrates diffusion in a setup where a plain diffusive forcing mechanism was essentially put in by hand. Diffusion appears already in very short time scales as a result of high frequency oscillators. This means that there is a shorter, unexplored time scale on which most of the oscillators live, hence the initial Hamiltonian with the Caldeira-Leggett limits should not be considered microscopic, rather mesoscopic. This problem is especially transparent if the heat bath is provided by phonons (crystal lattice vibrations) which have a physical ultraviolet cutoff (lattice spacing). In other words, for systems with UV cutoff and without time rescaling, Δ_v is not the correct diffusion operator.

In contrast to this diffusive mechanism, the source of the diffusion in more realistic models dealing with a moving test-particle interacting with many degrees of freedom is the *scaling limit*, especially time rescaling. This means that in these models the full frequency spectrum of the diffusion is collected over a long time from the cumulative effects of interactions with bounded frequency, and the diffusive behaviour is visible only on a much larger time (and sometimes space) scale than that of the microscopic interaction (collision) mechanism. This makes a key difference between the present model and other works dealing, for instance, with collisional models as scaling limits of microscopic dynamics, i.e. macroscopic long time behaviour of Schrödinger equations (see e.g. [62], [63], [44], [38], [25], [26], [27], [51], [52], [10], [11], [42] or also [5]).

We remedy this drawback of the CL scaling in Sections 2.4 and 2.5, as we indicate now.

2.1.2 Diffusion from Resonances in the Scaling Limit

In Section 2.4, we show that one can also recover a diffusive non-kinetic behaviour from the Caldeira-Leggett Hamiltonian under a more realistic space-time scaling limit. Namely, for a *fixed* cutoff in frequency Ω, and after the high-temperature limit, we consider the resulting dynamics for the test-particle for large time $t \sim \alpha^{-2}$ and large space and velocity variables x, $v \sim \alpha^{-1}$. Here $\alpha \to 0$ is a scaling parameter and we define $X = \alpha x$, $V = \alpha v$, $T = \alpha^2 t$ to be the macroscopic (or rescaled) position, velocity and time variables. We prove that the phase space density is subject to a heat equation both in the (rescaled) velocity and position variables. In particular, the energy of the test-particle increases up to α^{-2} due to the resonances with bath particles of high energy (but bounded frequency). Recall that the temperature of the heat bath is $\beta^{-1} \to \infty$, hence bath particles can have large energy even with bounded frequency.

In this case the diffusion indeed comes from the cumulative effect of bounded frequency interactions via a change of scale. This is in fact a high energy diffusion in phase space; the test-particle is heated up. The forcing frequency distribution can be quite arbitrary, the only condition is that it has to carry energy at the resonant frequency. The diffusion comes from a pure resonance effect, and this seems to be a more universal physical feature in this context (see [16]). However, the high temperature limit is still essential in this derivation.

In Section 2.5, we keep the temperature fixed and we rescale only time, $t = T\delta^{-1}$ (where $\delta \to 0$ plays the role of α^2 above), space and velocity remain unscaled. The reason is that the bath temperature is finite, hence the typical energy ("temperature") of the test-particle remains finite as well. Since the particle Hamiltonian is confining (energy level sets are compact in phase space), the particle remains effectively localized. As a result we get a small scale diffusion in phase space with friction, after integrating out the fast circular motion. Again the diffusion comes from resonance and is developed over a long time period, and the contributing bath frequencies are bounded.

One of the important features of these models is that the derivation is quite insensitive to the actual form of the spectral density $J(\omega)$ (2.5); the only relevant quantity is its value at the resonant frequency.

2.1.3 Comparison of the Three Models

The main goal of our investigation is to derive diffusion, i.e. a Δ_v term in the limiting equation. The time dependence of the mean square displacement of the characteristics (2.14) is quadratic for small time (unless $\Omega \to \infty$) and is linear for large time. To see diffusion on *all* times considered, there are two alternatives: either we take $\Omega \to \infty$ or we rescale time.

I.) If $\Omega \to \infty$, then the coupling λ must go to zero to keep the frequency shift $\lambda^2\Omega$ finite. Up to a positive time t, the total effect of the friction term is of order $\lambda^2 t$, while the diffusive (forcing) term is roughly of order $\lambda^2 t/\beta$ for larger times, see (2.61), however for short times it is only quadratic in t. Hence for finite times $\lambda^2 t \to 0$, the friction term vanishes. Moreover, the diffusive term vanishes as well, unless $\beta \to 0$ is chosen such that $\lambda^2 \sim \beta$, i.e. the weak coupling and high temperature limits must be related. The frequency shift is $\lambda^2\Omega$ and its actual size depends on the simultaneous limits $\lambda \to 0$, $\Omega \to \infty$. If $\lambda \to 0$ is taken first, then $\Omega \to \infty$ and the frequency shift vanishes. If $\lambda^2\Omega$ is kept at a positive constant along the limits, then we see a frequency shift. These two cases are described in Theorem 2.1, where frictionless Fokker-Planck equations are derived on the microscopic time scale.

II.) If we consider long times, i.e. $t = \alpha^{-2}T$, $\alpha \to 0$ and T is fixed, then the size of the diffusive term is roughly $\lambda^2\alpha^{-2}T/\beta$ for *all* T. To compensate for the blowup α^{-2}, we can either rescale space and velocity ($x = \alpha^{-1}X$, $v = \alpha^{-1}V$) or we set $\lambda^2 \sim \alpha^2$.

II/a. If we rescale space and velocity as well, then the friction term has a size $\lambda^2 T$ and the diffusion term is of order $\lambda^2 T/\beta$ (in the new variables). One would like to keep λ and β fixed to see both friction and diffusion. But since the phase shift, $\lambda^2\Omega$, has to be kept finite, it forces keeping Ω finite as well. This is the most realistic physical situation. However, the friction has a non-Markovian part, whose size is $\lambda^2 T$ if Ω is fixed (and it goes to zero only if $\Omega \to \infty$). Hence the limiting equation must have a term which is nonlocal in time. This is the extra term which is missing in (2.6), but its inclusion would lead to an integro-differential equation and not to Fokker-Planck.

To derive a differential equation, the non-Markovian friction part has to be killed. With finite Ω it is possible only if $\lambda \to 0$, and then the full friction is eliminated.

In order not to eliminate the diffusive term as well, $\beta \sim \lambda^2$ is necessary. This again leads to the high temperature limit, but now Ω is fixed and the diffusion comes from long-time cumulative resonance effects. The fast oscillator motion on the microscopic time scale has to be integrated out; either in time or by a radial averaging. This is the model in Section 2.4.

II/b. If we set $\lambda^2 \sim \alpha^2$ and keep β finite, then we see a finite diffusion on a microscopic space and velocity scale. The friction term $\lambda^2 t$ remains positive and the ratio of the friction to the diffusion is β, which gives Einstein relation. Hence Ω could be kept fixed to see the diffusion mechanism.

However, the non-Markovian part of the memory does not vanish unless $\Omega \to \infty$. The qualitative analysis of Section 2.5 shows that Ω can grow very slowly (like $|\log \alpha|^7$), i.e. the non-Markovian part of the friction is weak for large times and moderately large Ω. This was probably the heuristic idea of Caldeira and Leggett to neglect this term. However, this effect shows up only after time rescaling; for finite microscopic times t this term is not negligible.

Hence we let $\Omega \to \infty$, and assume that $\lambda^2 \Omega$ converges to a fixed number (possibly zero). This number gives the frequency shift. Again, we see that the size of the frequency shift delicately depends on the simultaneous limiting procedure. This is the model of Section 2.5 (where $\delta := \alpha^2$ is introduced for brevity).

We point out that in models II/a and II/b the origin of the diffusion is the time rescaling. Since the forcing frequencies are kept finite, there is no diffusion on the microscopic scale; it becomes visible only after the large time rescaling. Hence the physically questionnable limits, $\beta \to 0$, $\Omega \to \infty$ have nothing to do with the emergence of the diffusion in these models.

However, at least one of these limits is necessary to arrive at a differential equation instead of an integro-differential equation with time delayed memory term. In model II/a. (Section 2.4) we use $\beta \to 0$ and keep Ω fixed, while in II/b. (Section 2.5) we let $\Omega \to \infty$ and keep β finite.

We always consider nonnegative times $t \geq 0$. However, most of our computations are valid for *any* time, except those which are directly responsible for the emergence of the diffusion (Laplacian, or linear mean square displacement). We shall point out these steps. If time were evolved backward, $t < 0$, then the same argument would yield an opposite sign of the Laplacian (so that along the evolution it is regularizing) in the final limiting equations. This is the usual phenomenon of irreversibility of the parabolic equations.

2.2 Preliminary Results

2.2.1 The Wigner Formalism

The density matrix,

$$\rho^{N,\varepsilon} := \rho^{N,\varepsilon}(t,x,y,R,Q) \ , \tag{2.15}$$

which is the solution of,

$$i\partial_t \rho^{N,\varepsilon} = [H, \rho^{N,\varepsilon}] \ , \tag{2.16}$$

represents the state of the system "particle + reservoir" at time t with the reservoir variables $R = (R_1, \dots, R_{N\Omega})$, $Q = (Q_1, \dots, Q_{N\Omega})$. We index the density matrix by N and the superscript $\varepsilon = (\beta, \Omega, \lambda)$, which stands for all the other scaling parameters; recall that β is the inverse temperature, Ω is the frequency range and λ is the coupling strength in the Hamiltonian (2.7).

We take the initial data (independent of ε for simplicity),

$$\rho_A^0 \otimes e^{-\beta H_R} \ , \tag{2.17}$$

with $\rho_A^0 := \rho_A^{N,\varepsilon}(t=0)$. Here $H_R := \frac{1}{2}\sum_{k=1}^{N\Omega}\Big(- \Delta_{R_k} + \omega_k^2 R_k^2\Big)$ is the reservoir Hamiltonian and $\rho_A^{N,\varepsilon}(t,x,y)$ is the density matrix at time t of the test-particle. It is defined by

$$\rho_A^{N,\varepsilon}(t,x,y) := \int_{\mathbb{R}^{N\Omega}} \rho^{N,\varepsilon}(t,x,y,R,R)\, dR \ ,$$

with the obvious notation $dR = dR_1 \dots dR_{N\Omega}$. As usual, we do not distinguish between operators and their kernels in the notation. Following [8], we have to compute,

$$Tr_R\Big(e^{-itH}\big(\rho_A^0 \otimes e^{-\beta H_R}\big)e^{itH}\Big) \ ,$$

where Tr_R is the partial trace over the reservoir variables. We observe that the Hamiltonian (2.7) is quadratic, so that equation (2.16) can actually be transformed into a first order transport partial differential equation by using the Wigner transform. Indeed, let us define the Wigner transform $w^{N,\varepsilon}(t)$ of $\rho^{N,\varepsilon}(t)$ by,

$$\begin{aligned} w^{N,\varepsilon}(t,x,v,R,P) \quad &:= \quad \int_{\mathbb{R}^{N\Omega+1}} \rho^{N,\varepsilon}\Big(t, x+\frac{y}{2}, x-\frac{y}{2}, R+\frac{Q}{2}, R-\frac{Q}{2}\Big) \\ &\times \ \exp\Big(-i[yv+\sum_{k=1}^{N\Omega} Q_k P_k]\Big)\ dy\ dQ\ . \end{aligned} \tag{2.18}$$

Also, let us define the Wigner transform of $\rho_A^{N,\varepsilon}$ by,

$$w_A^{N,\varepsilon}(t,x,v) := \int_{\mathbb{R}} \rho_A^{N,\varepsilon}\Big(t, x+\frac{y}{2}, x-\frac{y}{2}\Big)\ \exp(-iyv)\ dy\ .$$

We have the well-known property,

$$w_A^{N,\varepsilon}(t,x,v) := \int_{\mathbb{R}^{2N\Omega}} w^{N,\varepsilon}(t,x,v,R,P)\ dR\ dP\ , \tag{2.19}$$

and the initial datum for $w^{N,\varepsilon}$ is easily computed from (2.17) and the Mehler kernel,

$$w^{N,\varepsilon}(t=0,x,v,R,P) = w_0(x,v) W_0^{N,\varepsilon}(R,P) \tag{2.20}$$

with

$$\begin{aligned} W_0^{N,\varepsilon}(R,P) \quad := \quad \prod_{k=1}^{N\Omega} \Bigg[\ & 4\pi\Big(\frac{\cosh(\beta\omega_k)-1}{\cosh(\beta\omega_k)+1}\Big)^{1/2} \ \exp\Big(-\{\frac{\omega_k(\cosh(\beta\omega_k)-1)}{\sinh(\beta\omega_k)}R_k^2\}\Big) \\ &\times \exp\Big(-\{\frac{\sinh(\beta\omega_k)}{\omega_k(\cosh(\beta\omega_k)+1)}P_k^2\}\Big)\ \Bigg]\ . \end{aligned}$$

Here, $w_0(x,v)$ is the initial datum for the test-particle, i.e. it is the Wigner transform of $\rho_A^0(x,y)$ and we shall assume the following regularity for w_0,

$$\widehat{w}_0(\xi,\eta) := \int_{\mathbb{R}^2} w_0(x,v) \exp(-i[x\xi+v\eta])\ dx\ dv \quad \in L^1(\mathbb{R}_\xi\times\mathbb{R}_\eta)\ . \tag{2.21}$$

It is well known that, if $\rho^{N,\varepsilon}$ satisfies the Von-Neumann equation (2.16) with Hamiltonian given by (2.7), then its Wigner transform (2.18) satisfies the following partial differential equation,

$$\begin{aligned} &\partial_t w^{N,\varepsilon} + v\ \partial_x w^{N,\varepsilon} - x\ \partial_v w^{N,\varepsilon} + \sum_{k=1}^{N\Omega}\Big(P_k\ \partial_{R_k} w^{N,\varepsilon} - \omega_k^2 R_k\ \partial_{P_k} w^{N,\varepsilon}\Big) \\ &-\frac{\lambda}{\sqrt{N}}\Big(\sum_{k=1}^{N\Omega}\omega_k R_k\Big)\ \partial_v w^{N,\varepsilon} - \frac{\lambda}{\sqrt{N}}\Big(\sum_{k=1}^{N\Omega}\omega_k x\ \partial_{P_k} w^{N,\varepsilon}\Big) = 0\ . \end{aligned} \tag{2.22}$$

As a conclusion we can now rephrase our original problem in the Wigner formalism: following [8], we want to derive a diffusive behaviour for $w_A^{N,\varepsilon}(t)$, the trace of $w^{N,\varepsilon}(t)$, in the thermodynamic limit ($N \to \infty$) and in certain limiting regimes of ε. Here, $w^{N,\varepsilon}$ satisfies (2.22) with initial datum (2.20).

2.2.2 Solution by Characteristics

Equation (2.22) can easily be solved by the method of characteristics. In fact, for all values of time t, and for all smooth, compactly supported test functions $\phi(x,v)$, we have,

$$\begin{aligned}
&\int_{\mathbb{R}^2} w_A^{N,\varepsilon}(t,x,v)\overline{\phi}(x,v)\,dx\,dv \\
=\;& \int_{\mathbb{R}^{2N\Omega+2}} w(t=0,x,v,R,P)\,\overline{\phi}(X(t),V(t))\,dx\,dv\,dR\,dP \\
=\;& \int_{\mathbb{R}^{2N\Omega+6}} \hat{w}_0(\xi,\eta)\overline{\hat{\phi}(\theta,\sigma)}e^{i(x\xi+v\eta)}e^{-i(X(t)\theta+V(t)\sigma)} \\
&\times W_0^{N,\varepsilon}(R,P)\,dx\,dv\,dR\,dP\,d\xi\,d\eta\,d\theta\,d\sigma,
\end{aligned} \tag{2.23}$$

where we have introduced the (forward) characteristics,

$$\begin{aligned}
X'(t) = V(t)\,, \quad & V'(t) = -X(t) - \frac{\lambda}{\sqrt{N}}\sum_{k=1}^{N\Omega}\omega_k R_k(t) \\
R_k'(t) = P_k(t)\,, \quad & P_k'(t) = -\omega_k^2 R_k(t) - \frac{\lambda}{\sqrt{N}}\omega_k X(t)\,,
\end{aligned} \tag{2.24}$$

with initial data $X(0)=x$, $V(0)=v$, $R_k(0)=R_k$ and $P_k(0)=P_k$. Here we used that the flow (2.24) preserves the Lebesgue measure over $\mathbb{R}^{2(N\Omega+1)}$. For simplicity, we did not index the characteristics by N, ε, but $X(t), V(t)$ in (2.23) depend on N, ε. However, sometimes we will use $X_N(t)$ for special emphasis.

Integrating with respect to $R_k(t)$ in (2.24) and inserting the result in the equation for $X(t)$ gives,

$$\begin{aligned}
X''(t) + X(t) \;=\;& -\frac{\lambda}{\sqrt{N}}\sum_{k=1}^{N\Omega}\omega_k\Big[R_k\cos\omega_k t + P_k\frac{\sin\omega_k t}{\omega_k}\Big] \\
&+\frac{\lambda^2}{N}\sum_{k=1}^{N\Omega}\int_0^t \omega_k \sin\omega_k(t-s)X(s)ds\,.
\end{aligned} \tag{2.25}$$

The right-hand-side of (2.25) is of the form 'forcing term + memory term'.

In view of (2.20) and (2.23), the partial trace over the oscillators is an integral with respect to a Gaussian distribution in R_k, P_k with (unnormalized) density,

$$\exp\Big[-\frac{\omega_k(\cosh\beta\omega_k - 1)}{\sinh\beta\omega_k}R_k^2 - \frac{\sinh\beta\omega_k}{\omega_k(\cosh\beta\omega_k + 1)}P_k^2\Big] . \tag{2.26}$$

Changing variables such that,

$$r_k = \sqrt{\frac{2\omega_k(\cosh\beta\omega_k - 1)}{\sinh\beta\omega_k}}R_k , \quad p_k = \sqrt{\frac{2\sinh\beta\omega_k}{\omega_k(\cosh\beta\omega_k + 1)}}P_k ,$$

we obtain (after normalization) the standard Gauss measure,

$$d\mu_N = \prod_{k=1}^{N\Omega}\frac{1}{2\pi}e^{-\frac{1}{2}(r_k^2+p_k^2)}dr_k dp_k , \tag{2.27}$$

i.e. r_k, p_k are independent standard Gaussian variables. The integration with respect to this probability measure will be denoted by $\mathbf{E}_N$.

Using these new variables and integration by parts with respect to s, the equation (2.25) for $X_N(t) = X(t)$ becomes,

$$X_N''(t) + X_N(t) = f_N(t) + \lambda^2\Omega X_N(t) - (M_N \star X_N')(t) - xM_N(t) , \tag{2.28}$$

with,

$$f_N(t) := -\frac{\lambda}{\sqrt{N}}\sum_{k=1}^{N\Omega}A_\beta(\omega_k)\Big[r_k\cos\omega_k t + p_k\sin\omega_k t\Big] , \tag{2.29}$$

and,

$$M_N(t) := \frac{\lambda^2}{N}\sum_{k=1}^{N\Omega}\cos\omega_k t . \tag{2.30}$$

Here we defined,

$$A(\omega) = A_\beta(\omega) := \sqrt{\frac{\omega(\cosh\beta\omega + 1)}{2\sinh\beta\omega}} .$$

We see that the memory term is split into three parts. The term $\lambda^2\Omega X_N$ induces a frequency shift of the test-particle oscillator, $M_N \star X_N'$ is the friction term and the last inhomogeneous term will be irrelevant. We define

$$a^2 = a_\varepsilon^2 := 1 - \lambda^2\Omega$$

(recall that ε stands for the triple (β, Ω, λ)), and we always assume that a_ε is uniformly separated from zero, i.e. $c_0 \le a_\varepsilon \le 1$ with some constant $c_0 > 0$. We can rewrite (2.28) as

$$X_N''(t) + a^2 X_N(t) = f_N(t) - (M_N \star X_N')(t) - x M_N(t) \ . \tag{2.31}$$

2.2.3 The Thermodynamic Limit

We now perform the limit $N \to \infty$. A possible way is to solve (2.25) (iteratively), and compute the limit in the corresponding formulae (see (2.50) later). This rigorously gives the thermodynamic limit but we present an alternative approach which is more illuminating to explain the asymptotic diffusion that we shall recover in Section 2.3. We first need an a priori bound.

