

# Quantum Theory of Linear Friction

Stig Stenholm

*Helsinki Institute of Physics*

*and the Academy of Finland P.O.Box 9, Siltavuorenpenger 20C*

*FIN-00014 University of Helsinki*

*Finland*

Received September 11, 1996

We consider the quantum theoretic description analogous with the classical Brownian motion. A Phenomenological Master Equation is found, which gives the same description as the classical theory up to the second moments of the dynamical variables. However, this is not of the generic Lindblad form, and it cannot be the basis for a simulation algorithm. The Master Equation is derived using the Born-Markov approach, and its form is discussed for various cases. Especially the slow particle limit and the harmonic oscillator case are investigated. In the slow limit, the fluctuation-dissipation relation must be of the classical form, except in very special ranges of the temperature. It may still be necessary to include quantum corrections to the dynamics. For the harmonic oscillator, only a narrow range of response frequencies of the reservoir are needed, and all cases seem possible. The approach is related to the general Lindblad formalism, and it is found that, when its formal requirements are implemented, the ensuing equations lead to questionable physical consequences which violate our physical intuition. The validity of the approach is discussed, and it is compared with earlier works in the field. In particular, we find differences between the conclusions deriving from strict reservoir assumptions and those following from models of coupled oscillators. I suggest that these differences may be real and contain information about the emergence of universal dissipative behavior in realistic physical systems.

## I. Introduction

Linear dissipation is the most usual model of irreversible dynamical time evolution. In classical mechanics, linear friction has become something of a paradigm for damped motion. In connection with the phenomenon of Brownian motion it became clear that the dissipation must be accompanied by unavoidable fluctuations. The physical situation was clarified by Einstein, whose theory later was developed into a full fledged mathematical description of random motion. In the classical domain, the phenomenon is well understood and the mathematical description is mature and sophisticated.

The quantum theory of dissipation is much less clear. Schrodinger time evolution is manifestly unitary, and no irreversible behaviour is found. In contrast to

the classical theory, the quantum description of time evolution does not allow any simple phenomenological extension to irreversible behaviour. Detailed theoretical investigations have been devoted to this problem, and by now we have some basic understanding of the mechanism for the appearance of irreversibility and the domain of validity of the various models proposed. However, the area of linear friction still continues to attract attention and new attempts at deriving the basic equations.

The earliest attempts to derive quantum analogs of Langevin equations was presented by Senitzky<sup>[1]</sup>. This approach has been widely used in Quantum Optics, and it does provide a useful and efficient tool for solving many problems in this field of physics. In many cases, however, the ensuing equations are hard to solve, and in

others the theoretical formulation is difficult to justify. A theory based on Master Equations is a viable alternative. In many cases these equations can be derived in more transparent ways and their use is less risky than the treatment of nonlinear operator equations.

The first dissipative quantum Master Equation was derived for nuclear induction by Wangsness and Bloch<sup>[2]</sup> using a perturbative approach. Their method has later been used widely in many areas of physics. For the quantum Brownian motion problem, however, theorists desired a more exact method. This can be seen as an attempt to compete with the well developed mathematical theory of classical Brownian motion. Typical representatives of this view are the papers [3] and [4]; there are however many others. A detailed investigation of friction was carried out by Ullersmaa<sup>[5]</sup>. At the same time, the problem was discussed widely in the area of Quantum Optics, and e.g. Agarwal<sup>[6]</sup> derived dissipative master equations both with and without the rotating-wave-approximation. The early developments in the field of irreversible Master Equations were reviewed by Haake<sup>[7]</sup>, Agarwal<sup>[8]</sup>, Dekker<sup>[9]</sup> and Grabert<sup>[10]</sup>.

In the beginning of the 1980s, Caldeira and Leggett applied their functional integration approach to linear friction<sup>[11]</sup> for the harmonic oscillator. This approach was used by Hakim and Ambegaokar<sup>[12]</sup> to investigate the case of a free particle. At the same time, many other approaches were introduced and developed, see e.g. [13] and [14]. The originator of the statistical mechanical theory, Ford, showed a renewed interest in the problem<sup>[15,16]</sup>, and the Quantum Optics community reconsidered the derivation of the Master Equations for coupled harmonic oscillators in [17,18]. A field theory approach was given by Unruh and Zurek<sup>[19]</sup>.

The stochastic Master Equation was considered from a different point of view by the Quantum Measurement program<sup>[20–22]</sup>. This approach has been further developed and applied to many problems, see e.g. [23–25]. Here the Master Equation is awarded a position

as fundamental in quantum mechanics. By coupling an external stochastic perturbation to the position variable of the system, one localizes the particle in real space, which is assumed to imply the transition to classical behaviour of quantum objects. The fundamental role of irreversibility in the interpretation of quantum mechanics is stressed by Zurek in the article<sup>[26]</sup>.

The approaches described above came together when it was realized that quantum systems modelled by Markovian Master Equations can be represented terms of ensembles of stochastically generated pure states. This was first realized by Mollow<sup>[27]</sup> for spontaneous radiative transitions. It has later been developed into an efficient computational method by Carmichael<sup>[28]</sup> and Moelmer et al.<sup>[29]</sup>. The ensuing simulation algorithm is eminently suitable for numerical computations, and it has become very popular recently; for a discussion and review see Ref. [30].

The simulation method is applicable to a wide range of dissipative Master Equations of the Markovian type. Lindblad<sup>[31]</sup> showed that a very general class of generic equations are of this form, and it is commonly expected that all physically relevant Master Equations fall into this class. The theory is discussed together with applications by Davis in [32]. This approach has been applied to the case of linear friction by Sandulescu and Scutaru<sup>[33]</sup> and Gallis<sup>[34]</sup>. The latter gives a Lindblad form Master Equation, which closely approximates the classical Brownian motion theory.