Lemma 2.1 *Let $X_N(t)$ solve (2.31) with initial conditions $X(0) = x$, $X'(0) = v$, and let*

$$F_N(t) := \sup_{s \le t} \mathbf{E}_N |X_N(s)| + \sup_{s \le t} \mathbf{E}_N |X_N'(s)| \ . \tag{2.32}$$

Then there is a constant $C > 0$ such that

$$F_N(t) \le C e^{Kt} \left(|x| + |v| + K|x| + \sup_{s \le t} \Big\{ s e^{-Ks} \Big\} \Big[\lambda^2 \Omega \Big(\beta^{-1} + \Omega \Big) \Big]^{1/2} \right) \ . \tag{2.33}$$

uniformly in N, where

$$K = K(\lambda, \Omega) := C \lambda^2 \Big(1 + \frac{1}{|\Omega - a|} \Big) \ . \tag{2.34}$$

and $a^2 = 1 - \lambda^2 \Omega \in (0, 1]$.

Proof. From the fundamental solution of (2.31), one has

$$\begin{aligned} X_N(t) &= x \cos at + v a^{-1} \sin at \\ &\quad + \int_0^t a^{-1} \sin a(t-s) \Big[f_N(s) - (M_N \star X_N')(s) - x M_N(s) \Big] ds \ , \\ X_N'(t) &= -xa \sin at + v \cos at \\ &\quad + \int_0^t \cos a(t-s) \Big[f_N(s) - (M_N \star X_N')(s) - x M_N(s) \Big] ds \ . \end{aligned} \tag{2.35}$$

First step. To estimate the memory term in (2.35), we write,

$$\begin{aligned}\textstyle\int_0^t \sin[a(t-s)](M_N \star X_N')(s)ds &= \Big(\sin(a\,\cdot\,) \star M_N \star X_N'\Big)(t) \\ &= \textstyle\int_0^t \Big(\int_0^s \sin[a(s-u)]M_N(u)du\Big)X_N'(t-s)ds\ ,\end{aligned}$$

An easy calculation shows that the inner integral is bounded by

$$\begin{aligned}\Big|\int_0^s \sin[a(s-u)]M_N(u)du\Big| &= \Big|\Big(M_N \star \sin(a\,\cdot\,)\Big)(s)\Big| \\ &\leq k\lambda^2\Big(1+\frac{1}{|a-\Omega|}\Big)\ ,\end{aligned} \tag{2.36}$$

with a universal constant k uniformly in N. Indeed, notice that,

$$\lim_{N\to\infty} M_N(s) = \lambda^2 \frac{\sin\Omega s}{s} =: M(s)\ , \tag{2.37}$$

uniformly for $s \in [0,t]$. Moreover $\int_0^s \sin[a(s-u)]M(u)du$ can be estimated by splitting the integration into two regimes $u \leq 1$ and $u \geq 1$ (or $u \leq s$ regime only if $s \leq 1$) and both regimes can be estimated by elementary integration by parts to obtain (2.36).

Hence the expected value of the integral of the memory terms in (2.35) is estimated by,

$$\begin{aligned}&\mathbf{E}_N\Big|\int_0^t a^{-1}\sin a(t-s)\Big[-(M_N \star X_N')(s) - xM_N(s)\Big]ds\Big| \\ &\qquad\leq a^{-1}k\lambda^2\Big(1+\frac{1}{|a-\Omega|}\Big)\Big[|x| + \int_0^t F_N(s)\,ds\Big]\ ,\end{aligned} \tag{2.38}$$

and similarly for the cosine term in (2.35).

Second step. For the forcing term one computes,

$$\mathbf{E}_N\Big|\int_0^t \sin[a(t-s)]f_N(s)ds\Big| \;\leq\; t\sup_{s\leq t}\Big(\mathbf{E}_N|f_N(s)|^2\Big)^{1/2}\ . \tag{2.39}$$

We have,

$$\mathbf{E}_N|f_N(s)|^2 = \frac{\lambda^2}{N}\sum_{k=1}^{N\Omega} A_\beta^2(\omega) \leq \hat{k}\lambda^2\Omega\Big(\beta^{-1}+\Omega\Big)\ , \tag{2.40}$$

where $\hat{k}$ is again some positive constant, independent of N. Indeed, this sum is an approximating Riemann sum for the integral,

$$\lambda^2 \int_0^\Omega A_\beta^2(\omega) d\omega = \lambda^2 \int_0^\Omega \frac{\omega(\cosh\beta\omega + 1)}{2\sinh\beta\omega}\, d\omega\ ,$$

which satisfies the estimate (2.40). Hence we obtain,

$$\begin{aligned} \mathbf{E}_N\Big[|X_N(t)| + |X_N'(t)|\Big] \quad &\le \quad |x| + |v| + k\lambda^2\Big(1 + \frac{1}{|a-\Omega|}\Big)\Big[|x| + \int_0^t F_N(s)\, ds\Big] \\ &\qquad + t\Big[\hat{k}\lambda^2\Omega\Big(\beta^{-1} + \Omega\Big)\Big]^{1/2} . \end{aligned} \tag{2.41}$$

By a standard Gronwall-type argument we conclude (2.33). ■

2.2.4 Digression on Stochastic Integrals

Stochastic integration is integration with respect to a random measure. Once the measure is specified, the integrals are defined as limits of integrals of stepfunctions. We do not develop this notion here, just indicate how it is related to the present problem.

Definition 2.1 *The ensemble of random variables $g(A)$, A running over the Borel sets of $\mathbb{R}$, is called standard Gaussian random measure if $g(A)$ is a centered real Gaussian random variable for all A and $\mathbf{E}g(A)g(B) = |A \cap B|$ where $|\cdot|$ is the Lebesgue measure.*

In the thermodynamic limit $N \to \infty$, the forcing term (2.29) converges in an $L^2(d\mu_N)$ sense towards the stochastic integral,

$$f(t) := -\lambda \int_0^\Omega A_\beta(\omega)\Big[r(d\omega)\cos\omega t + p(d\omega)\sin\omega t\Big]\ , \tag{2.42}$$

where $r(d\omega)$, $p(d\omega)$ are independent standard Gaussian random measures. The expectation with respect to their joint measure is denoted by $\mathbf{E}$. Clearly $f_N(t)$ is a Riemann sum approximation of $f(t)$ by choosing $r_k := N^{1/2} r\Big(\Big[\frac{k-1}{N}, \frac{k}{N}\Big]\Big)$ and $p_k := N^{1/2} p\Big(\Big[\frac{k-1}{N}, \frac{k}{N}\Big]\Big)$, since their distribution is $d\mu_N$ (see (2.27)). In particular we can realize all f_N's and f on a common probability space. Note that $f(t)$ is formally a white noise (see (2.12)) when the 'hyperbolic factor' $A_\beta(\omega)$ is replaced by one and $\Omega = \infty$.

Lemma 2.2 *For $1 < \Omega < \infty$ there exist a random function $X(t)$ such that,*

$$\lim_{N\to\infty}\Big(\sup_{s\le t}\mathbf{E}|X_N(s)-X(s)|+\sup_{s\le t}\mathbf{E}|X'_N(s)-X'(s)|\Big)=0\ , \tag{2.43}$$

and $X(t)$ almost surely satisfies the equation,

$$X''(t)+a^2X(t)=f(t)-(M\star X')(t)-xM(t)\ , \tag{2.44}$$

with initial conditions $X(0)=x$, $X'(0)=v$. Moreover,

$$F(t):=\sup_{s\le t}\mathbf{E}|X(s)|+\sup_{s\le t}\mathbf{E}|X'(s)|\ ,$$

satisfies the same estimate as $F_N(t)$ (see (2.33)),

$$F(t)\le Ce^{Kt}\left(|x|+|v|+K|x|+\sup_{s\le t}\Big\{se^{-Ks}\Big\}\Big[\lambda^2\Omega\Big(\beta^{-1}+\Omega\Big)\Big]^{1/2}\right)\ . \tag{2.45}$$

Proof. Let us define $X(t)$ by the integral equation,

$$\begin{aligned} X(t) &= x\cos at+va^{-1}\sin at \\ &\quad+\int_0^t a^{-1}\sin[a(t-s)]\Big[f(s)-(M\star X')(s)-xM(s)\Big]ds\ , \end{aligned} \tag{2.46}$$

Since,

$$\int_0^t\mathbf{E}|f(s)|^2ds=\lambda^2\int_0^\Omega\frac{\omega(\cosh\beta\omega+1)}{2\sinh\beta\omega}d\omega<\infty\ ,$$

$X(t)$ is well defined almost surely and satisfies (2.44). Moreover, the uniformity of (2.33) in N, and (2.43) shows that $F(t)$ satisfies (2.45). So we are left with proving (2.43).

Let $Z_N(s):=X_N(s)-X(s)$, then it satisfies (from (2.35) and (2.46)),

$$\begin{aligned} Z_N(t) &= \int_0^t a^{-1}\sin[a(t-s)]\Big[f_N(s)-f(s)-(M\star Z'_N)(s) \\ &\qquad -(M_N-M)\star X'_N(s)-x(M_N-M)(s)\Big]ds\ , \end{aligned}$$

and a similar formula holds $Z'_N(t)$. Clearly $Z_N(0)=Z'_N(0)=0$. Hence, similarly to (2.41),

$$\mathbf{E}\Big(|Z_N(s)|+|Z'_N(s)|\Big)\le K\textstyle\int_0^t\widetilde{F}_N(s)ds$$
$$+a^{-1}t\sup_{s\le t}\left(\Big\{|x|+t\sup_{u\le t}\mathbf{E}|X'_N(u)|\Big\}|M_N(s)-M(s)|+\mathbf{E}|f_N(s)-f(s)|\right)\ ,$$

with $\widetilde{F}_N(t) = \sup_{s\leq t} \mathbf{E}|Z_N(s)| + \sup_{s\leq t} \mathbf{E}|Z'_N(s)|$. We use again a Gronwall argument to obtain (2.43), based upon the control of $\sup_{u\leq t} \mathbf{E}|X'_N(u)|$ from Lemma 2.1 and the facts that $|M_N(s) - M(s)| \to 0$ (see (2.37)) and $\mathbf{E}|f_N(s) - f(s)| \to 0$ uniformly for $s \leq t$ as $N \to \infty$.

In order to check $\mathbf{E}|f_N(s) - f(s)| \to 0$, we observe that,

$$r_k = N^{1/2} r\Big(\Big[\frac{k-1}{N}, \frac{k}{N}\Big]\Big) = N^{1/2} \int \mathbf{1}\Big(\omega \in \big[\frac{k-1}{N}, \frac{k}{N}\big]\Big) r(d\omega) ,$$

to obtain,

$$\begin{aligned} &\mathbf{E}|f(s) - f_N(s)|^2 \\ &= \lambda^2 \int_0^\Omega \left[A_\beta(\omega) - \sum_{k=1}^{N\Omega} A_\beta(\omega_k) \cdot \mathbf{1}\Big(\omega \in \big[\frac{k-1}{N}, \frac{k}{N}\big]\Big) \right]^2 d\omega , \end{aligned} \tag{2.47}$$

which goes to zero as $N \to \infty$, uniformly in $s \leq t$. For uniformly spaced frequencies, $\omega_k = \frac{k}{N}$, (2.47) is straightforward. For frequencies satisfying only the uniform density condition (2.4) with $c = 1$, first one has to verify that

$$\lim_{N\to\infty} \frac{1}{N} \#\Big\{k \ : \ \big|\omega_k - \frac{k}{N}\big| \geq \eta\Big\} = 0$$

for any $\eta > 0$, and then using the continuity of the function $A_\beta(\omega)$ to conclude the result. ■

The conclusion of Section 2.2 is the,

Lemma 2.3 *Assume (2.4) with $c = 1$ and assume (2.21). Let $w_A^{N,\varepsilon}(t)$ be defined as (2.19), while $w^{N,\varepsilon}(t)$ is the solution of (2.22) with initial datum (2.20). Then, in the thermodynamic limit, we have for all $\phi(x,v) \in C_c^\infty(\mathbb{R}^2)$ locally uniformly for $t \in \mathbb{R}$,*

$$\lim_{N\to\infty} \int_{\mathbb{R}^2} w_A^{N,\varepsilon}(t,x,v)\overline{\phi}(x,v) dx\, dv = \int_{\mathbb{R}^2} w_A^\varepsilon(t,x,v)\overline{\phi}(x,v) dx\, dv , \tag{2.48}$$

where w_A^ε is defined by,

$$\begin{aligned} &\int_{\mathbb{R}^2} w_A^\varepsilon(t,x,v)\overline{\phi}(x,v) dx dv = \\ &\qquad = \mathbf{E} \int_{\mathbb{R}^6} \hat{w}_0(\xi,\eta) \overline{\hat{\phi}(\theta,\sigma)} e^{i(x\xi+v\eta)} e^{-i(X(t)\theta + X'(t)\sigma)} d\xi\, d\eta\, dx\, dv\, d\theta\, d\sigma , \end{aligned} \tag{2.49}$$

and X satisfies (2.44) .

For the proof one only has to observe that the dominated convergence theorem applies and use Lemma 2.2 and (2.23) (recalling that X is actually X_N in that formula). ■

Remark: As an alternative proof which avoids any reference to probabilistic concepts, we can easily compute the right-hand-side of (2.23) directly by performing a finite dimensional Gaussian integration with respect to $d\mu_N$ (again, $X(t)$ is actually $X_N(t)$ in (2.23)). In this case all the integrals $\int_0^{N\Omega}(\dots)d\omega$ are finite sums and the $N \to \infty$ limit is taken only after having performed the $d\mu_N$ integration. We easily find that the right-hand-side of (2.23) is equal to,

$$\begin{aligned}&\int_{\mathbb{R}^2} \hat{w}_0\Big(A(t)\theta + A'(t)\sigma\ ,\ B(t)\theta + B'(t)\sigma\Big)\ \overline{\hat{\phi}(\theta,\sigma)} \\ &\times \exp\Big[-\int_0^\Omega \frac{[A_\omega(t)\theta + A'_\omega(t)\sigma]^2}{2\lambda_\omega}\ d\omega - \int_0^\Omega \frac{[B_\omega(t)\theta + B'_\omega(t)\sigma]^2}{2\mu_\omega} d\omega\Big]\ d\theta\ d\sigma\ ,\end{aligned} \tag{2.50}$$

where $\lambda_\omega = [2\omega(\cosh(\beta\omega) - 1)]/[\sinh(\beta\omega)]$, $\mu_\omega = [2\sinh(\beta\omega)]/[\omega(\cosh(\beta\omega)+1)]$, and,

$$\begin{aligned}\Psi(t) &= \lambda^2 \int_0^\Omega \int_0^t \omega \sin(\omega[t-s])\sin(s)\ ds\ d\omega\ , \\ A(t) &= \cos(t) + (\Psi \star A)(t)\ , \\ B(t) &= \sin(t) + (\Psi \star B)(t)\ , \\ A_\omega(t) &= -\int_0^t \lambda\omega\cos(\omega s)\sin(t-s)\ ds + (\Psi \star A_\omega)(t)\ , \\ B_\omega(t) &= -\int_0^t \lambda \sin(\omega s)\sin(t-s)\ ds + (\Psi \star B_\omega)(t)\ .\end{aligned}$$

2.3 The Fokker-Planck Equation from the Original Caldeira-Leggett Model

2.3.1 Evolution Without Friction

In the spirit of [8], we would like to exhibit a scaling where the solution of (2.44) is close to the solution $\widetilde{X}(t)$ of the equation without friction term below. The scaling parameters are $\varepsilon = (\beta, \Omega, \lambda)$. The frictionless equation (compare with (2.44)) is,

$$\widetilde{X}''(t) + a^2\widetilde{X}(t) = f(t)\ , \qquad \text{with,} \qquad \widetilde{X}(0) = x\ ,\quad \widetilde{X}'(0) = v\ , \tag{2.51}$$

recalling that $a^2 = a_\varepsilon^2 = 1 - \lambda^2\Omega \in (0,1]$.

We need a continuity result ensuring that $X(t)$ and $\widetilde{X}(t)$ are close. If $Y(t) = X(t) - \widetilde{X}(t)$, then,

$$Y''(t) + a^2 Y(t) = -(M \star X')(t) - xM(t) \ ,$$

with initial conditions $Y(0) = Y'(0) = 0$. Given the bound (2.45) on $X(t)$ and (2.36) it is trivial to see that,

$$\begin{aligned}
&\mathbf{E}\Big(|Y(t)| + |Y'(t)|\Big) \qquad (2.52)\\
&\leq Kte^{Kt}\left(|x| + |v| + K|x| + \sup_{s\leq t}\Big\{se^{-Ks}\Big\}\Big[\lambda^2\Omega\Big(\beta^{-1} + \Omega\Big)\Big]^{1/2}\right) ,
\end{aligned}$$

where $K = C\lambda^2(1 + \frac{1}{|\Omega - a|})$ (see (2.34)). So in particular the solution of (2.44) tends to the solution of (2.51) in a very strong norm if the right-hand-side of (2.52) goes to zero. This happens for example for such limiting regimes of $\varepsilon = (\beta, \Omega, \lambda)$ that $\lambda \to 0$ and $\Omega \to \infty$ in such a way that $a^2 = 1 - \lambda^2\Omega \in (0,1]$ and $\lambda^2\beta^{-1/2} \to 0$.

Hence, as soon as one can ensure a small right-hand-side in (2.52), we can replace X by $\widetilde{X}$ in (2.48)-(2.49) by the Lebesgue theorem, since the x, v, θ, σ integrations range over a bounded domain (ϕ is compactly supported) and we assumed $\widehat{w}_0(\xi,\eta) \in L^1$ (see (2.21)). This proves

Lemma 2.4 *Let $\widetilde{w}_A^\varepsilon$ be defined as,*

$$\begin{aligned}
&\int_{\mathbb{R}^2} \widetilde{w}_A^\varepsilon(t,x,v)\overline{\phi}(x,v)dxdv \qquad (2.53)\\
&= \mathbf{E}\int_{\mathbb{R}^6} \hat{w}_0(\xi,\eta)\overline{\hat{\phi}(\theta,\sigma)}e^{i(x\xi+v\eta)}e^{-i(\widetilde{X}(t)\theta + \widetilde{X}'(t)\sigma)}d\xi\ d\eta\ dx\ dv\ d\theta\ d\sigma \ ,
\end{aligned}$$

analogously to (2.49). Then,

$$\lim_\varepsilon \int_{\mathbb{R}^2} \widetilde{w}_A^\varepsilon(t,x,v)\overline{\phi}(x,v)dxdv = \lim_\varepsilon \int_{\mathbb{R}^2} w_A^\varepsilon(t,x,v)\overline{\phi}(x,v)dxdv \ , \qquad (2.54)$$

for any limit of the parameters $\varepsilon = (\beta, \Omega, \lambda)$ for which the right hand side of (2.52) goes to zero. ■

2.3.2 Computing the Dynamics of the Test-Particle when the Memory Vanishes

In this section we compute $w^\varepsilon(t,x,v)$ when X is actually replaced by $\widetilde{X}$, the solution of (2.51), in (2.49). We have,

$$\begin{aligned}
\widetilde{X}(t) &= x\cos at + va^{-1}\sin at + \int_0^t a^{-1}\sin a(t-s)f(s)ds \ , \\
\widetilde{X}'(t) &= -xa\sin at + v\cos at + \int_0^t \cos[a(t-s)]f(s)ds \ .
\end{aligned}$$

Hence

$$\begin{aligned}
&\int\limits_{\mathbb{R}^2} \widetilde{w}_A^\varepsilon(t,x,v)\overline{\phi(x,v)}dx\ dv \qquad (2.55)\\
&= \mathbf{E}\int\limits_{\mathbb{R}^6} \widehat{w}_0(\xi,\eta)\overline{\widehat{\phi}(\theta,\sigma)}e^{i(x\xi+v\eta)}e^{-i(\widetilde{X}(t)\theta+\widetilde{X}'(t)\sigma)}\ d\xi\ d\eta\ dx\ dv\ d\theta\ d\sigma \\
&= \mathbf{E}\int_{\mathbb{R}^2} \widehat{w}_0\Big(\xi_{\theta,\sigma}(t),\eta_{\theta,\sigma}(t)\Big)\overline{\widehat{\phi}(\theta,\sigma)}e^{-i\int_0^t \eta_{\theta,\sigma}(t-s)f(s)ds}\ d\theta\ d\sigma \ ,
\end{aligned}$$

with,

$$\eta_{\theta,\sigma}(t) := \theta a^{-1}\sin at + \sigma\cos at \ , \qquad \xi_{\theta,\sigma}(t) := \theta\cos at - \sigma a\sin at \ , \qquad (2.56)$$

which are, by the way, harmonic oscillator trajectories,

$$\frac{d}{dt}\eta_{\theta,\sigma}(t) = \xi_{\theta,\sigma}(t) \ , \quad \frac{d}{dt}\xi_{\theta,\sigma}(t) = -a^2\eta_{\theta,\sigma}(t) \ .$$

After performing the expectation in (2.55), we arrive at

Lemma 2.5 *With the notations above, we have for any $t \geq 0$,*

$$\begin{aligned}
&\int_{\mathbb{R}^2} \widetilde{w}_A^\varepsilon(t,x,v)\overline{\phi(x,v)}\ dx\ dv \qquad (2.57)\\
&= \int_{\mathbb{R}^2} \widehat{w}_0\Big(\xi_{\theta,\sigma}(t),\eta_{\theta,\sigma}(t)\Big)\overline{\widehat{\phi}(\theta,\sigma)}e^{-\frac{1}{2}Q(t)}\ d\theta\ d\sigma \ ,
\end{aligned}$$

with

$$Q(t) := Q(t;\theta,\sigma;\beta,a) = \lambda^2\int_0^\Omega A_\beta^2(\omega)H(t,\omega)d\omega \ , \qquad (2.58)$$

$$H(t,\omega) := H(t,\omega;\theta,\sigma;a) = \Big| \int_0^t \eta_{\theta,\sigma}(s) e^{-i\omega s} ds \Big|^2 . \tag{2.59}$$

The functions $\xi_{\theta,\sigma}$, $\eta_{\theta,\sigma}$ are defined by (2.56). The function $H(t,\omega)$ satisfies the following estimate

$$H(t,\omega) \le \frac{\gamma^2}{4a^2} \left\{ \Big| \frac{e^{it(a-\omega)} - 1}{a-\omega} \Big|^2 + \frac{4}{(a+\omega)^2} \right\} \tag{2.60}$$

with $\gamma^2 := \theta^2 + a^2\sigma^2$. Assuming $\Omega > 1$ we also have

$$Q(t) = I\lambda^2 t \gamma^2 \frac{\cosh \beta a + 1}{2a \sinh \beta a} + \lambda^2 \gamma^2 B(t) \tag{2.61}$$

with $I := \frac{\pi}{2}$ and with a function B satisfying $B(0) = 0$ and

$$|B(t)| \le C\big[1 + \beta^{-1}\big]\big[1 + (\log t)_+\big]\big[1 + \log \Omega\big] \tag{2.62}$$

with a universal constant C. Also, we have the estimate:

$$Q(t) = \mathbf{E}\Big(f \star \eta_{\theta,\sigma}\Big)^2(t) = \mathbf{E}\Big(\theta \widetilde{X}(t) + \sigma \widetilde{X}'(t)\Big)^2 + \mathcal{O}\Big[(|x| + |v|)(|\theta| + |\sigma|)\Big] . \tag{2.63}$$

Remarks:

- Notice that $Q(t)$ grows quadratically in t for small t (since H does so). This means that the test-particle as described by the Wigner distribution w_A^ε has a ballistic behaviour when the memory effects disappear (quadratic growth of the mean squared displacement $\mathbf{E}\widetilde{X}^2(t)$). In the rest of this paper we show that, under several specific scaling limits, one can indeed replace w_A^ε with $\widetilde{w}_A^\varepsilon$ (see Lemma 2.4) *and* recover a linear growth for $Q(t)$, i.e. a diffusive behaviour for the test-particle. In particular, this is where the time asymmetric condition $t \ge 0$ is used.

- Suppose that the frequency distribution $\varrho(\omega)$ (see (2.4)) is not uniform (hence $J(\omega)$ is not linear). By the same calculation, we still obtain (2.57) except that $Q(t)$ is given by $\lambda^2 \int_0^\Omega A_\beta^2(\omega) H(t,\omega)\varrho(\omega) d\omega$. Assuming that $\varrho(\omega)$ is bounded and it is differentiable around the resonant frequency $\omega = a$, we obtain the analogue of (2.61),

$$Q(t) = I\lambda^2 t \gamma^2 \varrho(a) \frac{\cosh \beta a + 1}{2a \sinh \beta a} + \lambda^2 \gamma^2 B(t) ,$$

and the estimates (2.60), (2.62) remain valid. The proof is identical. This remark will be used in Sections 2.4 and 2.5.

Proof. We only have to show the estimates (2.60) and (2.62). These are straightforward calculations. We use the following notation,

$$a\sigma + i\theta = \gamma e^{i\phi} .$$

(i.e. $\theta = \gamma \sin\phi$, $a\sigma = \gamma\cos\phi$ and $\gamma^2 = \theta^2 + a^2\sigma^2$). Hence, from (2.56),

$$\eta_{\theta,\sigma}(t) = \frac{\gamma}{2a}\Big(e^{i(\phi-at)} + e^{-i(\phi-at)}\Big) ,$$

and

$$H(t,\omega) \;=\; \frac{\gamma^2}{4a^2}\Big|e^{2i\phi}\frac{e^{-it(a+\omega)}-1}{a+\omega} - \frac{e^{it(a-\omega)}-1}{a-\omega}\Big|^2 ,$$

which proves (2.60).

To prove (2.61)-(2.62), for any $\Omega > 1$ we obtain, by extracting the worst singularity

$$\begin{aligned} Q(t) &= \lambda^2\int_0^{\Omega}\frac{\omega(\cosh\beta\omega+1)}{2\sinh\beta\omega}H(t,\omega)d\omega \\ &= \lambda^2\frac{\gamma^2}{4a^2}\widetilde{B}(t) + \lambda^2\frac{\gamma^2}{4a^2}\int_0^{\Omega}\frac{\omega(\cosh\beta\omega+1)}{2\sinh\beta\omega}\Big|\frac{e^{it(a-\omega)}-1}{a-\omega}\Big|^2 d\omega , \end{aligned} \tag{2.64}$$

with,

$$\begin{aligned} \widetilde{B}(t) :=& \int_0^{\Omega}\frac{\omega(\cosh\beta\omega+1)}{2\sinh\beta\omega} \\ &\times\Big\{\Big|\frac{e^{-it(a+\omega)}-1}{a+\omega}\Big|^2 - 2\mathrm{Re}\Big(e^{2i\phi}\frac{e^{-it(a+\omega)}-1}{a+\omega}\frac{e^{it(a-\omega)}-1}{a-\omega}\Big)\Big\}d\omega , \end{aligned} \tag{2.65}$$

and $\widetilde{B}(0) = 0$. With the substitution $\omega' = t(a-\omega)$ in (2.65), one easily computes

$$|\widetilde{B}(t)| \le C\big[1+\beta^{-1}\big]\big[1+(\log t)_+\big]\big[1+\log\Omega\big] . \tag{2.66}$$

The second integral in (2.64) is proportional to t for large t since $\Omega > 1$. Obviously it becomes uniformly bounded if $\Omega < a \le 1$ (a trivial behaviour), and this is the very reason why we assumed $\Omega > 1$ in this section. Then the main contribution comes from $\omega \sim a$, and by the same change of variables as above, the result is,

$$Q(t) = \lambda^2 \gamma^2 B(t) + I \lambda^2 t \gamma^2 \frac{\cosh a\beta + 1}{2a \sinh a\beta} \tag{2.67}$$

with $I := \frac{\pi}{2}$, and $\widetilde{B}(t)$ is replaced by some $B(t)$ which also satisfies (2.66) and $B(0) = 0$. ■

2.3.3 The Caldeira-Leggett Limits: Obtaining the Fokker-Planck Equation

In this section we rigorously perform the scaling limit introduced in [8]. We prove the following,

Theorem 2.1 *Let w_A^ε be the Wigner distribution of the test-particle after the thermodynamic limit, as given by Lemma 2.3. We recall that ε stands for (β, Ω, λ). Let $\lambda = \lambda_0 \beta^{1/2}$ with some fixed λ_0.*

a) [Nonzero frequency shift.] *Assume that $a^2 = 1 - \lambda^2 \Omega = 1 - \lambda_0^2 \beta \Omega \in (0, 1]$ is fixed. Then for any $t \geq 0$ the following weak limit exists*

$$W(t, x, v) = \lim_{\substack{\Omega \to \infty, \beta \to 0 \\ \beta\Omega = (1-a^2)\lambda_0^{-2}}} w_A^\varepsilon(t, x, v) \ . \tag{2.68}$$

The limit holds in the topology of $C^0([0, \infty)_t; \mathcal{D}'_{x,v})$. Moreover, W satisfies the Fokker-Planck equation,

$$\partial_t W + v \partial_x W - a^2 x \partial_v W - \frac{\lambda_0^2 \pi}{2} \Delta_v W = 0 \ , \tag{2.69}$$

with initial datum $W(t = 0) = w_0$ satisfying (2.21)

b) [No frequency shift.] *For any $t \geq 0$ the following weak limit exists,*

$$W(t, x, v) = \lim_{\Omega \to \infty} \lim_{\beta \to 0} w_A^\varepsilon(t, x, v) \ . \tag{2.70}$$

[the order of limits cannot be interchanged], and W satisfies the Fokker-Planck equation,

$$\partial_t W + v \partial_x W - x \partial_v W - \frac{\lambda_0^2 \pi}{2} \Delta_v W = 0 \ , \tag{2.71}$$

with initial datum $W(t = 0) = w_0$ satisfying (2.21)

Proof. For the proof of part a) first notice that Lemma 2.4 applies since the right hand side of (2.52) goes to zero under the prescribed limits. Hence X can be replaced by $\widetilde{X}$ and we can therefore rely on Lemma 2.5 above. On the other hand, since we assumed $\lambda = \lambda_0 \beta^{1/2}$, we readily observe,

$$\begin{aligned} \lim{}^* Q(t) &= \lambda_0^2 \lim{}^* \int_0^\Omega \beta A_\beta^2(\omega) H(t,\omega) d\omega \\ &= \lambda_0^2 \int_0^\infty \Big| \int_0^t \eta_{\theta,\sigma}^2(s) e^{-i\omega s} ds \Big|^2 d\omega \ , \end{aligned} \tag{2.72}$$

where $\lim^*$ stands for the simultaneous limit $\beta \to 0$, $\Omega \to \infty$ such that $a^2 = 1 - \lambda_0^2 \beta \Omega \in (0,1]$ is fixed. Here we used that $\beta A_\beta(\omega)^2 \to 1$ in our limit if $\omega \leq \Omega^{1/2}$ and that $H(t,\omega) \in L^1(d\omega)$, see (2.60). The contribution $\omega \geq \Omega^{1/2}$ to the integral vanishes in the limit by the estimate (2.60) and the trivial bound $\frac{z \cosh z + 1}{\sinh z} \leq 2(1+z)$. Hence from the unitarity of the Fourier transform

$$\int_0^\infty \Big| \int_0^t g(s) e^{-i\omega s} ds \Big|^2 d\omega = \pi \int_0^t |g(s)|^2 ds \ , \tag{2.73}$$

which is valid for any real function g, we obtain

$$\lim{}^* Q(t) = \lambda_0^2 \pi \int_0^t \eta_{\theta,\sigma}^2(s) ds \ . \tag{2.74}$$

Here $t \geq 0$ is used, and this step is the origin of irreversibility. The end of the calculation is trivial. From Lemma 2.5 together with (2.74) we have,

$$\begin{aligned} \lim{}^* \int_{\mathbb{R}^2} w_A^\varepsilon(t,x,v) \overline{\phi(x,v)}\, dx\, dv &= \int_{\mathbb{R}^2} \widehat{w}_0 \Big(\xi_{\theta,\sigma}(t), \eta_{\theta,\sigma}(t) \Big) \\ &\quad \times \overline{\widehat{\phi}(\theta,\sigma)} e^{-I\lambda_0^2 \int_0^t \eta_{\theta,\sigma}^2(s) ds}\, d\theta\, d\sigma \ , \end{aligned} \tag{2.75}$$

where η and ξ are defined in (2.56) and $I = \frac{\pi}{2}$. We can define,

$$W(t,x,v) := \lim{}^* w_A^\varepsilon(t,x,v) \ , \tag{2.76}$$

as a weak limit given by (2.75). Then differentiating (2.75) gives (using (2.56)),

$$\begin{aligned} &\int_{\mathbb{R}^2} \partial_t W(t,x,v) \overline{\phi(x,v)} dx\, dv \\ &= \int_{\mathbb{R}^2} \partial_t \widehat{W}(t,\theta,\sigma) \overline{\widehat{\phi}(\theta,\sigma)} d\theta\, d\sigma \\ &= \int_{\mathbb{R}^2} \Big[-a^2 \eta_{\theta,\sigma}(t) \partial_\xi + \xi_{\theta,\sigma}(t) \partial_\eta - I \lambda_0^2 \eta_{\theta,\sigma}^2(t) \Big] \\ &\times \widehat{w}_0 \Big(\xi_{\theta,\sigma}(t), \eta_{\theta,\sigma}(t) \Big) \overline{\widehat{\phi}(\theta,\sigma)} e^{-I\lambda_0^2 \int_0^t \eta_{\theta,\sigma}^2(s) ds} d\theta\, d\sigma \ . \end{aligned} \tag{2.77}$$

Letting $t = 0$, we have,

$$\partial_t\Big|_{t=0}\widehat{W}(t,\theta,\sigma) = \Big[-a^2\sigma\partial_\theta + \theta\partial_\sigma - I\lambda_0^2\sigma^2\Big]\widehat{W}(t,\theta,\sigma)\Big|_{t=0} , \tag{2.78}$$

which is exactly the Fokker-Planck equation (2.71) after Fourier transforming,

$$\partial_t\Big|_{t=0}W(t,x,v) = \Big[a^2x\partial_v - v\partial_x + I\lambda_0^2\Delta_v\Big]W(t,x,v)\Big|_{t=0} . \tag{2.79}$$

Considering $t = 0$ is not a restriction, since the proof works for any L^1 initial condition.

The proof of part b) is completely analogous. We again notice that under the prescribed limits the right hand side of (2.52) goes to zero, hence Lemma 2.4 applies. Here $\eta_{\theta,\sigma}$ and $\xi_{\theta,\sigma}$ depend on the limiting parameters, since $a^2 = 1-\lambda^2\Omega = 1-\lambda_0^2\beta\Omega$. But $\lim_{\beta\to 0} a = 1$, hence

$$\lim_{\beta\to 0}\eta_{\theta,\sigma}(s) = \theta\sin s + \sigma\cos s , \qquad \lim_{\beta\to 0}\xi_{\theta,\sigma}(s) = \theta\cos s - \sigma\sin s \tag{2.80}$$

uniformly for $s \in [0,t]$. Therefore

$$\begin{aligned}
\lim_{\Omega\to\infty}\lim_{\beta\to 0} Q(t) &= \lambda_0^2\lim_{\Omega\to\infty}\int_0^\Omega\Big|\int_0^t\big[\theta\sin s + \sigma\cos s\big]e^{-i\omega s}ds\Big|^2 d\omega \\
&= \lambda_0^2\int_0^\infty\Big|\int_0^t\big[\theta\sin s + \sigma\cos s\big]e^{-i\omega s}ds\Big|^2 d\omega \\
&= \pi\lambda_0^2\int_0^t\big[\theta\sin s + \sigma\cos s\big]^2 ds .
\end{aligned} \tag{2.81}$$

Again, the last step is robust in a sense that it does not use the particular form of the function $\big[\theta\sin s + \sigma\cos s\big]$, instead it uses (2.73). But it is rigid in a sense that $\Omega = \infty$ is essential to get diffusive (linear) behaviour for the mean square displacement (2.63).

To conclude, we follow the calculation (2.75)-(2.79). In addition to the limit (2.81), we have to replace $\xi_{\theta,\sigma}(s), \eta_{\theta,\sigma}(s)$ by their limiting values (2.80) in the argument of $\widehat{w}_0$ to arrive at the analogue of (2.75). Dominated convergence theorem applies if we assume, additionally, that $\widehat{w}_0$ is continuous and bounded. However $\widehat{w}_0 \in L^1$, hence it can be approximated by such functions in L^1-norm. Using that the flow $(\theta,\sigma) \mapsto \Big(\xi_{\theta,\sigma}(s), \eta_{\theta,\sigma}(s)\Big)$ is measure preserving and that $\widehat{\phi}$ is bounded, one can easily see that the approximation error can be made arbitrarily small.

The rest of the calculation is identical to the proof of part a) and we obtain (2.71). ■

2.4 Scaling Limit at High Temperature: The Frictionless Heat Equation

We propose a different way to get diffusion from the Hamiltonian (2.7). As we mentioned, obtaining diffusion for the test-particle means that we have to extract linear dependence in time for $Q(t)$. In this section, linear growth is obtained from time rescaling and from the special form of linear combinations of $\sin s$ and $\cos s$ in Lemma 2.5. It relies on a resonance effect which comes from a singularity near $\omega \sim a$. The system $\widetilde{X}''(t) + a^2\widetilde{X}(t)$ (see (2.51)) picks up those modes from the forcing term $f(t)$ in (2.42) for which the frequency ω is close to its eigenfrequency. So, in this section we assume $\Omega > 1$ but finite, contrary to the previous section.

This effect is more robust (see the remark after (2.81)) in the sense that one *could* leave the hyperbolic functions βA_β^2 in (2.72) without ensuring a limit where it goes to 1. In other terms, we do not need the high temperature limit $\beta \to 0$ to obtain diffusion, unlike in Section 2.3, where this limit made the $d\omega$ measure uniform and we recovered a white noise forcing term.

Nevertheless, Lemma 2.5 needs the right-hand-side of (2.52) to go to zero in order to be applicable (one needs the friction to vanish), and this cannot be achieved keeping β fixed (cf. the comparison of the models in Section 2.1), hence we again set $\lambda = \lambda_0\beta^{1/2}$, $\beta \to 0$.

2.4.1 Large Space/Time Convergence of the Wigner Distribution

Let α be a small parameter. We describe the behaviour of the test-particle, as given by its Wigner distribution w_A^ε on time scales of order $1/\alpha^2$. We consider the diffusive scaling, i.e. the space coordinate scales as $1/\alpha$. Since the test-particle is a fast harmonic oscillator, and energies are transferred back and forth between space and velocity, we also have to consider velocities of order $1/\alpha$. Hence we introduce the following scaling,

$$t = T\alpha^{-2}, \qquad x = X\alpha^{-1}, \qquad v = V\alpha^{-1}\ , \tag{2.82}$$

where the capital letters are unscaled quantities (macroscopic variables). The rescaled reduced Wigner transform is defined as,

$$W_T^{\varepsilon,\alpha}(X, V) := w_A^\varepsilon(T\alpha^{-2}, X\alpha^{-1}, V\alpha^{-1})\ , \tag{2.83}$$

where w^ε_A is defined in Lemma 2.3 (after the thermodynamic limit). Its Fourier transform is,

$$\widehat{W}^{\varepsilon,\alpha}_T(\Theta,\Sigma) = \alpha^2 \widehat{w}^\varepsilon_A(T\alpha^{-2}, \Theta\alpha, \Sigma\alpha) \ , \tag{2.84}$$

where we use $\Theta = \theta\alpha^{-1}$ and $\Sigma = \sigma\alpha^{-1}$ rescaled dual variables. The initial condition is,

$$W^{\varepsilon,\alpha}_{T=0}(X,V) = W_0(X,V) \ , \qquad \widehat{W}^{\varepsilon,\alpha}_{T=0}(\Theta,\Sigma) = \widehat{W}_0(\Theta,\Sigma) \ , \tag{2.85}$$

and we assume that,

$$\widehat{W}_0(\Theta,\Sigma) \in L^1(\mathbb{R}_\Theta \times \mathbb{R}_\Sigma) \ . \tag{2.86}$$

The macroscopic testfunction $\Phi(X,V)$ is a smooth function with compact support, the microscopic testfunction is defined as,

$$\phi(x,v) = \Phi(x\alpha, v\alpha) = \Phi(X,V) \ ,$$

and in Fourier variables, $\widehat{\phi}(\theta,\sigma) = \alpha^{-2}\widehat{\Phi}(\theta\alpha^{-1},\ \sigma\alpha^{-1}) = \alpha^{-2}\widehat{\Phi}(\Theta,\Sigma)$.