In this paper, I wish to reconsider the case of linear dissipative motion in the quantum regime. The basic philosophy of my approach is presented in Sec. II together with its motivation. Section III discusses a phenomenological quantum Master Equation describing Brownian motion. Its formal derivation is discussed in Sec. IV. Section V considers the slow motion limit, and connects the result to the phenomenological description. The special case of a harmonic oscillator is discussed in Section VI. A general coupling potential is treated in Sec. VII, and the connection to the Lind-

blad formalism is presented in Sec. VIII. Section IX discusses the validity of the approach. A summary with some conclusions is presented in Sec. X. Some technical details are relegated to the Appendices.

## II. Basic approach

In view of all the work summarized in the Introduction, why do I want to reconsider the problem of linear friction? My original motivation stems from our work<sup>[35]</sup> on wave packet motion on adiabatic energy surfaces in molecules. The introduction of dissipation turned out to present unexpected numerical difficulties, that indicated some fundamental problem. Indeed, many investigators have suggested that Brownian motion can exist only in the classical, high temperature limit.

My attempts to resolve these difficulties made me dissatisfied with all discussions of Brownian motion Master Equations, and the present paper reports the results of my own effort. Many questions remain unclear, but it may be of interest to pinpoint the assumptions needed in the derivation and the obscure points of the result.

Firstly, we must conclude that the standard Master Equation used in Quantum Optics, see Refs. [37] and [8], does not do for a particle moving in a real physical potential. It is derived only for the case when the motion is purely harmonic, which is relevant for electromagnetic radiation modes. In addition, it distributes the dissipation equally between the variables  $x$  and  $p$ , which is correct in case they are quadrature components of the electric field. If  $x$  is a real position variable, it is not to be damped; no physical mechanism can force the system to the origin of the coordinate system.

Master Equations describing physical friction are discussed in among others the Refs. [6], [9], [11], [17], [18] and [19]. All these approaches do, however, use the model of linearly coupled harmonic systems. The problem is then formally exactly soluble, and the emergence of the Brownian motion limit can be scrutinized

in detail. The method has the advantage of being totally analytic, and the degree of mathematical rigour introduced is determined mainly by the point of view taken by the authors. However, choosing such a special case, the authors are unable to distinguish the generic features from those deriving from the solubility of the model. Ford and Kac<sup>[15]</sup> concede this point, but consider the derivations as existence proofs for such situations where the Brownian motion description is valid.

Considerable care has been devoted to the decay of initial correlations between the reservoir oscillators and the system of interest. The choice of initial state thus becomes very important, and certain specially correlated states have to be excluded. To complete the proof one should show that these states form a set of negligible measure; this seems intuitively obvious but it has never been proved, to the best of my knowledge.

There is an alternative to soluble harmonic oscillator models, which is chosen in this work. We follow the original idea of Wangsness and Bloch<sup>[2]</sup>, who ascribe the emergence of an irreversible master equation to the weak coupling of the system of interest to a large reservoir which is kept in thermal equilibrium unaffected by the influence of its perturbation by the system of interest.

The reservoir must be “large” in a very precise sense, which was elucidated early by Fano<sup>[36]</sup>: The interaction is weak and the calculation can be carried out to second order in the coupling constant (Born approximation). The ensuing perturbation of the reservoir must be so small that no back reaction of the reservoir on the system need be considered. Furthermore, the perturbation must be so rapidly distributed over the whole reservoir, that the time evolution lacks all memory effects (the Markov approximation). This requires the reservoir to have a continuous spectrum, which in a well understood manner leads to irreversible quantum behaviour. A derivation using these assumption is termed a Born-Markov calculation.

An additional consideration in this paper is the re-

quirement of universality of the results obtained. This derives from my opinion that dissipation is caused by real physical reservoirs into which our systems of interest are immersed. I look for cases where the damping and diffusion constants are characterized only by the properties of the reservoir and its interaction parameters but do not depend on the conservative forces acting on the system. This can be valid only in very particular cases; thus we are looking for these.

Operationally the universality requirement implies e. g. that we can suspend a particle harmonically in the reservoir and determine the dissipative parameters from its damping rate and its thermal motion once equilibrium has been achieved. These parameters can then be used to predict its rate of descent, when the particle is released in the same reservoir to fall under the influence of gravity. In the slow motion limit the prediction should be valid.

In this paper we adopt the reservoir assumptions uncritically. We regard the existence of reservoirs as a paradigm and investigate the consequences of this assumption. The reservoir acts like a stream of the external world flowing past our system of interest. Every time we interact with it, it has been reset to its initial state by an external source which we have no influence over; never can we retrieve the information once it has been transferred to the reservoir.

I assume the Born-Markov calculation to be valid, and look at the conditions necessary to obtain agreement with the classical Brownian motion behaviour. This contrasts our treatment to that of the soluble models, which can be considered to obtain their results as sufficient conditions for the validity of the Brownian motion description. The detailed validity of the reservoir assumption for special cases of physical interest is left for future discussions.

By choosing the approach outlined above, we can ask certain questions not possible within the framework of coupled oscillator models. We can see how generic their results are. We can ask why the friction is linear

in velocity? We can look for the conditions of validity of the Brownian motion description and whether it can stay valid in the quantum domain of motion. Finally the connection to the Lindblad theory and its recent developments can be investigated. These problems are discussed in the present paper.

### III. The phenomenological theory of friction

Linear friction is, perhaps, the best understood classical dissipative effect. The theory of Brownian motion is well developed, it describes the physics eminently and its mathematical apparatus is precise and sophisticated. Its most concise statement for a particle moving in the potential  $U(x)$  is in terms of the Langevin equations

$$\begin{aligned}\dot{x} &= -\frac{p}{m} \\ \dot{p} &= -gp - \frac{\partial U(x)}{\partial x} + \mathcal{L}(t),\end{aligned}\quad (3.1)$$

where the stochastic Langevin force  $\mathcal{L}(t)$  satisfies the conditions

$$\begin{aligned}\langle \mathcal{L}(t) \rangle &= 0 \\ \langle \mathcal{L}(t)\mathcal{L}(t') \rangle &= 2D\delta(t-t');\end{aligned}\quad (3.2)$$

all higher order correlation functions factorize in terms of these two. The process is taken to be Gaussian. This is a complete physical description of Brownian motion in the classical case.

We want to extend the theory of Eqs. (3.1-2) to quantum mechanical motion in a consistent and physically acceptable way. We already concluded that the form used in Quantum Optics is not correct. Thus a different Master Equation is needed.

It is simple to find the appropriate form of the Master Equation. We write (with Planck's constant  $\hbar$  set equal to unity)

$$\dot{\rho} = -i[H, \rho] - i\frac{\gamma}{2}[x, [p, \rho]_+] - D[x, [x, \rho]]. \quad (3.3)$$

This is supposed to hold for some class of Hamiltonians  $H$ ; the restrictions on the deterministic motion will

be discussed below. The symbol  $[\cdot]_+$  denotes the anti-commutator. It is easily verified that (3.3) reproduces

the average values of the classical equations (3.1), and it also gives the correct equations for the second moments

$$\begin{aligned}\frac{d}{dt} \langle x^2 \rangle &= \frac{1}{m} \langle (xp + px) \rangle \\ \frac{d}{dt} \langle (xp + px) \rangle &= -\gamma \langle (xp + px) \rangle + \frac{2}{m} \langle p^2 \rangle - 2 \left\langle x \frac{\partial U}{\partial x} \right\rangle \\ \frac{d}{dt} \langle p^2 \rangle &= -2\gamma \langle p^2 \rangle + 2D \left\langle \left( p \frac{\partial U}{\partial x} + \frac{\partial U}{\partial x} p \right) \right\rangle.\end{aligned}\quad (3.4)$$

Except for the operator ordering, these equations are exactly those that follow from the classical Langevin equations (3.1). Written out for the Wigner function, Eq. (3.3) also gives the dissipative terms in complete accordance with the classical Fokker-Planck equation. For this reason, I choose to call the equation (3.3) the Phenomenological Master Equation. This does not imply that it cannot be derived, it can, but that it leads to the same averaged equations of motion for the second moments as the classical Langevin system.

In the Lindblad form of the dissipative time evolution<sup>[31]</sup> the density matrix equation must be of the form

$$\dot{\rho} = -i[H, \rho] - \sum_q \alpha_q^2 (C_q^\dagger C_q \rho + \rho C_q^\dagger C_q - 2C_q \rho C_q^\dagger), \quad (3.5)$$

where the coefficients  $\alpha_q^2$  are explicitly positive, and  $q$  goes over some range of values. The advantage with this form is that it can always be subjected to a Monte Carlo simulation for the state vectors<sup>[28-29]</sup>.

In order to compare the Phenomenological Master Equation with the Lindblad form (3.5), we introduce the creation and annihilation operators according to

$$\begin{aligned}x &= \frac{1}{\sqrt{2m\omega}}(b + b^\dagger) \\ p &= \sqrt{\frac{m\omega}{2}} \left( \frac{b - b^\dagger}{i} \right).\end{aligned}\quad (3.6)$$

Some transformations of the friction term in Eq. (3.3) and the use of (3.6) give the form

$$\begin{aligned}\dot{\rho} &= -i[H, \rho] - i\frac{\gamma}{4}[(px + xp), \rho] - \frac{\gamma}{4}(b^\dagger b \rho + \rho b^\dagger b - 2b \rho b^\dagger) \\ &\quad + \frac{\gamma}{4}(bb^\dagger \rho + \rho bb^\dagger - 2b^\dagger \rho b) - D[x, [x, \rho]].\end{aligned}\quad (3.7)$$

The first two terms on the first line describe Hamiltonian time evolution including a renormalization term from the dissipative mechanism. The last term, the diffusion term, is of the Lindblad form as is the last term on the first line. However, the first term on the second line is not, it occurs with a negative probability, and no simulation can be based on it. We have also been unable to find any other splitting of the Master Equation (3.3) which would allow a simulation. The phenomenological form of the Master Equation is not of the generic Lindblad form.

The dissipative mechanism renormalizes the Hamiltonian. If we, for illustrative purposes, write out the result for a harmonic oscillator, we have

$$\begin{aligned}H_{\text{new}} &= H + \frac{\gamma}{4}(xp + px) \\ &= \Omega b^\dagger b + i\frac{\gamma}{4}(b^\dagger b^\dagger - bb).\end{aligned}\quad (3.8)$$

This can be diagonalized by the canonical transformation to new creation and annihilation operators  $a$ ,  $a^\dagger$  by setting

$$b = \sqrt{i}(\cosh(\theta/2)a - \sinh(\theta/2)a^\dagger). \quad (3.9)$$

where the parameter  $\theta$  is determined by

$$\tanh \theta = \frac{\gamma}{2\Omega} . \quad (3.10)$$

The resulting Hamiltonian is

$$H_{\text{new}} = \sqrt{\Omega^2 - \frac{\gamma^2}{4}} a^\dagger a . \quad (3.11)$$

This gives the correct oscillational frequency of a damped oscillator as derived in the classical theory. Thus the Phenomenological Master Equation contains this result too.

There are, however, many questions relating to the Master Equation (3.3). How can it be derived, what is its range of validity and why is it not of the Lindblad form? The last question relates to its inability to form the basis for a state vector simulation.