We are now in position to state the theorem of this section,

Theorem 2.2 *Define the large time/space scale Wigner distribution $W^{\varepsilon,\alpha}_T(X,V)$ as in (2.83). Assume (2.86) for the initial data. Assume that $\lambda = \lambda_0\beta^{1/2}$ with a fixed $\lambda_0 > 0$ and fix the frequency cutoff $\Omega > 1$. Hence the limits of the parameters $\varepsilon = (\beta,\Omega,\lambda)$ are reduced to $\beta \to 0$. Then:*

a) *The following high-temperature limit exists in the weak sense for any $T \geq 0$:*

$$W^\alpha_T(X,V) := \lim_{\beta\to 0} W^{\varepsilon,\alpha}_T(X,V) \ .$$

b) *Define the following time average of W^α over one cycle of the harmonic oscillator (2.56),*

$$W^{\#,\alpha}_T(X,V) := \frac{1}{2\pi\alpha^2}\int_T^{T+2\pi\alpha^2} W^\alpha_S(X,V)dS \ . \tag{2.87}$$

Then the weak limit,

$$W^+_T(X,V) := \lim_{\alpha\to 0} W^{\#,\alpha}_T(X,V) \ , \tag{2.88}$$

exists for each $T \geq 0$ and it satisfies the heat equation in phase space,

$$\partial_T W_T^+ = \frac{\pi\lambda_0^2}{4}(\Delta_X + \Delta_V) W_T^+ \ , \tag{2.89}$$

with initial condition $W_{T=0}^+(X,V)$ given by

$$\widehat{W}_0^+(X,V) = \frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(X\sin s + V\cos s,\ X\cos s - V\sin s\Big)ds \ . \tag{2.90}$$

c) *Define the radial average,*

$$W_T^{*,\alpha}(X,V) := \frac{1}{2\pi}\int_0^{2\pi} W_T^{\alpha}(R\cos s, R\sin s)ds \tag{2.91}$$

with $R := \sqrt{X^2+V^2}$, and clearly $W_T^{*,\alpha}$ depends on R only. Again, the weak limit,

$$W_T^{\dagger}(X,V) := \lim_{\alpha\to 0} W_T^{*,\alpha}(X,V) \ ,$$

exists and the radially symmetric function $W_T^{\dagger}$ satisfies the heat equation (2.89) with initial condition,

$$W_{T=0}^{\dagger}(X,V) := \frac{1}{2\pi}\int_0^{2\pi} W_0(R\cos s, R\sin s)ds \ .$$

Remarks:

- The same theorem is true if the frequency distribution function $\varrho(\omega)$ is not uniform (see (2.4)), but it is only bounded and with bounded derivative. In particular the sharp cutoff is not necessary. The right hand side of the equation (2.89) is multiplied by the resonant spectral density $\varrho(1)$. The proof relies on two modifications of the $\varrho \equiv 1$ proof given below. First, the memory kernel $M(t)$ (see (2.30) and (2.37)) is modified to $\lambda^2 \int_0^{\Omega} \cos(\omega t)\varrho(\omega)d\omega$, and it still satisfies an estimate similar to (2.36) which leads to Lemma 2.4, hence the memory can be eliminated. Further, the second remark after Lemma 2.5 gives the large time behavior of $Q(t)$ in the general case. The details are left to the reader.

- Here we identified the equation in a weak sense in the space and velocity variables, but in a strong sense in the time variable and some averaging ((2.87) or (2.91)) was needed to ensure the existence of the limit. If we want to consider the limit in a weak sense in time as well, then there is no need for averaging. Based upon part b), one can easily prove that $W_T^+(X,V)$ can also be identified as the weak limit in space, velocity and time, i.e. we have the following

Corollary 2.1 *Under the above conditions the weak limit*

$$W_T^+(X,V) := \lim_{\alpha\to 0}\lim_{\beta\to 0} W_T^{\varepsilon,\alpha}(X,V)$$

exists in the topology of $\mathcal{D}'\big(\ [0,\infty)_T \times \mathrm{I\!R}_X \times \mathrm{I\!R}_V\ \big)$, *it coincides with (2.88) and satisfies (2.89).* ■

Proof of Theorem 2.2. Using the rescaling and the definition of w_A^ε (2.49), we have,

$$\begin{aligned}
\langle W_T^{\varepsilon,\alpha}, \Phi\rangle &= \int_{\mathrm{I\!R}^2} W_T^{\varepsilon,\alpha}(X,V)\overline{\Phi(X,V)}dX\ dV \qquad (2.92)\\
&= \alpha^2 \int_{\mathrm{I\!R}^2} w_A^\varepsilon(T\alpha^{-2},x,v)\overline{\phi(x,v)}dx\ dv\\
&= \alpha^2\ \mathbf{E}\int_{\mathrm{I\!R}^6} \widehat{w}_0(\xi,\eta)\overline{\widehat{\phi}(\theta,\sigma)}e^{i(x\xi+v\eta)}e^{-i(\theta X(t)+\sigma X'(t))}d\xi\ d\eta\ dx\ dv\ d\theta\ d\sigma\\
&= \mathbf{E}\int_{\mathrm{I\!R}^6} \widehat{W}_0(\xi\alpha^{-1},\eta\alpha^{-1})\overline{\widehat{\Phi}(\Theta,\Sigma)}e^{i(x\xi+v\eta)}\\
&\quad \times e^{-i\alpha(\Theta X(t)+\Sigma X'(t))}d\xi\ d\eta\ dx\ dv\ d\Theta\ d\Sigma\ ,
\end{aligned}$$

where $t = T\alpha^{-2}$.

First Step: the limit $\beta \to 0$.

Due to the choice $\lambda = \lambda_0\beta^{1/2}$, we can replace $X(t)$ by $\widetilde{X}(t)$ in the $\beta \to 0$ limit. For, the right hand side of (2.52) goes to zero as $\beta \to 0$, hence Lemma 2.4 applies. Hence,

$$\begin{aligned}
&\lim_{\beta\to 0}\langle W_T^{\varepsilon,\alpha}, \Phi\rangle =\\
&= \lim_{\beta\to 0}\mathbf{E}\int_{\mathrm{I\!R}^6} \widehat{W}_0(\xi\alpha^{-1},\eta\alpha^{-1})\overline{\widehat{\Phi}(\Theta,\Sigma)}e^{i(x\xi+v\eta)}e^{-i\alpha(\Theta\widetilde{X}(t)+\Sigma\widetilde{X}'(t))}d\xi\ d\eta\ dx\ dv\ d\Theta\ d\Sigma\\
&= \lim_{\beta\to 0}\mathbf{E}\int_{\mathrm{I\!R}^2} \widehat{W}_0\Big(\xi_{\Theta,\Sigma}(T\alpha^{-2}),\eta_{\Theta,\Sigma}(T\alpha^{-2})\Big)\overline{\widehat{\Phi}(\Theta,\Sigma)}e^{-\frac{1}{2}Q(T\alpha^{-2})}\ d\Theta\ d\Sigma\ , \qquad (2.93)
\end{aligned}$$

where in the second step we also used Lemma 2.5 and the fact that $\alpha^{-1}\xi_{\alpha\Theta,\alpha\Sigma} = \xi_{\Theta,\Sigma}$ and $\alpha^{-1}\eta_{\alpha\Theta,\alpha\Sigma} = \eta_{\Theta,\Sigma}$ (see (2.56)).

Recall that both $Q(t)$ and the trajectories $\xi_{\Theta,\Sigma}, \eta_{\Theta,\Sigma}$ depend on β, since $a^2 = 1-\lambda^2\Omega = 1-\lambda_0^2\beta\Omega$ appears in their definition (see (2.56)). Similarly to the argument at the end of the proof of part b) of Theorem 2.1, using that $\widehat{W_0} \in L^1(d\Theta\ d\Sigma)$, $\widehat{\Phi} \in L^\infty \cap C^0$, $Q \geq 0$, we see that the limit can be taken inside the integral and the trajectories $\xi_{\Theta,\Sigma}, \eta_{\Theta,\Sigma}$ can be replaced by their limiting values (as $a \to 1$)

$$\eta^*_{\Theta,\Sigma}(s) := \theta \sin t + \sigma \cos t \qquad \xi^*_{\Theta,\Sigma}(s) := \theta \cos t - \sigma \sin t \; . \tag{2.94}$$

We also use (see (2.61)) that

$$\lim_{\beta \to 0} Q(t) = I\lambda_0^2 t\gamma^2 + \lambda_0^2\gamma^2 B_0(t) \; .$$

with $B_0(t)$ satisfying $B_0(0) = 0$ and

$$|B_0(t)| \leq C\big[1 + (\log t)_+\big]\big[1 + \log \Omega\big] \tag{2.95}$$

(see (2.62)). We also recall that $\gamma^2 = \theta^2 + \sigma^2 = \alpha^2(\Theta^2 + \Sigma^2) =: \alpha^2\Gamma^2$. Hence,

$$\begin{aligned} \lim_{\beta \to 0}\langle W_T^{\varepsilon,\alpha}, \Phi\rangle &= \int_{\mathbb{R}^2} \widehat{W_0}\Big(\xi^*_{\Theta,\Sigma}(T\alpha^{-2}), \eta^*_{\Theta,\Sigma}(T\alpha^{-2})\Big)\ \overline{\widehat{\Phi}(\Theta,\Sigma)} \times \\ &\quad \times \exp\Big\{ -\frac{1}{2}\Big[I\lambda_0^2 T\alpha^{-2} + \lambda_0^2 B_0(T\alpha^{-2})\Big]\alpha^2(\Theta^2+\Sigma^2)\Big\} d\Theta\ d\Sigma \; . \end{aligned} \tag{2.96}$$

This relation defines the Fourier transform,

$$\widehat{W_T^\alpha}(\Theta,\Sigma) := \lim_{\beta \to 0} \widehat{W_T^{\varepsilon,\alpha}}(\Theta,\Sigma) \; ,$$

as a weak limit, and its inverse Fourier transform,

$$W_T^\alpha(X,V) := \lim_{\beta \to 0} W_T^{\varepsilon,\alpha}(X,V) \; .$$

We can compute its time derivative in Fourier space,

$$\begin{aligned} \langle \partial_T \widehat{W_T^\alpha}, \widehat{\Phi}\rangle &= \int \alpha^{-2}\Bigg[- \eta^*_{\Theta,\Sigma}(T\alpha^{-2})\partial_\xi + \xi^*_{\Theta,\Sigma}(T\alpha^{-2})\partial_\eta - \\ &\quad -\frac{\alpha^2}{2}\Big[I\lambda_0^2 + \lambda_0^2 B_0'(T\alpha^{-2})\Big](\Theta^2+\Sigma^2)\Bigg]\widehat{W_0}\Big(\xi^*_{\Theta,\Sigma}(T\alpha^{-2}), \eta^*_{\Theta,\Sigma}(T\alpha^{-2})\Big) \\ &\quad \times \overline{\widehat{\Phi}(\Theta,\Sigma)} \exp\Big\{ -\frac{1}{2}\Big[I\lambda_0^2 T\alpha^{-2} + \lambda_0^2 B_0(T\alpha^{-2})\Big]\alpha^2(\Theta^2+\Sigma^2)\Big\} d\Theta\ d\Sigma \; . \end{aligned}$$

As usual, we can let $T = 0$ to obtain,

$$\begin{aligned} &\partial_T\Big|_{T=0} \widehat{W_T^\alpha}(\Theta,\Sigma) \\ &= \alpha^{-2}\Bigg[- \Sigma\partial_\Theta + \Theta\partial_\Sigma - \frac{\alpha^2}{2}\Big[I\lambda_0^2 + \lambda_0^2 B_0'(0)\Big](\Theta^2+\Sigma^2)\Bigg]\widehat{W_0}(\Theta,\Sigma) \; . \end{aligned} \tag{2.97}$$

Second Step: the macroscopic limit $\alpha \to 0$.

Now the difficulty in (2.97) is that the convective term is too big compared to the last diffusive term since the motion takes place on two different time scales. There is the fast (microscopic) time scale of the harmonic oscillator described by $\alpha^{-2}[-\Sigma\partial_\Theta + \Theta\partial_\Sigma]$. Then there is a slow, macroscopic diffusive scale. We present two ways to average out the fast motion.

Part b) of Theorem 2.2: Averaging over a cycle.

Here we define $W^{\#,\alpha}$ according to (2.87). Now for any T fixed the formula,

$$\begin{aligned}\lim_{\alpha\to 0}\langle \widehat{W}_T^{\#,\alpha}, \widehat{\Phi}\rangle &= \lim_{\alpha\to 0}\int \widehat{W}_T^{\#,\alpha}(\Theta,\Sigma)\overline{\widehat{\Phi}(\Theta,\Sigma)}d\Theta d\Sigma \\ = \lim_{\alpha\to 0}\int &\left[\frac{1}{2\pi\alpha^2}\int_T^{T+2\pi\alpha^2} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(S\alpha^{-2}), \eta^*_{\Theta,\Sigma}(S\alpha^{-2})\Big)\right. \\ &\left.\times e^{-I_1\lambda_0^2 S(\Theta^2+\Sigma^2)}dS\right]\overline{\widehat{\Phi}(\Theta,\Sigma)}d\Theta d\Sigma\ ,\end{aligned} \tag{2.98}$$

defines a function,

$$\widehat{W}_T^{+}(\Theta,\Sigma) := \lim_{\alpha\to 0}\widehat{W}_T^{\#,\alpha}(\Theta,\Sigma)\ , \tag{2.99}$$

weakly, as we show below. Here $I_1 := \frac{I}{2} = \frac{\pi}{4}$ for brevity. Note that in (2.98) we neglected the term involving B_0 in the exponential (see (2.96)) since the estimate (2.95) readily implies $\alpha^2 B_0(T\alpha^{-2}) \to 0$. The exponential factor in (2.96) converges to that in (2.98) uniformly for all $S \le T$. Using $\widehat{\Phi} \in L^1$, we can apply the dominated convergence theorem along with approximating $\widehat{W}_0$ by bounded functions, similarly to the argument at the end of the proof of Theorem 2.1.

We have to show that the limit on the right-hand-side of (2.98) exists,

$$\begin{aligned}\langle \widehat{W}_T^{\#,\alpha}, \widehat{\Phi}\rangle &= \int_{\mathbb{R}^2}\left[\frac{1}{2\pi\alpha^2}\int_T^{T+2\pi\alpha^2} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(S\alpha^{-2}), \eta^*_{\Theta,\Sigma}(S\alpha^{-2})\Big)e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}dS\right. \\ &+\frac{1}{2\pi\alpha^2}\int_T^{T+2\pi\alpha^2} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(S\alpha^{-2}), \eta^*_{\Theta,\Sigma}(S\alpha^{-2})\Big) \\ &\left.\times\Big[e^{-I_1\lambda_0^2 S(\Theta^2+\Sigma^2)} - e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}\Big]dS\right]\overline{\widehat{\Phi}(\Theta,\Sigma)}d\Theta d\Sigma\ .\end{aligned} \tag{2.100}$$

The first term in (2.100) is independent of α, because it is just the integral of $\widehat{W}_0(\xi^*(s), \eta^*(s))$ over one full cycle of the harmonic oscillator (2.94),

$$\frac{1}{2\pi\alpha^2}\int_T^{T+2\pi\alpha^2} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(S\alpha^{-2}), \eta^*_{\Theta,\Sigma}(S\alpha^{-2})\Big)dS$$
$$= \frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(s), \eta^*_{\Theta,\Sigma}(s)\Big)ds \ .$$

The second term in (2.100) vanishes in the limit $\alpha \to 0$ since,

$$\left| e^{-I_1\lambda_0^2 S(\Theta^2+\Sigma^2)} - e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)} \right| \leq 2\pi I_1 \lambda_0 \alpha^2 (\Theta^2+\Sigma^2) e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}$$

(use that $|S-T| \leq 2\pi\alpha^2$), which kills the factor α^{-2} in (2.100) and then the length of the integration interval goes to zero. Dominated convergence theorem again has to be applied after an approximation. This shows that the limit in (2.99) makes sense and,

$$\begin{aligned} \langle W_T^+, \Phi\rangle &= \langle \widehat{W}_T^+, \widehat{\Phi}\rangle \\ &= \int_{\mathbb{R}^2} \Big[\frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(s), \eta^*_{\Theta,\Sigma}(s)\Big)ds\Big] \\ &\quad \times e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}\overline{\widehat{\Phi}(\Theta,\Sigma)}d\Theta d\Sigma \ . \end{aligned} \tag{2.101}$$

The time derivative is,

$$\begin{aligned} \langle \partial_T W_T^+, \Phi\rangle &= -I_1\lambda_0^2 \int_{\mathbb{R}^2} (\Theta^2+\Sigma^2)\Big[\frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(\xi^*_{\Theta,\Sigma}(s), \eta^*_{\Theta,\Sigma}(s)\Big)ds\Big] \\ &\quad \times e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}\overline{\widehat{\Phi}(\Theta,\Sigma)}d\Theta d\Sigma \\ &= -I_1\lambda_0^2 \Big\langle \widehat{W}_T^+, (\Theta^2+\Sigma^2)\widehat{\Phi}\Big\rangle \\ &= -I_1\lambda_0^2 \Big\langle W_T^+, -(\Delta_X+\Delta_V)\Phi\Big\rangle \ , \end{aligned}$$

which completes the proof of (2.89). The initial condition (2.90) is easily obtained from (2.101) by setting $T=0$ and taking inverse Fourier transform.

Part c) of Theorem 2.2: Radial average

The other possibility to eliminate the fast modes is to use the radial function

$W_T^{*,\alpha}$ defined in (2.91). Now the formula,

$$\begin{aligned} &\lim_{\alpha\to 0}\langle \widehat{W}_T^{*,\alpha}, \widehat{\Phi}\rangle = \lim_{\alpha\to 0}\int \widehat{W}_T^{*,\alpha}(\Theta,\Sigma)\overline{\widehat{\Phi}(\Theta,\Sigma)}\, d\Theta\, d\Sigma \\ = \; &\lim_{\alpha\to 0}\int \left[\frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(\xi^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2}), \eta^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2})\Big) ds\right] \\ &e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}\overline{\widehat{\Phi}(\Theta,\Sigma)}\, d\Theta\, d\Sigma\ , \end{aligned} \tag{2.102}$$

(with $\Gamma := \sqrt{\Theta^2+\Sigma^2}$) defines a radial function,

$$\widehat{W}_T^{\dagger}(\Theta,\Sigma) := \lim_{\alpha\to 0}\widehat{W}_T^{*,\alpha}(\Theta,\Sigma)\ ,$$

(depending only on $\Theta^2+\Sigma^2$) as a weak limit, as we show below. Note that in (2.102) we again neglected the term involving B_0 in the exponential for the same reason as in (2.98).

We have to show that the limit on the right-hand-side of (2.102) exists. But,

$$\xi^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2}) = \Gamma\cos(s+T\alpha^{-2})\ , \qquad \eta^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2}) = \Gamma\sin(s+T\alpha^{-2})\ ,$$

hence,

$$\begin{aligned} &\frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0\Big(\xi^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2}), \eta^*_{\Gamma\cos s,\Gamma\sin s}(T\alpha^{-2})\Big) ds \\ &\quad = \frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_0(\Gamma\cos s,\Gamma\sin s) ds =: \widehat{W}_0^{\dagger}(\Theta,\Sigma)\ , \end{aligned}$$

independently of α, which is the "radialized" initial condition in Fourier space.

So it is clear that the limit on the right-hand-side of (2.102) exists,

$$\lim_{\alpha\to 0}\langle \widehat{W}_T^{*,\alpha}, \widehat{\Phi}\rangle = \int \widehat{W}_0^{\dagger}(\Theta,\Sigma) e^{-I_1\lambda_0^2 T(\Theta^2+\Sigma^2)}\overline{\widehat{\Phi}(\Theta,\Sigma)}\, d\Theta\, d\Sigma =: \langle \widehat{W}_T^{\dagger}, \widehat{\Phi}\rangle\ ,$$

and clearly $W_T^{\dagger}$ also satisfies the heat equation (2.89). This ends the proof of Theorem 2.2. ■

2.5 Heat Equation with Friction at Finite Temperature

Here we choose a scaling where the Markovian part of the friction term does not vanish, i.e. we can keep β fixed and still get finite diffusion. Again we look at large time $t = T\delta^{-1}$ but now we do not scale the space variable. To eliminate the fast mode, we again integrate the angle. The result is a radial Fokker-Planck equation with friction. While the test-particle performs many cycles, it slowly diffuses out, and this diffusion is slowed down by a friction. The diffusion comes from resonance.