#### IV. Derivation of Master Equations

Following the discussion in Sec. II, we immerse our system of interest into a vast reservoir, which we assume to be totally unaffected by the interaction. We write the Hamiltonian of the total system in the form

$$H_{\text{tot}} = H + H_R + H_{\text{int}} . \quad (4.1)$$

Here  $H$  is the Hamiltonian for the system of interest,  $H_R$  that of the reservoir, and the interaction is taken to be of the form

$$H_{\text{int}} = \lambda V(x) \Gamma . \quad (4.2)$$

Here  $\lambda$  is a coupling constant and  $\Gamma$  is an operator on the reservoir degrees of freedom. More general forms could be introduced by adding further terms coupled to other reservoir operators, but no new physical considerations would emerge.

The system of interest is taken to be a simple particle with the Hamiltonian

$$H = \frac{p^2}{2m} + U(x) . \quad (4.3)$$

The Heisenberg equations of motion are then

$$\begin{aligned} \dot{x} &= -i[H, x] = \frac{p}{m} \\ \dot{p} &= -i[H, p] = -\frac{\partial U}{\partial x} - \lambda \frac{\partial V}{\partial x} \Gamma . \end{aligned} \quad (4.4)$$

The last term here serves as the Langevin term in the classical problem (3.1). It transmits the fluctuations of the reservoir to the motion of the system of interest.

From the equations (4.4) we see immediately that the coupling potential  $V(x)$  should not depend on the momentum  $p$ ; this would give a correction term to the equation for  $\dot{x}$ , which would not admit an interpretation in terms of a random force. No physical reservoir is expected to make the particle jump in space, it can only provide momentum kicks.

The quantum analog of the strict Langevin case (3.1) can only be achieved by taking

$$V(x) = x, \quad (4.5)$$

when the Langevin force in (4.4) becomes independent of position. This is an important special case which I will refer to as the Langevin case in the following. I do, however, not attach any significance to the Heisenberg point of view from now on; I will concentrate on the derivation of a Master Equation. Especially, no quantum Langevin equation is discussed or derived.

The derivation of the Master Equation is carried out to second order in the coupling constant  $\lambda$  and by assuming that the correlation time  $\tau_c$  of the reservoir is so short that no memory effects can be transmitted through the reservoir; this is the Born-Markov approximation, which is taken for granted. It assumes the reservoir band width  $B(\propto \tau_c^{-1})$  to be the largest frequency in the problem. The Master Equation can be obtained by many derivation methods, but one which is convenient for our purposes is given in Appendix I. The reader only interested in the result, need not look up the details of the calculation.

The result (I.19) of the derivation can be written

$$\dot{\rho}(t) = i \frac{\lambda^2}{2} [V(t), [V_\chi(t), \rho(t)]_+] - \lambda^2 [V(t), [V_D(y), \rho(t)]] , \quad (4.6)$$

where the influence of the reservoir in the Master Equation is through the convoluted operators

$$\begin{aligned} V_D(t) &= \int_0^t d\tau D(\tau) V(t-\tau) \\ V_\chi(t) &= \int_{-\infty}^t d\tau \chi(\tau) V(t-\tau) . \end{aligned} \quad (4.7)$$

We call the equation (4.6) the proto-master equation.

All operators in Eq.(4.6) are taken in the interaction picture with respect to the system Hamiltonian  $H$ , and going back to the Schrödinger picture, we obtain the system time evolution generated by  $H$  as in the Master Equation (3.3). The operators  $V$  are then given in the Schrödinger picture. The influence of the reservoir is seen in the correlation functions. The fluctuations of the operator  $\Gamma$  are described by  $D(\tau)$  and its linear response by the susceptibility  $\chi(\tau)$ . Both are assumed to decay to zero after times larger than the reservoir correlation time, and the time dependence from the upper limits in the integrals Eqs. (4.7) disappears from the equation. Thus it should be used only over times  $t$  clearly longer than  $\tau_c$ .

The time dependence in the potential  $V(t)$  is actually through the position variable

$$V(t) = V(x(t)). \quad (4.8)$$

and its time scale relates to the time scale of the dy-

namic evolution in the system of interest. This time dependence is slow, i. e. it contains only small frequencies in its Fourier spectrum, when the motion  $x(t)$  is slow enough. This is taken to be equivalent with a low energy content in the dynamic degrees of freedom. We consider this case in the next section.

## V. The slow motion limit

We expect the linear friction to appear in a physical system when the motion is slow enough that only small frequency components are needed to describe the time evolution. Then an expansion in the frequency of the Fourier transform variable  $\omega$  is expected to be valid and we can simplify the Master Equation. In Appendix II we derive some formal properties for the reservoir correlation functions and, in particular, the Fourier transform of the susceptibility is found to be of the form

$$\begin{aligned} \chi(\omega) &= \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{1}{\omega' - \omega - i\epsilon} \sum_{j=1}^{\infty} a_j \omega'^{2j-1} \\ &= \chi'(\omega) + \frac{i}{2} \sum_{j=1}^{\infty} a_j \omega^{2j-1} . \end{aligned} \quad (5.1)$$

The operators (4.7) can now be expressed in terms of the coefficients  $a_j$ .

We find with (4.7) and (5.1)

$$\begin{aligned} V_\chi(t) &= \int_{-\infty}^{\infty} d\tau \chi(\tau) V(t-\tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi(\omega) \tilde{V}(\omega) \\ &= V'_\chi + \frac{i}{2} \sum_{j=1}^{\infty} a_j \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \omega^{2j-1} \tilde{V}(\omega) \end{aligned}$$

$$\begin{aligned}
&= V'_\chi + \frac{1}{2} \sum_{j=1}^{\infty} a_j i^{2j} \left( \frac{\partial}{\partial t} \right)^{2j-1} V(t) \\
&= V'_\chi - \frac{1}{2} a_1 \frac{\partial V}{\partial t} + O \left( \frac{\partial}{\partial t} \right)^3 .
\end{aligned} \tag{5.2}$$

In the slow motion limit, we can show that the term  $V'_\chi$  gives only a renormalization of the Hamiltonian time evolution. We write

$$V'_\chi = P \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} A(\omega') \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\tilde{V}(\omega)}{\omega' - \omega} e^{-i\omega t} . \tag{5.3}$$

We now remember that the time dependence of  $V(t)$  derives from the Heisenberg evolution of  $x(t)$ , and we can conclude that in the slow motion limit the spectrum of  $\tilde{V}(\omega)$  can be taken to be much narrower than that of the bath response  $A(\omega)$ . Thus, over most of the integration range, we can assume that  $\omega'$  is much larger than  $\omega$  in the denominator. Then we obtain

$$V'_\chi = P \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega'} V(t) = \Lambda V(t) . \tag{5.4}$$

The principal value integral exists because of the expansion (II.9). In the equation of motion (4.6), this contributes a term

$$i \frac{\lambda^2}{2} \Lambda [V, [V, \rho]_+] = i \frac{\lambda^2}{2} \Lambda [V^2, \rho] . \tag{5.5}$$

This is clearly an energy shift by the amount

$$\Delta E = -\frac{\lambda^2}{2} \Lambda V^2 = -\frac{\lambda^2}{2} V \left\langle \frac{1}{\omega} \right\rangle V . \tag{5.6}$$

The latter form represents the origin of the factor  $\Lambda$  in symbolic form. The similarity of this energy shift with a second order perturbation result is obvious. In the following, we neglect this shift.

Using the formula (II.8) and proceeding in the same way as before, we obtain

$$\begin{aligned}
V_D(t) &= \int_0^\infty d\tau D(\tau) V(t-\tau) = V'_D + \frac{1}{2} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} d(\omega) \tilde{V}(\omega) \\
&= \frac{1}{4} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \coth \left( \frac{\beta\omega}{2} \right) \sum_{j=1}^{\infty} a_j \omega^{2j-1} \tilde{V}(\omega) \\
&= \frac{1}{4} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \left( \frac{2}{\beta\omega} + \frac{\beta\omega}{6} + \dots \right) (a_1\omega + a_2\omega^3 + \dots) \tilde{V}(\omega) \\
&= \frac{a_1}{2\beta} V(t) - \frac{1}{2} \left( \frac{a_2}{\beta} + \frac{\beta a_1}{12} \right) \frac{d^2}{dt^2} V(t) + \dots .
\end{aligned} \tag{5.7}$$

In these calculations we have neglected the term  $V'_D$ . In the slow motion limit this can be justified by writing

$$\begin{aligned}
V'_D &= P \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} d(\omega') \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\tilde{V}(\omega)}{\omega' - \omega} e^{-i\omega t} \\
&\simeq P \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{d(\omega')}{\omega'} V(t) .
\end{aligned} \tag{5.8}$$

The principal value integral vanishes exactly because  $d(\omega)$  is an even function.

If we neglect time derivatives higher than the first, we obtain the Master Equation

$$\dot{\rho} = -i \frac{\lambda^2 a_1}{4} [V, [\dot{V}, \rho]_+] - \frac{\lambda^2 a_1}{2\beta} [V, [V, \rho]] \tag{5.9}$$

If we choose the Langevin case (4.5), i.e.  $V(x) = x$ , we find directly from Eq. (5.9)

$$\dot{\rho} = -i \frac{\lambda^2 a_1}{4m} [x, [p, \rho]_+] - \frac{\lambda^2 a_1}{2\beta} [x, [x, \rho]] . \quad (5.10)$$

Going back to the Schrödinger picture, we find that this is the Phenomenological Master Equation (3.3) with the damping coefficient

$$\gamma = \frac{\lambda^2 a_1}{2m} , \quad (5.11)$$

and the diffusion coefficient is

$$D = \frac{\lambda^2 a_1}{2\beta} , \quad (5.12)$$

Combining these we obtain the correct Einstein relation

$$D = \frac{m\gamma}{\beta} = m\gamma kT . \quad (5.13)$$

Because we have used an expansion in the variable

$$\beta\omega = \frac{\omega}{kT} \leq \frac{B}{kT} , \quad (5.14)$$

we have obtained a high temperature expansion. A small value of  $\beta B$  is sufficient in order to get the simple results (5.7) and (5.8). In the slow motion limit, however, the transform of the potential  $\tilde{V}(\omega)$  is supposed to provide a frequency cut-off, and we may hope that the results remain valid also for  $\beta B \gg 1$ . If we have to retain higher order  $\omega$  terms in the expansions in Eqs. (5.2) and (5.7), we obtain higher derivatives with

respect to the potential. Thus even in the Langevin case (4.5) we obtain relaxation dependent on  $(d^3x/dt^3)$ , which is known from radiative damping to cause problems. For the diffusion we obtain terms proportional to  $(d^2x/dt^2)$ . The influence of such terms has not been discussed to the best of my knowledge.

## VI. The harmonic oscillator

Most derivations of Brownian motion Master Equations have treated the harmonic oscillator. In order to see what happens we want to look how this case fits into our approach. We choose to treat the problem only in the Langevin case (4.5), when all results can be obtained explicitly. In this case, we can proceed directly from Eqs.(4.6) and (4.7).