In this scaling limit the solution of (2.44) is close to the solution $\widetilde{X}(t)$ of an equation without a time delayed (non-Markovian) friction term, but a Markovian friction term will be present. Let us choose,

$$\lambda := \lambda_0 \delta^{1/2} ,$$

with some $\lambda_0 < 1$ fixed. We compare the solution of (2.44) to that of

$$\widetilde{X}''(t) + I\lambda^2 \widetilde{X}'(t) + a^2 \widetilde{X}(t) = f(t) ; \qquad \widetilde{X}(0) = x , \quad \widetilde{X}'(0) = v , \tag{2.103}$$

with $a^2 := 1 - \lambda^2 \Omega = 1 - \lambda_0^2 \delta^{-1} \Omega$, and,

$$I = \int_0^\infty \frac{\sin \Omega s}{s} ds = \frac{\pi}{2} . \tag{2.104}$$

We choose the scaling such that $a \in (0, 1]$, hence we always assume that $\Omega \le \delta^{-1}$, but to exploit resonance, we also assume $\Omega > 2$. The new term $\lambda^2 I \widetilde{X}'(t)$ for the approximate characteristic is due to the fact that $M(t) \sim \lambda^2 I \delta_0(t)$ as $\Omega \to 0$, where δ_0 denotes the Dirac delta measure. This term is the main part of the full friction $(M \star X')$ in (2.44). Notice that it is small compared with the pure harmonic oscillator terms, $\widetilde{X}'' + a^2 \widetilde{X}$, but it is not negligible, since we will consider long times $t \sim \lambda^{-2}$.

2.5.1 A Priori Bounds and Continuity Results

As in Section 2.3 we need a priori estimates for X, i.e. for,

$$F(t) := \sup_{s \le t} \mathbf{E}|X(s)| + \sup_{s \le t} \mathbf{E}|X'(s)| ,$$

and estimates on the difference between $\widetilde{X}(t)$ and $X(t)$. The estimate (2.45) in Lemma 2.2 (which originates in (2.33) in Lemma 2.1), however, is not precise enough for large times. The following estimate is a more precise version of Lemma 2.2.

Lemma 2.6 *Let* $t = T\delta^{-1}$, $\lambda = \lambda_0 \delta^{1/2}$ *with fixed* $\lambda_0 < 0$ *and* $T \ge 0$ *and we assume that* $2 \le |\log \delta|^7 \le \Omega \le \delta^{-1}$ *We also fix* $\beta > 0$, *hence the limit of scaling parameters* $\varepsilon = (\beta, \Omega, \lambda)$ *is reduced to* $\delta \to 0$, $\Omega \to \infty$ *with the side condition that* $\Omega \in \big[|\log \delta|^7, \delta^{-1}\big]$.

Let X be the solution to (2.44), then,

$$F(T\delta^{-1}) \leq C(\beta, \lambda_0, T)\Big(1 + |x| + |v|\Big) , \tag{2.105}$$

where C is monotone increasing in T. Moreover, if $\widetilde{X}$ is the solution to (2.103), then the difference $Y(t) =: X(t) - \widetilde{X}(t)$ satisfies,

$$\lim_{\delta\to 0}\Big(\sup_{s\leq T\delta^{-1}} \mathbf{E}|Y(s)| + \sup_{s\leq T\delta^{-1}} \mathbf{E}|Y'(s)|\Big) = 0 . \tag{2.106}$$

In particular,

$$\lim_{\delta\to 0}\int_{\mathbb{R}^2} \widetilde{w}^{\varepsilon}_A(s,x,v)\overline{\phi}(x,v)dxdv = \lim_{\delta\to 0}\int_{\mathbb{R}^2} w^{\varepsilon}_A(s,x,v)\overline{\phi}(x,v)dxdv , \tag{2.107}$$

uniformly for all $s \leq T\delta^{-1}$, where $\widetilde{w}^{\varepsilon}_A(t,x,v)$ is the Wigner transform corresponding to $\widetilde{X}$, defined exactly as (2.53), but $\widetilde{X}(t)$ now being the solution to (2.103).

Proof. We follow essentially the proof of Lemma 2.1. The characteristics (2.44) fulfill

$$\begin{aligned} X(t) &= x\cos at + va^{-1}\sin at \\ &\quad + \int_0^t a^{-1}\sin a(t-s)\Big[f(s) - (M\star X')(s) - xM(s)\Big]ds , \\ X'(t) &= -xa\sin at + v\cos at \\ &\quad + \int_0^t \cos a(t-s)\Big[f(s) - (M\star X')(s) - xM(s)\Big]ds . \end{aligned} \tag{2.108}$$

Similarly to the proof of (2.38) one obtains

$$\mathbf{E}\Big|\int_0^t a^{-1}\sin a(t-s)\Big[(M\star X')(s) + xM(s)\Big]ds\Big| \leq K\Big[\int_0^t F(s)ds + |x|\Big] , \tag{2.109}$$

recalling the value of K (2.34), and the cosine term in $X'(t)$ is similar.

Now we estimate the random forcing term. First we use

$$\mathbf{E}\Big|\int_0^t f(s)\ a^{-1}\sin a(t-s)\ ds\Big| \leq \left(\mathbf{E}\Big|\int_0^t f(s)\ a^{-1}\sin a(t-s)\ ds\Big|^2\right)^{1/2} , \tag{2.110}$$

then notice that $a^{-1}\sin a(t-s) = \eta_{\theta,\sigma}(t-s)$ with $\theta = 1$, $\sigma = 0$ (see (2.56)). Hence (cf. (2.59))

$$\mathbf{E}\Big|\int_0^t f(s)a^{-1}\sin a(t-s)\,ds\Big|^2 \le \lambda^2 \int_0^\Omega A_\beta^2(\omega)H(t,\omega;1,0;a) \tag{2.111}$$

which is just $Q(t) = Q(t;1,0;\beta,a)$, see (2.58). Hence from (2.61), (2.62) we get

$$\mathbf{E}\Big|\int_0^t f(s)\ a^{-1}\sin a(t-s)\,ds\Big|^2 \le C_1^2(\beta,\lambda_0,T) \tag{2.112}$$

using the relations among the parameters; $t = T\delta^{-1}$, $\lambda = \lambda_0\delta^{1/2}$ and $\Omega \le \delta^{-1}$. Similar estimate is valid for the cosine term.

The estimates (2.109), (2.110) and (2.112) lead to the a priori bound,

$$F(t) \le |x| + |v| + K\Big[\int_0^t F(s)ds + |x|\Big] + C_1(\beta,\lambda_0,T)\ , \tag{2.113}$$

and by the standard Gronwall argument we obtain,

$$F(t) \ \le\ C_2(\beta,\lambda_0,T)\Big(1 + |x| + |v|\Big)\ . \tag{2.114}$$

By monotonicity of C_2 in T, we get the a priori bound (2.105) on $X(t)$ and $X'(t)$.

From the equation (2.44) we also get a similar bound for $X''(t)$. We estimate

$$\mathbf{E}|X''(t)| \ \le\ a^2\mathbf{E}|X(t)| + \Big(\mathbf{E}|f(t)|^2\Big)^{1/2} + |x||M(t)| + \int_0^t |M(s)|\ \mathbf{E}|X'(t-s)|ds\ .$$

For the forcing term we use

$$\mathbf{E}|f(t)|^2 = \lambda^2\int_0^\Omega \frac{\omega(\cosh\beta\omega + 1)}{2\sinh\beta\omega}\ d\omega \le C_3(\beta)\lambda^2\Omega^2$$

(see (2.40)) and that

$$|M(s)| = \lambda^2\Big|\frac{\sin\Omega s}{s}\Big| \le \frac{2\Omega\lambda^2}{1+\Omega s}\ . \tag{2.115}$$

These estimates, along with $t = T\delta^{-1}$, $\lambda = \lambda_0\delta^{1/2}$ and $\Omega \le \delta^{-1}$, give that

$$\sup_{s\le T\delta^{-1}} \mathbf{E}|X''(s)| \le C_4(\beta,\lambda_0,T)\Big(|x| + |v| + \Omega^{1/2}\Big)\ , \tag{2.116}$$

using the a priori bounds (2.45), and C_4 is monotone in T.

For the continuity result, notice that $Y(t) := X(t) - \widetilde{X}(t)$ satisfies the equation,

$$Y''(t) + I\lambda^2 Y'(t) + a^2 Y(t) = I\lambda^2 X'(t) - (M \star X')(t) - xM(t) \ , \qquad (2.117)$$

with initial conditions $Y(0) = Y'(0) = 0$. Using (2.104) we obtain,

$$\begin{aligned} \Big| I\lambda^2 X'(s) - (M \star X')(s) \Big| \ &\leq \ \lambda^2 \Big| \int_0^s \frac{\sin \Omega u}{u} \Big(X'(s) - X'(s-u) \Big)\, du \Big| \\ &\quad + \lambda^2 \, |X'(s)| \, \Big| \int_s^\infty \frac{\sin \Omega u}{u} \, du \Big| \ . \qquad (2.118) \end{aligned}$$

The second term is estimated by $(const)\lambda^2 |X'(s)|$ with a universal constant if $s \leq 1$ and by $(const)\lambda^2 (\Omega s)^{-1} |X'(s)| \leq (const)\lambda^2 \Omega^{-1} |X'(s)|$ if $s \geq 1$.

In the first term we split the integration domain. For $u \geq \Omega^{-2/3}$ we use integration by parts, (2.45) and (2.116)

$$\begin{aligned} &\lambda^2 \, \mathbf{E} \, \Big| \int_{\Omega^{-2/3}}^s \frac{d}{du} \Big(\frac{\cos \Omega u}{\Omega} \Big) u^{-1} \Big(X'(s) - X'(s-u) \Big) \, du \Big| \\ &\leq C_5(\beta, \lambda_0, T) \delta |\log \delta| \Omega^{-1/3} \Big(1 + |x| + |v| \Big) \qquad (2.119) \end{aligned}$$

for all $s \leq T\delta^{-1}$. For the domain $0 \leq u \leq \Omega^{-2/3}$, we use Taylor expansion: $|X'(s) - X'(s-u)| \leq |u| \sup_{\sigma \leq s} |X''(\sigma)|$ and the bound (2.116). We obtain finally, using (2.45),

$$\mathbf{E} \, \Big| I\lambda^2 X'(s) - (M \star X')(s) \Big| \ \leq \ C_6(\beta, \lambda_0, T, x, v) \delta |\log \delta| \Omega^{-1/6} \ , \qquad (2.120)$$

if $1 \leq s \leq T\delta^{-1}$ and

$$\begin{aligned} \mathbf{E} \, \Big| I\lambda^2 X'(s) - (M \star X')(s) \Big| \ &\leq \ \pi \lambda_0^2 \delta F(t) \\ &\leq \ C_7(\beta, \lambda_0, x, v) \delta \Big(1 + |\log \delta| \Omega^{-1/6} \Big) \ , \qquad (2.121) \end{aligned}$$

if $s < 1$.

We now introduce the two fundamental solutions φ and ψ of $Y'' + I\lambda^2 Y' + a^2 Y = 0$ with $\varphi(0) = 0$, $\varphi'(0) = 1$ and $\psi(0) = 1, \psi'(0) = 0$. They are explicitly given as,

$$\varphi(t) = b^{-1} e^{-I\lambda^2 t/2} \sin bt \ , \qquad \psi(t) = e^{-I\lambda^2 t/2} \cos bt + \frac{I\lambda^2}{2} \varphi(t) \ , \qquad (2.122)$$

with $b := (a^2 - I^2\lambda^4/4)^{1/2}$. Note that they are bounded functions for small enough δ. Hence, by (2.115), (2.120) and (2.121),

$$\begin{aligned}
\mathbf{E}\,|Y(t)| &= \mathbf{E}\,\Big|\int_0^t \varphi(t-s)\Big(I\lambda^2 X'(s) - (M\star X')(s) - xM(s)\Big)\,ds\Big| \\
&\leq \Bigg(C_8(\beta,\lambda_0,T,x,v)|\log\delta|\Omega^{-1/6} \\
&\qquad +C_7(\beta,\lambda_0,x,v)\delta + 2\lambda^2|x|\Big[1+(\log\Omega t)_+\Big]\Bigg)\|\phi\|_\infty \\
&\leq C_9(\beta,\lambda_0,T,x,v)\Omega^{-1/6}|\log\delta|\ . \qquad (2.123)
\end{aligned}$$

The constants C_8 and C_9 can be chosen monotone in T, so the same estimate is valid for $\sup_{s\leq T\delta^{-1}}\mathbf{E}\,|Y(s)|$. The argument for Y' is similar, which proves (2.106). ■

2.5.2 Transport Equation Before Scaling Limits

Armed with (2.107), it is enough to compute $\widetilde{w}_A^\varepsilon(t,x,v)$. The calculation is the same as in Section 2.3 except for the different fundamental solutions φ and ψ given in (2.122). We redefine,

$$\begin{aligned}
\eta_{\theta,\sigma} &:= \theta\varphi(t) + \sigma\varphi'(t)\ , \qquad (2.124)\\
\xi_{\theta,\sigma} &:= \theta\psi(t) + \sigma\psi'(t)\ ,
\end{aligned}$$

and in complete analogy to Lemma 2.5 we state the,

Lemma 2.7 *We have for $t\geq 0$,*

$$\begin{aligned}
&\int_{\mathbb{R}^2}\widetilde{w}_A^\varepsilon(t,x,v)\overline{\phi(x,v)}\,dx\,dv \\
&= \int_{\mathbb{R}^2}\widehat{w}_0\Big(\xi_{\theta,\sigma}(t),\eta_{\theta,\sigma}(t)\Big)\overline{\widehat{\phi}(\theta,\sigma)}e^{-\frac{1}{2}Q(t)}\,d\theta\,d\sigma\ ,
\end{aligned}$$

with

$$Q(t) := \lambda^2\int_0^\Omega A_\beta^2(\omega)H(t,\omega)d\omega\ ,$$

and H is given again as $H(t,\omega) = \left|\int_0^t \eta_{\theta,\sigma}(s)e^{-is\omega}ds\right|^2$, but with the new $\eta_{\theta,\sigma}$ defined in (2.124). We also have exactly the same estimate as (2.63), but with the redefined quantities. ■

2.5.3 Obtaining Diffusion from Scaling Limit

In this section, and with similar arguments as in Section 2.4, we again obtain linear dependence in time of $Q(t)$ for large t. Indeed, we first write,

$$\varphi(t) = \frac{1}{2ib}\Big(e^{tu} - e^{t\bar{u}}\Big) , \qquad \text{with,} \quad u := -\frac{I\lambda^2}{2} + ib \, .$$

With these notations, we have,

$$\eta_{\theta,\sigma}(t) = \frac{1}{2ib}\Bigg(\theta\Big(e^{tu} - e^{t\bar{u}}\Big) + \sigma\Big(ue^{tu} - \bar{u}e^{t\bar{u}}\Big)\Bigg) ,$$

hence,

$$H(t,\omega) \;\; = \;\; \frac{1}{4b^2}\left|(\theta+\sigma u)\frac{e^{t(u-i\omega)}-1}{u-i\omega} - (\theta+\sigma\bar{u})\frac{e^{t(\bar{u}-i\omega)}-1}{\bar{u}-i\omega}\right|^2 .$$

We now take the scaling $t = T\delta^{-1}$ for a fixed T and $\delta \to 0$. The terms with denominator $\bar{u} - i\omega = -I\lambda^2/2 - i(\sqrt{a^2 - I^2\lambda^4/4} + \omega)$ have no singularity (they are bounded) so the first term of H is the main term. Extracting the main term, we can write (cf. (2.64)),

$$H(t,\omega) = (\theta^2 + a^2\sigma^2)\left[\frac{1}{4a^2}\left|\frac{e^{t(u-i\omega)}-1}{u-i\omega}\right|^2 + U(t,\omega)\right] .$$

Using $u = ai + O(\delta)$, $0 < a^2 \le 1$, $b^2 = a^2 + O(\delta^2)$ we obtain for small enough δ that,

$$\int_0^\infty \big|U(T\delta^{-1},\omega)\big|d\omega \le C_{10}(a,\beta,\lambda_0,T)|\log\delta| \, .$$

With some elementary calculations this implies,

$$\begin{aligned}
& Q(T\delta^{-1}) \\
= \;\; & \lambda^2(\theta^2+a^2\sigma^2)\left[\frac{1}{4a^2}\int_0^\Omega A_\beta^2(\omega)\left|\frac{e^{T\delta^{-1}(u-i\omega)}-1}{u-i\omega}\right|^2 d\omega + B_1(T\delta^{-1})\right] \\
= \;\; & \lambda^2(\theta^2+a^2\sigma^2)\left[\frac{A_\beta^2(a)}{4a^2}\int_{a+\sqrt{\delta}}^{a-\sqrt{\delta}} \left|\frac{e^{T\delta^{-1}(u-i\omega)}-1}{u-i\omega}\right|^2 d\omega + B_3(T\delta^{-1})\right] ,
\end{aligned}$$

where the functions B_j ($j = 1,2,3$) satisfy $|B_j(T\delta^{-1})| \le C_{11}(a,\beta,\lambda_0,T)\delta^{-1/2}$. We used that the function $\omega \mapsto A_\beta^2(\omega)$ is bounded with a bounded derivative around

$\omega \sim a$, and that the function $z \mapsto (e^{tz}-1)/z$ is uniformly bounded by t in the vicinity of the imaginary axis.

Since the derivative of $z \mapsto |(e^{tz}-1)/z|^2$ is bounded by t^2, one can replace u by ai in the last integral at the expense of an error $2\sqrt{\delta}|u-ia|t^2 = O(\delta^{-1/2})$. Finally one can evaluate,

$$\int_{a+\sqrt{\delta}}^{a-\sqrt{\delta}} \left| \frac{e^{T\delta^{-1}(a-\omega)i}-1}{a-\omega} \right|^2 d\omega = 2\pi T\delta^{-1} + O(\delta^{-1/2})$$

At this step $T \geq 0$ is used. In summary, we obtained,

$$Q(T\delta^{-1}) = (\theta^2 + a^2\sigma^2)\Big(\lambda_0^2 T \,\frac{\pi(\cosh(\beta a)+1)}{4a\sinh\beta a} + B_4(T\delta^{-1})\Big)\ . \tag{2.125}$$

The error satisfies $\big|B_4(T\delta^{-1})\big| \leq C_{12}(\beta,\lambda_0,T)\delta^{1/2}$, hence,

$$\lim_{\delta\to 0} Q(T\delta^{-1}) = c_\beta \lambda_0^2 \gamma^2 T\ , \tag{2.126}$$

with $\gamma := \theta^2 + \breve{a}^2\sigma^2$ and

$$c_\beta := \frac{\pi(\cosh(\beta\breve{a})+1)}{4\breve{a}\sinh\beta\breve{a}}\ , \tag{2.127}$$

assuming that

$$\breve{a} := \lim_{\delta\to 0,\Omega\to\infty} a \ = \lim_{\delta\to 0,\Omega\to\infty} \big(1-\lambda_0\Omega\delta^{-1}\big) \tag{2.128}$$

exists, and $\breve{a} \in (0,1]$.

Since we will keep β fixed and choose $\lambda = \lambda_0\delta^{1/2}$ with a fixed λ_0, δ and Ω are left as a scaling parameters from the triple $\varepsilon = (\beta,\Omega,\lambda)$. Like in Section 2.4 (cf.(2.83)) we introduce,

$$W_T^\varepsilon(x,v) := w_A^\varepsilon(T\delta^{-1},x,v)\ , \tag{2.129}$$

and notice that only the time is rescaled. We will assume that $\Omega \to \infty$ along with $\delta \to 0$ in such a way that the limit (2.128) exists and $\Omega \in \big[|\log\delta|^7, \delta^{-1}\big]$. Clearly either $\Omega \sim \delta^{-1}$, in which case $\breve{a} < 1$, or $\Omega \ll \delta^{-1}$, when $\breve{a} = 1$. In the latter case, however, we need $\Omega \geq |\log\delta|^7$.

2.5.4 Derivation of the Limiting Equation

We need the notion of "radial" function with respect to the elliptical phase space trajectories of the oscillator $Y'' + \check{a}^2 Y$. As usual, the dual variables to the phase space coordinates (x,v) are (θ,σ). With $\check{a} > 0$ fixed, let

$$\gamma = \gamma(\theta,\sigma) := \sqrt{\theta^2 + \check{a}^2\sigma^2}\ , \qquad r = r(x,v) := \sqrt{x^2 + \check{a}^{-2}v^2}\ ,$$

which will be considered either variables or functions, depending on the context. If a function $u(x,v)$ depends only on $x^2+\check{a}^{-2}v^2$, then it can be written as $u(x,v) = u^*(r)$ with some function u^* defined on $\mathbb{R}_+$. Then the *two dimensional* Fourier transform $\widehat{u}(\theta,\sigma) = \int \exp\big[-i(\theta x + \sigma v)\big]u(x,v)dxdv$ is a function of $\theta^2 + \check{a}^2\sigma^2$ only, hence it can be written as $\widehat{u}(\theta,\sigma) = \widetilde{u}^*(\gamma)$. Here $\widetilde{u}^*$ can be thought of as the "elliptical-radial" Fourier transform of u^*, but in order to avoid confusion, we will always perform Fourier transforms on $\mathbb{R}^2$, i.e. between $u(x,v) \leftrightarrow \widehat{u}(\theta,\sigma)$, even if these functions are "radial".

For any function $u(x,v)$ we can form the "radial" average of its Fourier transform $\widehat{u}(\theta,\sigma)$ by defining

$$\widehat{u}^{\#}(\theta,\sigma) := \frac{1}{2\pi}\int_0^{2\pi} \widehat{u}\big(\gamma\cos s, \check{a}^{-1}\gamma\sin s\big)ds \qquad \left(= \frac{1}{2\pi\gamma}\int_{\tilde{\theta}^2+\check{a}^2\tilde{\sigma}^2=\gamma^2} \widehat{u}(\tilde{\theta},\tilde{\sigma})d\tilde{\theta}d\tilde{\sigma} \right),$$

which is a function of γ, hence it can be written as

$$\widehat{u}^{\#}(\theta,\sigma) = \widetilde{u}^{\#,*}(\gamma)\ .$$

In this notation $\#$ refers to "radial" averaging, and $*$ indicates that we consider the radial part of the function. Tilde indicates that it comes from the two dimensional Fourier transform $\widehat{u}$ of the original function u.

Theorem 2.3 *Define the large time scale Wigner function $W_T^\varepsilon(x,v)$ as in (2.129). Assume that $\lambda = \lambda_0\delta^{1/2}$, $\lambda_0 < 1$ and fix $\beta > 0$, $\check{a} \in (0,1]$. The initial condition $W_0^\varepsilon(x,v) = w_0(x,v)$ satisfies $\widehat{w}_0(\theta,\sigma) \in L^1(\mathbb{R}_\theta \times \mathbb{R}_\sigma)$. Consider the "radial" average of $\widehat{W_T^\varepsilon}$,*

$$\widetilde{W}_T^{\#,\varepsilon}(\gamma) := \frac{1}{2\pi}\int_0^{2\pi} \widehat{W}_T^\varepsilon(\gamma\cos s, \check{a}^{-1}\gamma\sin s)ds\ .$$

Then for any $T \geq 0$ the limit,

$$\widehat{W}_T^+(\theta,\sigma) := \lim_{\substack{\delta\to 0,\Omega\to\infty \\ 1-\lambda_0^2\Omega\delta\to\check{a} \\ \Omega\geq|\log\delta|^7}} \widetilde{W}_T^{\#,\varepsilon}(\theta,\sigma) \;, \tag{2.130}$$

exists in a weak sense and it is a function of $\gamma = (\theta^2 + \check{a}^2\sigma^2)^{1/2}$ only. Hence, its inverse Fourier transform $W_T^+(x,v)$ is a function of $r = (x^2 + \check{a}^{-2}v^2)^{1/2}$ only and it can be written as $W_T^{+,*}(r) := W_T^+(x,v)$. This function satisfies the "radial" Fokker-Planck equation,

$$\partial_T W_T^{+,*} = \frac{\pi\lambda_0^2}{4}\,\partial_r(rW_T^{+,*}) + \frac{c_\beta\lambda_0^2}{2}\,\Delta_r W_T^{+,*} \;, \tag{2.131}$$

(c_β is given in (2.127)) with initial condition $W_0^{+,*}(r) := W_{T=0}^+(x,v)$ whose Fourier transform $\widehat{W}_0^+(\theta,\sigma)$ is given by,

$$\widehat{W}_0^+(\theta,\sigma) := \widehat{w}_0^{\#}(\theta,\sigma) = \frac{1}{2\pi}\int_0^{2\pi} \widehat{w}_0\big(\gamma\cos s, \check{a}^{-1}\gamma\sin s\big)ds \;. \tag{2.132}$$

Remarks:

- The weak limit $\lim^{**}\widehat{W}_T^{\varepsilon}(\theta,\sigma)$ (without averaging over the angular variables) does not exist (here $\lim^{**}$ stands for the same limit as in (2.130)). However, time averaging can again replace angular averaging (see Corollary 2.1 and the remark there), i.e. our method easily proves that $\lim^{**}W_T^{\varepsilon}(x,v)$ exists in a weak sense in all variables (x,v,T), i.e. in the topology of $\mathcal{D}'\big(\,\mathbb{R}_x\times\mathbb{R}_v\times[0,\infty)_T\,\big)$, and it satisfies (2.131) weakly in space, velocity and time.

- Since the diffusion coefficient $\frac{1}{2}\lambda_0^2 c_\beta$ in (2.131) behaves as β^{-1} for small β (high temperature), we see that Einstein's relation is satisfied at high temperatures. At small temperatures the diffusion does not disappear ($\lim_{\beta\to\infty} c_\beta > 0$), which is due to the ground state quantum fluctuations of the heat bath.

- Similarly to the first remark after Theorem 2.2, one can investigate how this theorem is modified if ϱ is not uniform (in particular if the cutoff is not sharp). The diffusive mechanism is not affected by this generalization, thanks to the second remark after Lemma 2.5, the only change is an extra $\varrho(\check{a})$ factor in the second term on the right hand side of (2.131). But the modified memory kernel,

$M(s) = \lambda^2 \int_0^\Omega \cos(\omega s)\varrho(\omega)d\omega$, does not converge to the delta function $\delta_0(t)$ as $\Omega \to \infty$, hence the nonuniform frequency distribution makes the memory term nonlocal in time. The details are left to the reader.

Proof. The proof is similar to the proof of Theorem 2.2, hence we skip certain steps. Let $\phi(x,v) \in C_0^\infty(\mathbb{R} \times \mathbb{R})$. Similarly to (2.92) we obtain from (2.49),

$$\begin{aligned} \langle W_T^\varepsilon, \phi \rangle &= \int \widehat{w}_A^\varepsilon(T\delta^{-1}, \theta, \sigma)\overline{\widehat{\phi}(\theta,\sigma)} d\theta\, d\sigma \\ &= \mathbf{E} \int \widehat{w}_0(\xi,\eta)\overline{\widehat{\phi}(\theta,\sigma)} e^{i(x\xi+v\eta)} e^{-i(\theta X(t)+\sigma X'(t))} d\xi\, d\eta\, dx\, dv\, d\theta\, d\sigma\ . \end{aligned}$$

Thanks to (2.107), in the limit $\delta \to 0$ we can replace X by $\widetilde{X}$ and to take the limiting value (2.126) of Q in the formulae (we again have to approximate $\widehat{w}_0$ by bounded functions first). We obtain (cf. (2.93)),

$$\begin{aligned} \lim{}^{**} \langle W_T^\varepsilon, \phi \rangle &= \lim{}^{**} \mathbf{E} \int \widehat{w}_0(\xi,\eta)\overline{\widehat{\phi}(\theta,\sigma)} e^{i(x\xi+v\eta)} \\ &\quad \times e^{-i(\theta\widetilde{X}(T\delta^{-1})+\sigma\widetilde{X}'(T\delta^{-1}))} d\xi\, d\eta\, dx\, dv\, d\theta\, d\sigma \\ &= \lim{}^{**} \int \widehat{w}_0\Big(\xi_{\theta,\sigma}(T\delta^{-1}), \eta_{\theta,\sigma}(T\delta^{-1})\Big)\overline{\widehat{\phi}(\theta,\sigma)} e^{-\frac{1}{2}Q(T\delta^{-1})} d\theta\, d\sigma \end{aligned} \tag{2.133}$$

where $\lim^{**}$ stands for the limit in (2.130). Recall that the functions $\xi_{\theta,\sigma}$ and $\eta_{\theta,\sigma}$ now depend on the limiting parameters, since φ and ψ do, and they are oscillating, which again prevents the existence of the weak limit in the last line of (2.133) without averaging.

Time averaging is analogous to part b) of Theorem 2.2, and it gives the weak limit in space, velocity and time. We skip the details of the proof of the statement of the first remark.

Performing a radial avegaring (with respect to the limiting ellipses given by the level curves of $r = r(x,v)$ or $\gamma = \gamma(\theta,\eta)$) is the same as using "radial" testfunctions ϕ which depend only on r; i.e. $\widehat{\phi}(\theta,\sigma)$ depends only on γ hence it can be written as $\widehat{\phi}(\theta,\sigma) = \widetilde{\phi}^*(\gamma)$. In this case

$$\langle \widehat{W}_T^{\#,\varepsilon}, \widehat{\phi} \rangle = \langle \widehat{W}_T^\varepsilon, \widehat{\phi} \rangle\ .$$

From the explicit formulas (2.122), (2.124) it is straightforward to check that

$$\lim{}^{**} \sup_{s\le T\delta^{-1}} \Bigg| \Big(\big[\xi_{\theta,\sigma}(s)\big]^2 + \check{a}^2 \big[\eta_{\theta,\sigma}(s)\big]^2 \Big) - e^{-I\lambda_0^2 s\delta} \Big(\big[\check{\xi}_{\theta,\sigma}(s)\big]^2 + \check{a}^2 \big[\check{\eta}_{\theta,\sigma}(s)\big]^2 \Big) \Bigg| = 0 \;, \tag{2.134}$$

where $\check{\xi}$ and $\check{\eta}$ are the solutions to $Y'' + \check{a}^2 Y = 0$, i.e.

$$\check{\xi}_{\theta,\sigma}(s) := \theta\cos(\check{a}s) - \sigma\check{a}\sin(\check{a}s) \;, \qquad \check{\eta}_{\theta,\sigma}(s) := \theta\check{a}^{-1}\sin(\check{a}s) + \sigma\cos(\check{a}s) \;.$$

Since the flow $(\theta,\sigma) \mapsto \Big(\xi_{\theta,\sigma}(s), \eta_{\theta,\sigma}(s)\Big)$ is measure preserving, one can change variables

$$\begin{aligned} &\int_{\mathbb{R}^2} \widehat{w}_0\Big(\xi_{\theta,\sigma}(t), \eta_{\theta,\sigma}(t)\Big) \overline{\widehat{\phi}(\theta,\sigma)} e^{-\frac{1}{2}Q(t)}\, d\theta\, d\sigma \\ = \;& \int_{\mathbb{R}^2} \widehat{w}_0(\theta,\sigma) \overline{\widehat{\phi}\Big(\xi^*_{\theta,\sigma}(t), \eta^*_{\theta,\sigma}(t)\Big)} e^{-\frac{1}{2}Q^*(t)}\, d\theta\, d\sigma \;, \end{aligned}$$

where $\eta^*(t) := \eta(-t)$, $\xi^*(t) := \xi(-t)$ are the backward trajectories. In this way we pushed the trajectories into the argument of $\widehat{\phi}$, where only their $\xi^2 + \check{a}^2\eta^2$ combination matters, and we can apply (2.134) to replace ξ, η by $\check{\xi}, \check{\eta}$, finally we can change variables backwards, now along these new trajectories.

Hence together with (2.126) and with $c'_\beta := c_\beta/2$ for simplicity, we have

$$\begin{aligned} \lim{}^{**} \langle \widehat{W}_T^{\#,\varepsilon}, \widehat{\phi} \rangle &= \lim{}^{**} \langle \widehat{W}_T^{\varepsilon}, \widehat{\phi} \rangle \\ &= \lim{}^{**} \int_{\mathbb{R}^2} \widehat{w}_0 \Big(e^{-I\lambda_0^2 T/2} \check{\xi}_{\theta,\sigma}(T\delta^{-1}) \,, e^{-I\lambda_0^2 T/2} \check{\eta}_{\theta,\sigma}(T\delta^{-1}) \Big) \\ &\quad \times \overline{\widetilde{\phi}^*(\gamma)} e^{-c'_\beta \lambda_0^2 T \gamma^2} d\theta\, d\sigma \;, \end{aligned}$$

if we can show that this latter limit exists. But the right hand side above is in fact independent of the limiting parameters δ, Ω, since we can first integrate on ellipses $\theta^2 + \check{a}^2\sigma^2 = (const)$, similarly to the same calculation in the proof of part c), Theorem 2.2. Hence,

$$\begin{aligned} &\int_{\mathbb{R}^2} \widehat{w}_0 \Big(e^{-I\lambda_0^2 T/2} \check{\xi}_{\theta,\sigma}(T\delta^{-1}) \,, e^{-I\lambda_0^2 T/2} \check{\eta}_{\theta,\sigma}(T\delta^{-1}) \Big) \overline{\widetilde{\phi}^*(\gamma)} e^{-c'_\beta \lambda_0^2 T \gamma^2} d\theta\, d\sigma \\ &\qquad = \int_{\mathbb{R}^2} \widetilde{W}_0^{+,*} \Big(\gamma e^{-I\lambda_0^2 T/2} \Big) \overline{\widetilde{\phi}^*(\gamma)} e^{-c'_\beta \lambda_0^2 T \gamma^2} d\theta\, d\sigma \;, \end{aligned}$$

where we recall the definition of $\widetilde{W}_0^+$ (2.132), which depends only on $\gamma^2 = \theta^2 + \check{a}^2\sigma^2$, and we let $\widetilde{W}_0^{+,*}(\gamma) := \widetilde{W}_0^+(\theta,\sigma)$. Therefore, the relation,

$$\lim{}^{**}\langle \widehat{W}_T^{\#,\varepsilon}, \widehat{\phi}\rangle = \int_{\mathbb{R}^2} \widetilde{W}_0^{+,*}\Big(\gamma e^{-I\lambda_0^2 T/2}\Big)\overline{\widetilde{\phi}^*(\gamma)}e^{-c'_\beta \lambda_0^2 T\gamma^2} d\theta\, d\sigma$$

defines the weak limit,

$$\widehat{W}_T^+(\theta,\sigma) := \lim{}^{**}\widehat{W}_T^{\#,\varepsilon}(\theta,\sigma)$$

and it is a function depending only on $\theta^2 + \check{a}^2\sigma^2$, i.e. it can be written as $\widetilde{W}_T^{+,*}(\gamma) := \widehat{W}_T^+(\theta,\sigma)$. Also, we readily obtain the equation satisfied by $\widetilde{W}_T^{+,*}(\gamma)$ by computing,

$$\begin{aligned}
&\Big\langle \partial_T\Big|_{T=0}\widehat{W}_T^+, \widehat{\phi}\Big\rangle \\
= \;& \partial_T\Big|_{T=0}\int_{\mathbb{R}^2} \widetilde{W}_0^{+,*}\Big(\gamma e^{-I\lambda_0^2 T/2}\Big)\overline{\widetilde{\phi}^*(\gamma)}e^{-c'_\beta \lambda_0^2 T\gamma^2} d\theta\, d\sigma \\
= \;& \int_{\mathbb{R}^2}\Big[-\frac{I\lambda_0^2}{2}\gamma\partial_\gamma - c'_\beta\lambda_0^2\gamma^2\Big]\widetilde{W}_0^{+,*}(\gamma)\overline{\widetilde{\phi}^*(\gamma)} d\theta\, d\sigma\ ,
\end{aligned}$$

from which (2.131) follows, recalling that $I = \frac{\pi}{2}$ and the value of $c'_\beta = c_\beta/2$ from (2.127). ■

3 Electron in a Harmonic Ionic Lattice

One of the physical situations described by the Caldeira-Leggett Hamiltonian is a single localized electron interacting with phonons. If a semiconductor is modeled as a perfect crystal, the electrons moving in the crystal are not scattered by the lattice ions at all. Because of thermal energy the ions do not remain stationary but each ion moves in a region of space centered at its lattice point. The strong forces which are provided by the interaction of an ion with all the other ions act on this ion when it is not at its lattice point. This leads to lattice vibrations which can be approximated by harmonic oscillations. The independent normal modes of these oscillations are called phonons which can be considered as particles (bosons, cf. [58], [67]).

For simplicity, we considered in the abstract model treated above only the one dimensional situation. In that case the phonons are generated by a periodic chain of ions, sitting at the the points of $\Lambda = \{\frac{j}{\Omega} \ : \ j = 0, 1, 2, \ldots N\Omega\} \subset T_N$ where the points 0 and N are identified. Here T_N is the 1 dimensional torus of length N. Let $\Lambda^* = \{\frac{j}{N} \ : \ j = 0, 1, 2, \ldots N\Omega\} \subset T_\Omega$ be the dual lattice. Assuming nearest neighbor harmonic coupling, the Hamiltonian of the lattice vibrations is exactly H_R in (2.1) written in normal variables, R_j, which are the Fourier transforms of the ion displacements (see e.g. [58]). After linearization in the phonon variables the interaction of an electron with the crystal lattice is,

$$H_I = \sum_{k \in \Lambda^*} C_k \cdot R_k \exp(ik \cdot x) \ , \tag{3.1}$$

where C_k is the k-th Fourier component of the electron-phonon interaction, which comes from a two-body interaction between the electron and the ions.

The essential point in (3.1) is that this interaction is non-linear in x. One can reach linear coupling by assuming that the quantity $k \cdot x$ in (3.1) remains small during the full evolution of the system, and linearize the exponential accordingly. This means that the wavelength ($= O(|\text{wavevector}|^{-1}) = O(|k|^{-1})$) of the crystal oscillation should be bigger than the displacement of the particle (x) during its full evolution. Furthermore, in the original Caldeira-Leggett model (as well as in Section 2.3) the ultraviolet cutoff was removed ($\Omega \to \infty$) in order to obtain diffusion (see Section 2.1). Therefore, we are led to assume big frequencies together with big wavelengths, wherease their product, the sound speed, is a bounded physical constant.

On the level of the Hamiltonian, notice that if C_k were frequency independent (equivalently, $J(\omega) \sim \omega^{-1}$) then $\sum_{k\in\Lambda^*} R_k$, to which the particle coordinate is coupled (2.1), is just the displacement of the ion at the origin as the normal modes are the Fourier transforms of the displacement vectors. In other words, the test-particle is assumed to remain in the vicinity of the origin, and it is assumed to interact with only one single ion of the crystal lattice for all its dynamics (see e.g. [19]). On the other hand, if we wish to derive a diffusive equation for the electron, then for large values of time it is expected to move away from the origin. Even if the diffusion appears only in the velocity (see (1.5)), the large velocity implies large fluctuation in the configuration variable as well.

Coupling depending linearly on the frequency, $C_j \sim \omega_j$, considered in [8], corresponds to $J(\omega) \sim \omega$. Theoretically, it can be obtained from a three dimensional phonon model with radial coupling. In this case R_j is the sum of all modes R_k with the same frequency ω_j, where k runs through the dual of the three dimensional lattice Λ. However, we should remark that the Ohmic law $J(\omega) \sim \omega$ breaks down for large frequencies in real systems.

In summary, the linear model effectively involves an implicit mean-field assumption by requiring that the test-particle is coupled to the same mode for all its evolution, which seems incompatible with the finite sound speed of the metals along with the removed UV cutoff. This leaves a serious doubt on the applicability of the linear coupling assumption for diffusion models for electron propagation in an ionic lattice (see also [2] for a brief criticism of this assumption).

3.1 Second Quantization

We now want to give a physically more relevant model for the electron – phonon interaction [33]. Two interaction processes occur: the electron can be scattered such that either a phonon is emitted or a phonon is absorbed, where in both processes the total wave number remains constant. Due to these scattering events the number of phonons is not conserved. To deal with this non-constant number of particles one uses the procedure of 2^{nd} quantization, which was originally introduced in quantum field theory. So although our model is purely non-relativistic we use the formalism of field quantization [7].

For the sake of simplicity we again use a one-electron model which means that we neglect electron-electron interactions and are just interested in the dynamics of one electron. We will also neglect the effects of the periodical potential of the stationary lattice, thus obtaining the so called Fröhlich Hamiltonian. Moreover we model the phonon Hamiltonian such that it has states of thermal equilibrium.