The time dependence of the potential is determined by the Heisenberg time evolution in the system of interest, and for the harmonic oscillator we have the equations

$$\begin{aligned} \dot{x} &= \frac{p}{m} \\ \dot{p} &= -m\Omega_0^2 x . \end{aligned} \quad (6.1)$$

From these we obtain the expression

$$x(t - \tau) = x(t) \cos \Omega_0 \tau - \frac{p(t)}{m\Omega_0} \sin \Omega_0 \tau \quad (6.2)$$

When this is inserted into Eqs. (5.7), and we use the properties of  $D(\tau)$  and  $\chi(\tau)$ , we find the formulae

$$\int_0^\infty d\tau D(\tau) \cos \Omega_0 \tau = \frac{1}{2} \int_{-\infty}^\infty d\tau e^{i\Omega_0 \tau} D(\tau) = \frac{1}{2} d(\Omega_0) \quad (6.3)$$

$$\int_0^\infty d\tau \chi(\tau) \sin \Omega_0 \tau = \frac{1}{2i} [\chi(\Omega_0) - \chi(-\Omega_0)] = \chi''(\Omega_0) = \frac{A(\Omega_0)}{2} , \quad (6.4)$$

because  $\chi(-\Omega) = \chi(\Omega)^*$ ; see Appendix II.

In addition to these we have two integrals involving principal values. The first one is

$$\int_{-\infty}^{+\infty} d\tau \chi(\tau) \cos \Omega_0 \tau = \frac{1}{2} [\chi(\Omega_0) - \chi(-\Omega_0)] = \chi'(\Omega_0) . \quad (6.5)$$

This goes together with the term proportional to

$$[x, [x, \rho]_+] = [x^2, \rho] , \quad (6.6)$$

which clearly gives a shift of the oscillational frequency of the harmonic oscillator.

We also have the term

$$\int_0^\infty d\tau D(\tau) \sin \Omega_0 \tau = \frac{1}{2i} \left[ \int_0^\infty d\tau D(\tau) e^{i\Omega_0 \tau} - \int_0^\infty d\tau D(\tau) e^{-i\Omega_0 \tau} \right] . \quad (6.7)$$

Using the result from Eq.(II.12) in Appendix II, we find

$$\int_0^\infty d\tau D(\tau) \sin \Omega_0 \tau = P \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{d(\omega)}{\Omega_0 - \omega} . \quad (6.8)$$

For very small oscillator frequencies  $\Omega_0$ , this goes to zero like in Eq.(5.8). It also vanishes for  $\Omega_0$  going to infinity. In the intermediate region, it does not necessarily vanish.

The effective range of integration is determined by the correlation time  $\tau_c$  of the reservoir. This is supposed to be much shorter than the oscillator period, and we can expand the trigonometric functions in the integral in (6.8). This is consequently seen to be small of the order

$$\Omega_0 \tau_c \propto \frac{\tau_c}{T_0} \ll 1 . \quad (6.9)$$

The finite value of the integral (6.8) is something of an embarrassment, because the integral stands in front of a commutator expression of the form  $[x, [\rho, p]]$ , which, in the Wigner function Master Equation gives a mixed derivative in the position and momentum variables. It is no comfort that the coefficient of such a term may be small; however small it is, it makes the diffusion tensor nonpositive. The exact role of such mixed derivatives in Master Equations is still obscure.

Collecting the results into the Master Equation (4.6) we obtain the result

$$\dot{\rho} = -i\Delta\Omega^2[x^2, \rho] - i\frac{\lambda^2 \chi''}{2m\Omega_0}[x, [p, \rho]_+] - \frac{\lambda^2 d(\Omega_0)}{2}[x, [x, \rho]] \quad (6.10)$$

In the Schrödinger picture, this is exactly the form of the Phenomenological Master Equation (3.3) with the energy shift

$$\Delta\Omega^2 = -\frac{\lambda^2}{2}\chi'(\Omega_0) , \quad (6.11)$$

and the damping

$$\gamma = \frac{\lambda^2 \chi''(\Omega_0)}{m\Omega_0} \quad (6.12)$$

and diffusion coefficient

$$D = \frac{\lambda^2 d(\Omega_0)}{2} \quad (6.13)$$

The term proportional to the (small) quantity (6.8) is omitted.

Using Eqs. (II.7) and (II.11) we obtain the fluctuation-dissipation relation

$$D = \frac{\gamma m \Omega_0}{2} \coth \left( \frac{\beta \Omega_0}{2} \right) \quad (6.14)$$

in the high temperature limit, this reduces correctly to the result (5.13).

## VII. The non-Langevin case

We noticed in Sec. III that we needed the potential to be of the form  $V(x) = x$  to obtain the quantum counterpart of the simple Langevin equation (3.1). Here we are going to consider the effects of the more general potential

$$V(x) = \sum_q e^{iqx} V_q . \quad (7.1)$$

The reality of  $V(x)$  implies that the  $q$ -sum is symmetric around  $q = 0$ .

We derive the Master Equation only in the slow motion limit of Sec. V, which is given in Eq. (5.9). There we need

$$\dot{V} = \sum_q i q V_q \left( e^{iqx} \frac{p}{m} \right)_s . \quad (7.2)$$

where  $(\dots)_s$  means the symmetrically ordered product.

Introducing the notation

$$g = \frac{\lambda^2 a_1}{2} , \quad (7.3)$$

we can write the Master Equation (5.9) in the form

$$\dot{\rho} = -\frac{g}{\beta} \left[ V, \left\{ \left( 1 + i \frac{\beta}{2} \frac{\partial}{\partial t} \right) V \rho - \rho \left( 1 - i \frac{\beta}{2} \frac{\partial}{\partial t} \right) V \right\} \right] \quad (7.4)$$

Using the expansions (7.1) and (7.2) we find

$$\dot{\rho} = -\frac{g}{\beta} \sum_{q, q'} V_q V_{q'} [e^{iqx}, (e^{-\beta q' p/2m} e^{iq' x} \rho - \rho e^{\beta q' p/2m} e^{iq' x})] , \quad (7.5)$$

where we have used the fact that the term proportional to  $p$  is supposed to be used in the slow motion limit only.

We now introduce some further assumptions about the potential (7.1). We postulate that it has randomly distributed phases so that we can take an ensemble average in the Master Equation. A weak form of translational invariance assumes the ensemble average  $\overline{V(x)V(x')}$  to be a function of  $(x - x')$  only. We find

$$\begin{aligned} \overline{V_q V_{q'}} &= \int \int \frac{dx dx'}{(2\pi)^2} e^{-i(qx + q'x')} \overline{V(x)V(x')} \\ &= \delta(q + q') \int \frac{dx'}{2\pi} e^{-iqx'} \overline{V(0)V(x')} \\ &= \overline{V_q^2} \delta(q + q') . \end{aligned} \quad (7.6)$$

In addition, it follows from Eq.(2.1) that the distribution of  $q$  values is symmetric

$$\overline{V_q^2} = \overline{V_{-q}^2} . \quad (7.7)$$

Introducing these assumptions into the Eq.(7.5) we obtain

$$\dot{\rho} = -\frac{g}{\beta} \sum_q \overline{V_q^2} (\rho e^{-\beta qp/2m} - e^{iqx} \rho e^{-\beta qp/2m} e^{-iqx} - e^{iqx} e^{-\beta qp/2m} \rho e^{-iqx} + e^{\beta qp/2m} \rho) . \quad (7.8)$$

Using the relation (7.7) we can change the sign of the summation variable in Eq.(7.8) and obtain the equation

$$\dot{\rho} = -\frac{g}{\beta} \sum_q \overline{V_q^2} (C_q^\dagger C_q \rho + \rho C_q^\dagger C_q - 2C_q \rho C_q^\dagger) \quad (7.9)$$

with

$$C_q = e^{iqx} e^{-\beta qp/4m} . \quad (7.10)$$

In these equations we have neglected some commutators between  $\rho$  and  $p$  in order to obtain the result.

This approximation is discussed in Appendix III.

The result (7.9) is clearly of the Lindblad form. The operator (7.10) shifts the momentum by the amount  $q$ , which is thus a random kick transmitted from the reservoir to the system of interest. A discussion of this situation has been given by Dalibard and Castin<sup>[38]</sup>.

To see that (7.9) is consistent with the phenomenological theory of damping we calculate the expectation values

$$\begin{aligned}
\frac{d}{dt} \langle x \rangle &= 0 \\
\frac{d}{dt} \langle p \rangle &= \frac{2g}{\beta} \sum_q \overline{V_q^2} q \langle e^{-\beta q p / 2m} \rangle \\
&= \frac{2g}{\beta} \sum_q \overline{V_q^2} q \left( 1 - \frac{\beta q}{2m} \langle p \rangle \right) \\
&= -\gamma \langle p \rangle ,
\end{aligned} \tag{7.11}$$

where the damping coefficient is

$$\gamma = \frac{g}{m} \sum_q \overline{V_q^2} q^2 \geq 0 . \tag{7.12}$$

For small momenta  $\langle p \rangle$ , this expansion is assumed valid; see, however, the discussion in the following section.

Assuming that the momentum distribution  $\overline{V_q^2}$  is sufficiently short ranged in momentum space, i. e. the potential is exceedingly smooth, we can express everything using its second moment as in Eq. (7.12). We expand the terms in the Master Equation (7.9) and obtain

$$\begin{aligned}
[V, [V, \rho]] &= \sum_q \overline{V_q^2} [e^{-iqx}, e^{iqx}, \rho] \\
&= \sum_q \overline{V_q^2} q^2 [x, [x, \rho]]
\end{aligned} \tag{7.13}$$

$$\begin{aligned}
[V, [\dot{V}, \rho]_+] &= -\frac{i}{m} \sum_q \overline{V_q^2} [e^{iqx}, [(pe^{iqx}), \rho]_+] \\
&= \frac{1}{m} \sum_q \overline{V_q^2} q^2 [x, [p, \rho]_+] .
\end{aligned} \tag{7.14}$$

Inserting these expressions into (7.9) and going to the Schrödinger picture, we obtain the phenomenological master equation with the damping given in Eq.(7.12) and the diffusion coefficient

$$D = \frac{g}{\beta} \sum_q \overline{V_q^2} q^2 . \tag{7.15}$$

As a check on the consistency of the procedure, we note that the results (7.12) and (7.15) satisfy the correct

form (5.13) of the fluctuation-dissipation relation. This concludes our derivation of the Master Equation for the general non-Langevin case.

The dimensionless expansion parameter in this section has been the quantity in (7.11) which we can write as

$$\left( \frac{\beta q p}{2m} \right)^2 = \left( \frac{q^2/2\mu}{kT} \right) \left( \frac{p^2/2m}{kT} \right) \left( \frac{\mu}{m} \right) , \tag{7.16}$$

where  $\mu$  is a typical mass relating to the particles constituting the reservoir. Near thermal equilibrium, the first two factors on the right hand side of (7.16) are of order unity and the expansion parameter is small if the reservoir particles are much lighter than the system of interest. This is just the limit when the classical Brownian motion prevails.

We have used the potential expansion (7.1) to derive the Master Equation in the form (7.9). In order to obtain the Langevin limit we should let  $V(x)$  equal  $x$ , Eq. (4.5), which implies

$$V_q = i \frac{\partial}{\partial q} \delta(q) . \tag{7.17}$$

With this result, it is difficult to make sense of the assumption (7.6), but the derivations in (7.13) and (7.14) prove that it suffices that  $V_q$  is short ranged in momentum space, i.e. the reservoir delivers only small momentum kicks to the system.