This means, we consider a modified version of the Fröhlich-Hamiltonian

$$H_{SQ} = H_A + H_R + H_I,$$

which is again of the form (1.14) but the Hamiltonian acts now on wave-functions which lie in the state space

$$\mathcal{S} = L^2(\mathbb{R}^3_x) \otimes \mathcal{F}_S,$$

where $\mathcal{F}_S$ is the Boson-Fock Space (see [57]). This means that a wave function $\psi \in \mathcal{S}$ is actually a sequence of functions $\psi = (\psi^{(n)})_{n=0}^{\infty}$, where $\psi^{(n)} = \psi^{(n)}(x, q_1, \ldots, q_n)$ (for $n \geq 1$) is invariant under permutation of $q_1, \ldots, q_n$ (clearly $\psi^{(0)} = \psi^{(0)}(x)$) . $\mathcal{S}$ is a separable Hilbert-Space with the inner product given by

$$\langle \phi, \psi \rangle_{\mathcal{S}} := \int_{\mathbb{R}^3_x} \phi^{(0)}(x) \overline{\psi^{(0)}(x)}\, dx + \sum_{n=1}^{\infty} \int_{\mathbb{R}^3_x} \int_{\mathbb{R}^{3n}_{q^{(n)}}} \phi^{(n)}(x, q^{(n)}) \overline{\psi^{(n)}(x, q^{(n)})}\, dx dq^{(n)} ,$$

where $q^{(n)} := (q_1, \ldots, q_n)$ for $n \geq 1$.

The physical interpretation of $|\psi^{(n)}(x, q_1, \ldots, q_n)|^2$ is the probability of finding the electron in an infinitesimal neighbourhood of x (electron position space) and n phonons in an infinitesimal neighbourhood of $q^{(n)}$ (phonon momentum space). The electron position density is given by

$$n(x) = \left|\psi^{(0)}(x)\right|^2 + \sum_{n=1}^{\infty} \int_{\mathbb{R}^{3n}_{q^{(n)}}} \left|\psi^{(n)}(x, q^{(n)})\right|^2 dq^{(n)} , \tag{3.2}$$

and the current density by

$$\begin{aligned} J(x) =& \frac{\hbar}{m^*} \mathrm{Im} \left(\overline{\psi^{(0)}(x)} \nabla_x \psi^{(0)}(x) \right) \\ &+ \frac{\hbar}{m^*} \sum_{n=1}^{\infty} \int_{\mathbb{R}^{3n}_{q^{(n)}}} \mathrm{Im} \left(\overline{\psi^{(n)}(x, q^{(n)})} \nabla_x \psi^{(n)}(x, q^{(n)}) \right) dq^{(n)} , \end{aligned} \tag{3.3}$$

where $\hbar$ is the Planck-constant and m^* the electron mass.

The three terms of the Hamiltonian H_{SQ} have the following form:

$$H_A = -\frac{\hbar^2}{2m^*} \Delta + V(x), \tag{3.4}$$

$V(x)$ denoting a given realvalued external potential. The Hamiltonian for the phonons is

$$H_R = \hbar \int_{\mathbb{R}^3_q} a_q^+ a_q \Big(\omega(q) + Z(D_q) \Big) \, dq \; , \tag{3.5}$$

with the annihilation and creation operators

$$\begin{aligned} (a_q \phi)^{(n)}(x, q^{(n)}) &= \sqrt{n+1} \, \phi^{(n+1)}(x, q, q^{(n)}) \quad n = 0, 1, \dots \, , \\ (a_q^+ \phi)^{(n)}(x, q^{(n)}) &= \begin{cases} \frac{1}{\sqrt{n}} \sum_{l=1}^n \delta(q - q_l) \phi^{(n-1)}(x, {}_l q^{(n)}) & n = 1, 2, \dots \\ 0 & n = 0 \, , \end{cases} \end{aligned}$$

where we introduced the notation ${}_l q^{(n)} := (q_1, \dots, q_{l-1}, q_{l+1}, \dots, q_n)$.

In the phonon-Hamiltonian $\omega(q)$ is the realvalued phonon-frequency and as a modification of the usual Hamiltonian we introduced the pseudodifferential operator $Z(D_q)$ which describes the phonon-phonon interactions. The mathematical reason for introducing $Z(D_q)$ is that we would like to have an orthonormal basis (ONB) of $\mathcal{F}_S$ consisting of eigenfunctions of H_R, which can be physically interpreted that the phonons are driven into states of thermal equilibrium. If we use the definition of the annihilation and creation operators then H_R can be written as

$$\begin{aligned} (H_R \psi)^{(n)}(x, q^{(n)}) &= \hbar \sum_{l=1}^n \omega(q_l) \psi^{(n)}(x, q^{(n)}) \\ &\quad + \frac{\hbar}{(2\pi)^3} \sum_{l=1}^n \int_{\mathbb{R}^3_q} \hat{Z}(q_l - q) \psi^{(n)}(x, q, {}_l q^{(n)}) \, dq, \end{aligned}$$

where $\hat{Z}$ denotes the Fourier transform of the function Z. $\hat{Z}$ is supposed to be realvalued. Here and in the sequel we set $\sum_{l=1}^0 c_l := 0$. Finally the electron-phonon interaction Hamiltonian is given by

$$H_I = i\hbar \int_{\mathbb{R}^3_q} F(q) \Big(a_q e^{iqx} - a_q^+ e^{-iqx} \Big) \, dq \; , \tag{3.6}$$

where the term with the annihilation operator models phonon absorption and the one with the creation operator models phonon emission. The realvalued function $F(q)$ describes the details of the electron-phonon interaction. Again using the definitions of a_q and a_q^+ the interaction term reads

$$\begin{aligned}(H_I\psi)^{(n)}(x,q^{(n)}) &= i\hbar\sqrt{n+1}\int_{\mathbb{R}^3_q} F(q)e^{iqx}\psi^{(n+1)}(x,q,q^{(n)})\,dq \\ &\quad -\frac{i\hbar}{\sqrt{n}}\sum_{l=1}^{n} F(q_l)e^{-iq_lx}\psi^{(n-1)}(x,{}_lq^{(n)}).\end{aligned}$$

Remark: Since $V,\hat{Z},F$ and ω are real-valued easy calculations show that the Hamiltonian H_{SQ} is formally self-adjoint (for H_I see also [57], p.209f, Segal quantization).

To study the dynamics of the system we introduce the density operator $\rho:\mathcal{S}\to\mathcal{S}$ which fulfills the von-Neumann equation

$$i\hbar\rho_t = [H_{SQ},\rho],$$

where $[A,B]:=AB-BA$ denotes the commutator of the operators A and B. The operator ρ is self-adjoint, positive and trace-class, therefore there exists an ONB $\{\rho_l\,|\,l\in\mathbb{N}\}$ of eigenfunctions of ρ such that

$$\rho\psi = \sum_{l=1}^{\infty}\mu_l\langle\psi,\rho_l\rangle_{\mathcal{S}}\,\rho_l,$$

where $\mu_l\geq 0$ are the corresponding eigenvalues. Using the eigenfunctions ρ_l we introduce the density matrix elements

$$r_{(n,m)}(x,q^{(n)};y,p^{(m)},t) := \sum_{l=1}^{\infty}\mu_l\rho_l^{(m)}(y,p^{(m)},t)\overline{\rho_l^{(n)}(x,q^{(n)},t)}\quad n,m=0,1,\dots$$

which determine the density operator ρ by

$$(\rho\psi)^{(n)}(x,q^{(n)},t) = \sum_{m=0}^{\infty}\int_{\mathbb{R}^3_y}\int_{\mathbb{R}^{3m}_{p^{(m)}}}\psi^{(m)}(y,p^{(m)},t)\overline{r_{(n,m)}\Big(x,q^{(n)};y,p^{(m)},t\Big)}\,dydp^{(m)}.$$

It is easy to show that the eigenfunctions of ρ fulfill the equation

$$i\hbar\frac{\partial}{\partial t}\rho_l = H_{SQ}\rho_l\ , \tag{3.7}$$

which gives the connection between the von-Neumann dynamics and the Schrödinger picture(cf. [45]). Using (3.7) we obtain the equation

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t} r_{(n,m)}(x,q^{(n)};y,q^{(m)},t) = \sum_{l=1}^{\infty} \mu_l \Big[& (H_{SQ}\rho_l)^{(m)}(y,p^{(m)},t)\overline{\rho_l^{(n)}(x,q^{(n)},t)} \\
& - \rho_l^{(m)}(y,p^{(m)},t)\overline{(H_{SQ}\rho_l)^{(n)}(x,q^{(n)},t)}\Big],
\end{aligned} \tag{3.8}
$$

which describes the dynamics of the density matrix. As a first step to obtain a transport equation for the electrons we introduce

$$
\begin{aligned}
& W_{(n,m)}(x,v,q^{(n)};p^{(m)},t) \\
& \qquad := \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3_\eta} r_{(n,m)}\Big(x+\frac{\hbar}{2m^*}\eta, q^{(n)}; x-\frac{\hbar}{2m^*}\eta, p^{(m)},t\Big) e^{iv\cdot\eta}\, d\eta.
\end{aligned}
$$

The matrix $W := (W_{(n,m)})_{n,m=0,1,\ldots}$ is called Wigner Matrix. It is the Wigner-transformation of the density-matrix $r = (r_{(n,m)})_{n,m=0,1,\ldots}$ with respect to the electron coordinates x and y. Note that

$$
n(x,t) = \int_{\mathbb{R}^3_v} W_{(0,0)}(x,v,t)\,dv + \sum_{n=1}^{\infty} \int_{\mathbb{R}^3_v}\int_{\mathbb{R}^{3n}_{q^{(n)}}} W_{(n,n)}\Big(x,v,q^{(n)};q^{(n)},t\Big)\,dq^{(n)}dv\ ,
$$

and

$$
J(x,t) = \int_{\mathbb{R}^3_v} vW_{(0,0)}(x,v,t)\,dv + \sum_{n=1}^{\infty} \int_{\mathbb{R}^3_v}\int_{\mathbb{R}^{3n}_{q^{(n)}}} vW_{(n,n)}\Big(x,v,q^{(n)};q^{(n)},t\Big)dq^{(n)}dv.
$$

The transport equation satisfied by $W_{(n,m)}$ is easily derived from equation (3.8):

$$
\frac{\partial}{\partial t}W_{(n,m)} + v\cdot\nabla_x W_{(n,m)} + \theta_\hbar[V]W_{(n,m)} = Q_p W_{(n,m)} + (Q_{e-p}W)_{(n,m)}\ . \tag{3.9}
$$

The operator

$$
\begin{aligned}
\theta_\hbar[V]W_{(n,m)}(x,v,q^{(n)},p^{(m)},t) := \frac{i}{(2\pi)^3}\int & \frac{V(x+\frac{\hbar}{2m^*}\eta) - V(x-\frac{\hbar}{2m^*}\eta)}{\hbar} \\
& \times\ W_{(n,m)}(x,v',q^{(n)};p^{(m)},t)e^{i(v-v')\cdot\eta}\,dv'd\eta
\end{aligned}
$$

is the usual pseudo-differential operator which stems from the external potential of the electron. The phonon-Hamiltonian gives the operator

$$
\begin{aligned}
&Q_p W_{(n,m)}(x,v,q^{(n)};p^{(m)},t) \\
&\qquad := -i\Big(\sum_{k=1}^{m}\omega(p_k)-\sum_{k=1}^{n}\omega(q_k)\Big)W_{(n,m)}(x,v,q^{(n)};p^{(m)},t) \\
&\qquad\quad -\frac{i}{(2\pi)^3}\left[\sum_{k=1}^{m}\int_{\mathbb{R}^3_p}\hat{Z}(p_k-p)W_{(n,m)}(x,v,q^{(n)};p,{}_kp^{(m)},t)dp\right. \\
&\qquad\quad \left.-\sum_{k=1}^{n}\int_{\mathbb{R}^3_q}\hat{Z}(q_k-q)W_{(n,m)}(x,v,q,{}_kq^{(n)};p^{(m)},t)dq\right] ,
\end{aligned}
\tag{3.10}
$$

and finally we obtain for the electron-phonon interaction operator

$$
\begin{aligned}
&(Q_{e-p}W)_{(n,m)} \\
&\qquad := \quad Q_1^- W_{(n,m+1)} + Q_2^- W_{(n+1,m)} - Q_1^+ W_{(n,m-1)} - Q_2^+ W_{(n-1,m)} ,
\end{aligned}
\tag{3.11}
$$

with

$$
\begin{aligned}
Q_1^- W_{(n,m+1)} &= \sqrt{m+1}\int_{\mathbb{R}^3_p} F(p)e^{ip\cdot x}W_{(n,m+1)}(x,v-\frac{\hbar}{2m^*}p,q^{(n)};p,p^{(m)},t)\,dp, \\
Q_2^- W_{(n+1,m)} &= \sqrt{n+1}\int_{\mathbb{R}^3_q} F(q)e^{-iq\cdot x}W_{(n+1,m)}(x,v-\frac{\hbar}{2m^*}q,q,q^{(n)};p^{(m)},t)\,dq, \\
Q_1^+ W_{(n,m-1)} &= \frac{1}{\sqrt{m}}\sum_{k=1}^{m} F(p_k)e^{-ip_k\cdot x}W_{(n,m-1)}(x,v+\frac{\hbar}{2m^*}p_k,q^{(n)};{}_kp^{(m)},t), \\
Q_2^+ W_{(n+1,m)} &= \frac{1}{\sqrt{n}}\sum_{k=1}^{n} F(q_k)e^{iq_k\cdot x}W_{(n-1,m)}(x,v+\frac{\hbar}{2m^*}q_k,{}_kq^{(n)};p^{(m)},t).
\end{aligned}
$$

We now introduce the phonon trace of the (Wigner)matrix W

$$
w(x,v,t) := (\mathrm{tr}\,_pW)(x,v,t) := W_{(0,0)}(x,v,t)+\sum_{n=1}^{\infty}\int_{\mathbb{R}^{3n}_{q^{(n)}}} W_{(n,n)}(x,v,q^{(n)};q^{(n)},t)\,dq^{(n)},
$$

which acts as the quantum-equivalent of the phase space distribution function of the electron in classical mechanics. Taking the phonon trace of (3.9) leads (after some calculations) to the transport equation

$$
\begin{aligned}
w_t + v \cdot \nabla_x w + \theta_\hbar[V]w =& 2\sum_{n=0}^{\infty} \sqrt{n+1} \int_{\mathbb{R}^3_q} \int_{\mathbb{R}^{3n}_{q^{(n)}}} F(q) \\
& \cdot \mathrm{Re} \left[e^{iq\cdot x} \left(W_{(n,n+1)}(x, v - \frac{\hbar}{2m^*}q, q^{(n)}; q, q^{(n)}, t) \right.\right. \\
& \left.\left. - W_{(n,n+1)}(x, v + \frac{\hbar}{2m^*}q, q^{(n)}; q, q^{(n)}, t) \right) \right] dq^{(n)} dq.
\end{aligned}
\tag{3.12}
$$

Remarks:

- Note that $\mathrm{tr}_p(Q_p W) = 0$.
- In the right hand side of (3.12) the subdiagonal elements $W_{(n,n+1)}$ are still present, which means that we do not have a closed equation for $w(x,v,t)$.
- Note that $n(x,t) = \int_{\mathbb{R}^3_v} w(x,v,t)dv$ and $J(x,t) = \int_{\mathbb{R}^3_v} v w(x,v,t)dv$.

3.2 Weak Electron-Phonon Interaction

To derive an approximating closed equation for $w(x,v,t)$ we now assume that the electron-phonon interaction is small. Therefore we write in (3.6) $\varepsilon F(q)$ instead of $F(q)$ with $0 < \varepsilon \ll 1$ and treat the problem with methods of asymptotic analysis for $\varepsilon \to 0$. The now ε-dependent Wigner matrix is solution of the transport equation

$$
LW^\varepsilon = Q_p W^\varepsilon + \varepsilon Q_{e-p} W^\varepsilon \ , \tag{3.13}
$$

where we introduced the Wigner transport operator

$$
L := \frac{\partial}{\partial t} + v \cdot \nabla_x + \theta_\hbar[V].
$$

Q_p and Q_{e-p} are now considered to act on the Wigner matrix W^ε as defined in (3.9). For W^ε we make the ansatz

$$
W^\varepsilon := W^0 + \varepsilon W^1 + \varepsilon^2 W^2 + \varepsilon^3 W^3 + O(\varepsilon^4). \tag{3.14}
$$

For the initial condition we assume

$$
W^\varepsilon(t=0) = w_I^0 A \ , \tag{3.15}
$$

where $w_I^0 = w^0(t=0)$ is a given (Wigner)function of x and v and A is defined as the density matrix corresponding to the operator (cf. [3])

$$T := \frac{1}{\mathrm{tr}_p(e^{-\beta H_R^0})} e^{-\beta H_R^0}, \quad \text{with } H_R = \mathrm{Id}_x \otimes H_R^0 \, .$$

H_R^0 is the phonon operator acting on $\mathcal{F}_S$. The exact definition of A will be given after we have introduced a special ONB in Lemma 3.1. The operator T describes the phonons in a state of thermal equilibrium, where β is a constant (indirectly proportional to the lattice temperature), this means we have the same initial conditions for the reservoir as in the Caldeira Leggett model. Note that T is normalized such that $\mathrm{tr}_p T = 1$.

We make the following assumption on H_R^0:

(A1) $\omega(q)$ and $\hat{Z}(q)$ are such that there exists an ONB of realvalued eigenfunctions $\{\psi_k(q) | k \in \mathbb{N}\}$ in $L^2(\mathbb{R}_q^3)$ and eigenvalues $\lambda_k \in \mathbb{R}$ such that

$$\hbar\omega(q)\psi_k(q) + \frac{\hbar}{(2\pi)^3} \int_{\mathbb{R}_{q'}^3} \hat{Z}(q-q')\psi_k(q')\, dq' = \lambda_k \psi_k(q).$$

Note that (A1) holds if growth conditions on $\omega(q)$ and on $Z = Z(x)$ at $x = q = \infty$ are imposed (confinement of phonons). The eigenfunctions can be chosen realvalued because $\omega(q)$ and $\hat{Z}$ are realvalued. With this assumption we have the following

Lemma 3.1 *If (A1) holds, then there exists an ONB of $\mathcal{F}_S$ consisting of eigenfunctions of H_R^0.*

PROOF: Define

$$\psi_{\vec{k}}^{(n)}(q_1, \dots, q_n) := \frac{1}{\sqrt{n!}} \sum_{\sigma \in P^n} \psi_{k_{\sigma(1)}}(q_1) \cdot \ldots \cdot \psi_{k_{\sigma(n)}}(q_n) \, ,$$

where $\vec{k} = (k_1, \dots, k_n)$ is a multiindex and P^n is the permutation group of n elements. Because of the structure of H_R it is obvious that

$$H_R^0 \psi_{\vec{k}}^{(n)}(q^{(n)}) = \lambda_{\vec{k}} \psi_{\vec{k}}^{(n)}(q^{(n)}) \quad \text{with } \lambda_{\vec{k}} := \sum_{j=1}^n \lambda_{k_j},$$

λ_{k_j} being the eigenvalue corresponding to ψ_{k_j}.

By definition the functions $\psi_{\vec{k}}(q_1, \dots, q_n)$ are invariant under permutation of the arguments and therefore

$$\psi_{\vec{k}} := (0, \dots, 0, \psi_{\vec{k}}^{(n)}(q^{(n)}), 0, \dots) \in \mathcal{F}_S \ .$$

Adding the vacuum state $\psi^0 := (1, 0, 0, \dots)$ we finally find that the so constructed set $\{\psi_{\vec{k}}\}$ is an ONB of $\mathcal{F}_S$ because $(\psi_k)_{k\in\mathbb{N}}$ is an ONB of $L^2(\mathbb{R}_q^3)$, cf. [56]. □

Now we use the ONB constructed above to represent the matrix A of the initial condition (3.15). To obtain a unique representation we use only multiindices $\vec{k} = (k_1, \dots, k_n)$ ordered such that $k_1 \leq \dots \leq k_n$. We thus obtain $\forall \phi \in \mathcal{F}_S$:

$$(H_R^0\phi)^{(n)}(q^{(n)}) = \sum_{\substack{\vec{k}\in\mathbb{N}^n \\ k_1\leq\dots\leq k_n}} \lambda_{\vec{k}} \int_{\mathbb{R}^{3n}_{p^{(n)}}} \phi^{(n)}(p^{(n)})\psi_{\vec{k}}^{(n)}(p^{(n)})\, dp^{(n)} \psi_{\vec{k}}^{(n)}(q^{(n)}).$$

Using the definition of the operator T we can write

$$(T\phi)^{(n)}(q^{(n)}) = \sum_{m=1}^{\infty} \int_{\mathbb{R}^{3m}_{p^{(m)}}} \phi^{(m)}(p^{(m)}) A_{(n,m)}(q^{(n)}, p^{(m)})\, dp^{(m)} \ ,$$

where we have

$$A_{(n,n)}(q^{(n)}, p^{(n)}) = \frac{1}{Tr} \sum_{\substack{\vec{k}\in\mathbb{N}^n \\ k_1\leq\dots\leq k_n}} e^{-\beta\lambda_{\vec{k}}} \psi_{\vec{k}}^{(n)}(p^{(n)})\psi_{\vec{k}}^{(n)}(q^{(n)}) \quad n = 1, 2, , \dots$$

with $Tr := \sum_n \sum_{\substack{\vec{k}\in\mathbb{N}^n \\ k_1\leq\dots\leq k_n}} e^{-\beta\lambda_{\vec{k}}}$ and because of the construction of the ONB it is clear that

$$A_{(n,m)}(q^{(n)}, p^{(m)}) = 0 \quad n \neq m.$$

Plugging the ansatz (3.14) into equation (3.13) we obtain by equating the coefficients of equal powers of ε:

$$\begin{aligned} LW^0 - Q_pW^0 &= 0 \ , \\ LW^1 - Q_pW^1 &= Q_{e-p}W^0 \ , \\ LW^2 - Q_pW^2 &= Q_{e-p}W^1 \ , \\ LW^3 - Q_pW^3 &= Q_{e-p}W^2 \ , \end{aligned} \tag{3.16}$$

and from (3.15) we obtain the initial conditions

$$\begin{aligned} W^0(t=0) =& w^0 A \ , \\ W^1(t=0) =& W^2(t=0) = W^3(t=0) = 0 \ . \end{aligned} \tag{3.17}$$

Using the first equation of (3.16) and the initial condition for W^0 the separation ansatz $W^0_{n,m} = w^0(x,v,t)M_{n,m}(q^n,p^m)$ shows that $M = A$, i.e. $W^0 = w^0 A$. A short calculation gives $Q_p A = 0$, therefore also $Q_p W^0 = 0$.

In the following we will use the convention that for a superscript $\alpha \in \{0,1,2,3,\varepsilon\}$ the function w^α will denote the phonon trace of the matrix W^α, i.e. $w^\alpha := \mathrm{tr}_p W^\alpha$.

Remarks:

- Note that this notation is consistent for W^0 because of the normalization of A, $tr_p A = 1$.
- The interpretation of the structure of $W^0 = w^0 A$ is that if there is no electron-phonon interaction at all (i.e. $\varepsilon = 0$) the phonons will be in a state of thermal equilibrium which is given by the operator T.

If we take the phonon traces of equations (3.16) we are thus led to the equations

$$\begin{aligned} Lw^0 &= 0 \ , \\ Lw^1 &= \mathrm{tr}_p(Q_{e-p}W^0) \ , \\ Lw^2 &= \mathrm{tr}_p(Q_{e-p}W^1) \ , \\ Lw^3 &= \mathrm{tr}_p(Q_{e-p}W^2) \ . \end{aligned} \tag{3.18}$$

We have already used $\mathrm{tr}_p(Q_p W^\alpha) = 0$ and another calculation shows that also $\mathrm{tr}_p(Q_{e-p}W^0) = 0$. Actually this can be seen easily by taking into account the fact that $A_{(n,m)} = 0$ for $n \neq m$ and therefore $(Q_{e-p}W^0)_{(n,n)} = 0, \forall n \geq 0$. With a similar argument one can see that $\mathrm{tr}_p(Q_{e-p}W^2) = 0$. So taking into account the initial conditions (3.17) we have found $w^1 \equiv w^3 \equiv 0$ and, formally,

$$Lw^\varepsilon = \varepsilon^2 \mathrm{tr}_p(Q_{e-p}W^1) + O(\varepsilon^4) \ ,$$

where we have of course $w^\varepsilon = \mathrm{tr}_p W^\varepsilon = w^0 + \varepsilon^2 w^2 + O(\varepsilon^4)$.

3.2.1 The Case of a Constant Potential: $V \equiv \mathrm{const.}$

W^1 is now calculated from

$$LW^1 - Q_p W^1 = Q_{e-p}(w^\varepsilon A) \ , \tag{3.19}$$

which is the second equation of (3.16) with w^0 replaced by w^ε. If we are able to solve equation (3.19) for W^1 we will have a closed equation for w^ε which is exact up to the order ε^4. To do so we assume now $V \equiv$ const. which means $\theta_\hbar[V] \equiv 0$. In this simple case equation (3.19) becomes

$$\frac{\partial}{\partial t} W^1 + v \cdot \nabla_x W^1 - Q_p W^1 = Q_{e-p}(w^\varepsilon A) \ ,$$

which can be solved explicitely by means of a separation ansatz and the variation of the constants formula. Using the orthogonality properties of the eigenfunctions of H_R^0 one finally obtains after long calculations

$$\begin{aligned} \operatorname{tr}_p(Q_{e-p}W^1) = \frac{2}{Tr} \int_{\tau=0}^{t} \int_{\mathbb{R}_p^3} \int_{\mathbb{R}_q^3} \sum_{n=0}^{\infty} \sum_{\substack{\vec{k}\in\mathbb{N}^{n+1} \\ k_1\le\ldots\le k_{n+1}}} \sum_{j=1}^{n+1} \mathrm{Re} \Big\{ e^{i(q-p)\cdot x + ip\cdot v\tau} \\ \cdot F_{k_j}(p) F_{k_j}(q) e^{\frac{i}{\hbar}\lambda_{k_j}\tau} \Big(e^{-\beta\lambda_{\vec{k}}} D_1^0 - e^{-\beta\lambda_{j\vec{k}}} D_2^0 \Big) \Big\} \, dq \, dp \, d\tau \ , \end{aligned} \tag{3.20}$$

with $F_{k_j}(p) := F(p)\psi_{k_j}(p)$ and

$$\begin{aligned} D_1^0 \ &:= \ e^{-i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon \Big(x - (v - \frac{\hbar}{2m^*}q)\tau, v - \frac{\hbar}{2m^*}(p+q), t-\tau \Big) \\ &- \ e^{i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon \Big(x - (v + \frac{\hbar}{2m^*}q)\tau, v - \frac{\hbar}{2m^*}(p-q), t-\tau \Big) \ , \\ D_2^0 \ &:= \ e^{-i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon \Big(x - (v - \frac{\hbar}{2m^*}q)\tau, v + \frac{\hbar}{2m^*}(p-q), t-\tau \Big) \\ &- \ e^{i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon \Big(x - (v + \frac{\hbar}{2m^*}q)\tau, v + \frac{\hbar}{2m^*}(p+q), t-\tau \Big). \end{aligned}$$

So in the case of $V \equiv$ const. we obtain the transport equation for w^ε

$$\frac{\partial}{\partial t} w^\varepsilon + v \cdot \nabla_x w^\varepsilon = \varepsilon^2 I_{scat}^0 + O(\varepsilon^4) \ , \tag{3.21}$$

where I_{scat}^0 is the term on the right hand side of (3.20).

Remarks:

- The most important property of I_{scat}^0 is the non-locality in time. This expresses the fact that the scattering term has a memory of the whole history of the states of the system, i.e. phonon scattering is nonlocal in time when a fully quantistic viewpoint is taken.

- An easy calculation shows that if $F_j(q)$ is either symmetric or antisymmetric, i.e. $F_j(q) = F_j(-q)$ or $F_j(q) = -F_j(-q)$, then equation (3.21) (without the

$O(\varepsilon^4)$-term) is time reversible (i.e. the equation is invariant under the transformation $t \to -t, v \to -v$). F_j has such symmetry properties, for example, if F is symmetric or antisymmetric and ψ_j is symmetric which is the case if ω and $\hat{Z}$ are symmetric.

3.2.2 The Case of a Constant Electric Field: The Barker-Ferry Equation

We now consider a linear potential $V = -E \cdot x$ where E is the constant electric field. In this case the pseudo-differential operator $\theta_\hbar[V]$ becomes the differential operator $-\frac{1}{m^*}E \cdot \nabla_v$ which means that the operator L is the Vlasov transport operator

$$L = \frac{\partial}{\partial t} + v \cdot \nabla_x - B \cdot \nabla_v, \quad B = \frac{E}{m^*} \ .$$

So we can again solve equation (3.19) by the method of characteristics and by similar calculations as in the case of $V \equiv$ const. we derive the transport equation

$$\frac{\partial}{\partial t} w^\varepsilon + v \cdot \nabla_x w^\varepsilon - B \cdot \nabla_v w^\varepsilon = \varepsilon^2 I^B_{scat} + O(\varepsilon^4) \ ,$$

where we have to replace D^0_1 and D^0_2 in the expression (3.20) by

$$\begin{aligned}
D^B_1 :=& \ e^{ip\frac{B}{2}\tau^2 - i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon\Big(x - (v - \frac{\hbar}{2m^*}q)\tau - \frac{B}{2}\tau^2, v - \frac{\hbar}{2m^*}(p+q) + B\tau, t-\tau\Big) \\
&- e^{ip\frac{B}{2}\tau^2 + i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon\Big(x - (v + \frac{\hbar}{2m^*}q)\tau - \frac{B}{2}\tau^2, v - \frac{\hbar}{2m^*}(p-q) + B\tau, t-\tau\Big), \\
D^B_2 :=& \ e^{ip\frac{B}{2}\tau^2 - i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon\Big(x - (v - \frac{\hbar}{2m^*}q)\tau - \frac{B}{2}\tau^2, v + \frac{\hbar}{2m^*}(p-q) + B\tau, t-\tau\Big) \\
&- e^{ip\frac{B}{2}\tau^2 + i\frac{\hbar}{2m^*}p\cdot q\tau} w^\varepsilon\Big(x - (v + \frac{\hbar}{2m^*}q)\tau - \frac{B}{2}\tau^2, v + \frac{\hbar}{2m^*}(p+q) + B\tau, t-\tau\Big).
\end{aligned}$$

Remark: In the physical literature the Ferry-Barker equation is quite well known (see e.g.[6]). It is a transport equation for an electron in a constant electric field with a scattering term describing the electron-phonon interaction for the space homogenous case. If we take a space homogenous function $w^\varepsilon = w^\varepsilon(v,t)$ and then integrate I^B_{scat} with respect to x we are led to a scattering operator which is structurally analogous to the one appearing in the Ferry-Barker equation.

We can write the scattering term also in pseudo-differential operator (PDO) form. For this purpose we introduce

$$\begin{aligned} f(x,k) &:= \int_{\mathbb{R}^3_q} e^{-iqx} F(q)\psi_k(q)\, dq, \\ \delta f(x,\eta,k) &:= f(x+\eta,k) - f(x-\eta,k), \\ \mu f(x,\eta,k) &:= f(x+\eta,k) + f(x-\eta,k). \end{aligned}$$

Using this notation we obtain

$$\begin{aligned} I^B_{scat} = \frac{1}{Tr}\int_{\tau=0}^{t} \sum_{n=0}^{\infty} \sum_{\substack{\vec{k}\in\mathbb{N}^{n+1} \\ k_1\le\ldots\le k_{n+1}}} \sum_{j=1}^{n+1} \mathrm{R}e \Bigg\{ & e^{\frac{i}{\hbar}\lambda_{k_j}\tau} \overline{\delta f(x, \frac{\hbar}{2m^* i}\nabla_v, k_j)} \\ & \Bigg(\left(e^{-\beta\lambda_{\vec{k}}} + e^{-\beta\lambda_{{}_j\vec{k}}}\right) \delta f(x - \frac{B}{2}\tau^2 - v\tau, \frac{\hbar}{2m^* i}\nabla_{v,2}, k_j) \\ & + \left(e^{-\beta\lambda_{\vec{k}}} - e^{-\beta\lambda_{{}_j\vec{k}}}\right) \mu f(x - \frac{B}{2}\tau^2 - v\tau, \frac{\hbar}{2m^* i}\nabla_{v,2}, k_j) \Bigg) \\ & w^\varepsilon(x - \frac{B}{2}\tau^2 - v\tau, v + B\tau, t-\tau) \Bigg\} d\tau \ , \end{aligned} \tag{3.22}$$

where the notation $\nabla_{v,2}$ signifies that the PDO acts only on the second argument of w.

3.3 Scaling limits

We shall assume in this chapter that $Tr = 1$. For the independent variables we introduce the scaling

$$t = \nu\tilde{t}, \quad x = \gamma_x\tilde{x}, \quad v = \gamma_v\tilde{v}, \quad q = \alpha\tilde{q} \ ,$$

and for the other occuring quantities we have

$$\begin{aligned} & w^\varepsilon(x,v,t) = \tilde{w}^\varepsilon(\tilde{x},\tilde{v},\tilde{t}), \quad \psi_k(q) = \alpha^{-\frac{3}{2}}\tilde{\psi}_k(\tilde{q}), \\ & E = A_E\tilde{E}, \quad F(q) = A_F\tilde{F}(\tilde{q}), \quad \lambda_{\vec{k}} = A_P\tilde{\lambda}_{\vec{k}} \ . \end{aligned}$$

The scaling is chosen such that the set $\{\tilde{\psi}_k\}$ is an ONB of $L^2(\mathbb{R}^3_{\tilde{q}})$. Note that

$$[\psi^{(n)}] = (m^3)^{\frac{n-1}{2}}, \quad [q] = m^{-1}, \quad [E] = kg\, ms^{-2}, \quad [F] = m^{3/2}s^{-1}.$$

We introduce the 3 dimensionless parameters

$$\varepsilon := \gamma_v m^* \frac{A_F}{A_E} \alpha^{\frac{3}{2}}, \quad \sigma := \frac{m^* \gamma_v}{\nu A_E}, \quad \kappa := \alpha \gamma_x.$$

Setting $\nu = \frac{\gamma_x}{\gamma_v}$, $\gamma_x = \frac{\hbar}{m^* \gamma_v}$ and $\gamma_v = \frac{\hbar A_E}{m^* A_P}$ we obtain the scaled equation

$$\begin{aligned}
\sigma w_t + \sigma v \cdot \nabla_x w - E \cdot \nabla_v w& \\
= \varepsilon^2 \sum_{n=0}^{\infty} \sum_{\substack{\vec{k} \in \mathbb{N}^{n+1} \\ k_1 \leq \ldots \leq k_{n+1}}} \sum_{j=1}^{n+1} \int_{\tau=0}^{\frac{t}{\sigma}} &\mathrm{Re} \Bigg\{ e^{i\sigma\lambda_{k_j}\tau} \overline{\delta f(\kappa x, \frac{\kappa}{2i} \nabla_v, k_j)} \\
&\Bigg(\left(e^{-\beta\lambda_{\vec{k}}} + e^{-\beta\lambda_{j\vec{k}}} \right) \delta f(\kappa x - \sigma \frac{E}{2} \tau^2 - \sigma v \tau, \frac{\kappa}{2i} \nabla_{v,2}, k_j) \\
&+ \left(e^{-\beta\lambda_{\vec{k}}} - e^{-\beta\lambda_{j\vec{k}}} \right) \mu f(\kappa x - \sigma \frac{E}{2} \tau^2 - \sigma v \tau, \frac{\kappa}{2i} \nabla_{v,2}, k_j) \Bigg) \\
&w^\varepsilon(x - \sigma \frac{E}{2} \tau^2 - \sigma v \tau, v + E\tau, t - \sigma\tau) \Bigg\} d\tau \ ,
\end{aligned} \tag{3.23}$$

where we have dropped "~" for the scaled quantities. The scaling is chosen such that σ is indirectly proportional to the strength of the electric field, κ is proportional to the scaling parameter of q and ε is proportional to the strength of the electron-phonon interaction.

Limit 1

Taking the limit $\sigma \to 0$ (which means we consider strong electric fields) and $\frac{\varepsilon^2}{\sigma} \sim$ *const* we formally obtain the limiting equation

$$\begin{aligned}
w_t + v \cdot \nabla_x w - \frac{1}{\sigma} E \cdot \nabla_v w = \frac{\varepsilon^2}{\sigma} \sum_{n=0}^{\infty} \sum_{\substack{\vec{k} \in \mathbb{N}^{n+1} \\ k_1 \leq \ldots \leq k_{n+1}}} \sum_{j=1}^{n+1} \int_{\tau=0}^{\infty} &\mathrm{Re} \Bigg\{ \overline{\delta f(\kappa x, \frac{\kappa}{2i} \nabla_v, k_j)} \\
&\Bigg(\left(e^{-\beta\lambda_{\vec{k}}} + e^{-\beta\lambda_{j\vec{k}}} \right) \delta f(\kappa x, \frac{\kappa}{2i} \nabla_v, k_j) \\
&+ \left(e^{-\beta\lambda_{\vec{k}}} - e^{-\beta\lambda_{j\vec{k}}} \right) \mu f(\kappa x, \frac{\kappa}{2i} \nabla_v, k_j) \Bigg) \\
&w^\varepsilon(x, v + E\tau, t) \Bigg\} d\tau.
\end{aligned} \tag{3.24}$$

If we then take the limit $\kappa \to 0$ (small wave vectors q) the PDOs become differential operators:

$$\begin{aligned} \delta f(\kappa x, \frac{i\kappa}{2}\nabla_v, k_j)w(x,v,t) &= i\kappa \nabla_x f(0,k_j)\cdot\nabla_v w(x,v,t) + O(\kappa^3), \\ \mu f(\kappa x, \frac{i\kappa}{2}\nabla_v, k_j)w(x,v,t) &= 2f(0,k_j)w(x,v,t) + O(\kappa^2). \end{aligned}$$

Assuming that $F_{k_j}(q) = F(q)\psi_{k_j}(q)$ is antisymmetric we conclude $f(0,k_j) = 0$ and in the limit δf dominates. Thus we derive

$$w_t + v\cdot\nabla_x w - \frac{1}{\sigma}E\cdot\nabla_v w = \frac{\varepsilon^2\kappa^2}{\sigma}\int_{\tau=0}^{\infty} \nabla_v^T M \nabla_v w(x, v+E\tau, t)d\tau \qquad (3.25)$$

with the matrix

$$\begin{aligned} M &= \sum_{n=0}^{\infty} \sum_{\substack{\vec{k}\in\mathbb{N}^{n+1} \\ k_1\le\ldots\le k_{n+1}}} \sum_{j=1}^{n+1} \left(e^{-\beta\lambda_{\vec{k}}} + e^{-\beta\lambda_{{}_j\vec{k}}}\right) G_{k_j}\otimes G_{k_j}, \\ G_{k_j} &= \int_{\mathbb{R}^3_q} F(q)\psi_{k_j}(q) q\, dq\ . \end{aligned}$$

Using the equality

$$\int_{\tau=0}^{\infty}\int_{\mathbb{R}_\xi} h(\xi+\tau)h(\xi)d\xi\, d\tau = \frac{1}{2}\left(\int_{\mathbb{R}_\xi} h(\xi)d\xi\right)^2,$$

we can proof easily that the scattering term in (3.25) is dissipative.

Limit 2

We obtain another simplified scattering term if we are only interested in the equation for small times. We set $\sigma = 1$ (electric field strength of order one) and take first the limit $\kappa \to 0$ which leads to the approximation

$$w_t + v\cdot\nabla_x w - E\cdot\nabla_v w = \varepsilon^2\kappa^2 \int_{\tau=0}^{t} cos(\lambda_{k_j}\tau)\nabla_v^T M \nabla_{v,2} w(x+\frac{E}{2}\tau^2 - v\tau, v+E\tau, t-\tau)d\tau.$$

Taylor expansion with respect to t gives the equation

$$w_t + v\cdot\nabla_x w - E\cdot\nabla_v w = \varepsilon^2\kappa^2 t \nabla_v^T M\nabla_v w(x,v,t) + o(\varepsilon^2\kappa^2 t). \qquad (3.26)$$

Taking only the leading term of this expansion gives a dissipative (Fokker-Planck) scattering term.

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