However, another problem arises from non-Langevin forms of the potential  $V(x)$ . This derives from the loss of translational invariance of the reservoir force; the influence of the reservoir depends on position. Only on the average, can we restore the invariance. This changes the relationship between the system and the reservoir, and it is not obvious to what extent the physics is changed from the pure Langevin case. In the literature, see e.g. Ref. [16], there are several methods to restore the translational invariance; it remains to be seen if such modifications of the theory will affect the physical conclusions.

### VIII. Connection with the Lindblad form

In this section we want to compare the results of the previous section with the general Lindblad form (3.5). In a recent publication<sup>[34]</sup> Gallis has derived a Lindblad form compatible with the result we desire for a Brownian motion with linear damping. I start by restating his conclusions in the notation used in the present paper.

Gallis uses the Lindblad form (3.5) with  $\alpha_q = 1$  and

$$C_q = \frac{1}{\sqrt{2}} e^{iqx} (A(q) - B(q)qp), \quad (8.1)$$

where  $A(q)$  and  $B(q)$  are even complex functions of their argument  $q$ . The form is supposed to be an expansion in the momentum variable  $p$ , and it is hence compatible with our low energy expansion in Sec. V.

The conditions imposed by Gallis on the Lindblad form determine the dissipative terms in the Master Equation (Gallis<sup>[34]</sup> Eq.(3.15))

$$\begin{aligned} \dot{\rho} = & - \sum_q |A(q)|^2 (\rho - e^{iqx} \rho e^{-iqx}) - \sum_q \text{Re}(A^*(q)B(q)) q e^{iqx} [p, \rho]_+ e^{-iqx} \\ & - \frac{1}{2} \sum_q |B(q)|^2 q^2 (p^2 \rho + \rho p^2 - 2e^{iqx} p \rho p e^{-iqx}) - \sum_q \text{Im}(A^*(q)B(q)) q e^{iqx} [p, \rho] e^{iqx} \end{aligned} \quad (8.2)$$

In order to compare this result with our work we rewrite the dissipative part of the Eq.(7.8) in the form

$$\dot{\rho} = -\frac{2g}{\beta} \sum_q \overline{V_q^2} (\rho - e^{iqx} \rho e^{iqx}) - \frac{g}{2m} \sum_q \overline{V_q^2} q e^{iqx} [p, \rho]_+ e^{-iqx} ; \quad (8.3)$$

in order to obtain this form we have used the evenness of respect to  $q$ . In Appendix III, we discuss the influence of noncommutativity of  $p$  and  $x$  on this equation

We find that the first two terms on the right hand side of Eq.(8.2) reproduce the result (8.3) if we set

$$\begin{aligned} |A(q)|^2 &= \frac{2g}{\beta} \overline{V_q^2} , \\ \text{Re}(A^*(q)B(q)) &= \frac{g}{2m} \overline{V_q^2} , \end{aligned} \quad (8.4)$$

The latter condition is most easily satisfied by the choice

$$B(q) = \frac{\beta}{4m} A(q). \quad (8.5)$$

This has the advantage that we have

$$\text{Im}(A^*(q)B(q)) = 0 , \quad (8.6)$$

leading to the vanishing of the last term in the Master Equation (8.2).

With the choices (8.4) and (8.5) we can compare the momentum damping constant  $\gamma$  with that derived in Gallis Eq. (3.13)

$$\begin{aligned} \gamma &= 2 \sum_q \text{Re}(A^*(q)B(q)) q^2 \\ &= \frac{g}{m} \sum_q \overline{V_q^2} q^2 , \end{aligned} \quad (8.7)$$

which agrees with the result (7.12). Gallis also derives the equation for the kinetic energy of the motion in the form

$$\begin{aligned} \frac{d}{dt} \langle p^2 \rangle &= \frac{d}{dt} \langle p^2 \rangle + \frac{d}{dt} \langle (p - \langle p \rangle)^2 \rangle \\ &= -\Gamma \langle p^2 \rangle + 2D . \end{aligned} \quad (8.8)$$

The diffusion coefficient  $D$  is given by

$$D = \frac{1}{2} \sum_q |A(q)|^2 q^2 = \frac{g}{\beta} \sum_q \overline{V_q^2} q^2 \quad (8.9)$$

in agreement with Eq. (7.15).

For the energy damping constant  $\Gamma$  Gallis obtains the expression

$$\begin{aligned}\Gamma &= 2\gamma - \sum_q |B(q)|^2 = 2\gamma - \frac{\beta g}{8m^2} \sum_q \overline{V_q^2} q^4 \\ &= \frac{2g}{m} \sum_q \overline{V_q^2} q^2 \left(1 - \frac{\beta}{16m} q^2\right) .\end{aligned}\quad (8.10)$$

The first term in (8.10) is the expected  $2\gamma$ , but the correction term is unexpected. Assuming that  $q_0$  is some typical momentum exchange in a single encounter with the reservoir, we estimate the correction term to be of the order

$$\frac{q_0^2 \beta}{2m} = \left(\frac{q_0^2/2\mu}{kT}\right) \left(\frac{\mu}{\beta}\right) . \quad (8.11)$$

where  $\mu$  is a typical mass of the reservoir particles; see Eq.(7.16). As the quantity (8.11) is proportional to the

expansion parameter of the theory, (7.16), we expect the correction term in (8.10) to be small. The same conclusion follows, of course, if we assume the potential  $\overline{V_q^2}$  to be short ranged as in the previous section.

Finally we need to consider terms proportional to higher powers of  $p$  in Eq. (8.2). They are necessary to assure that the Master Equation is of the Lindblad form, but they have no counterpart in our result (3.3). Their form is, however, such that no corrections of order  $< p^2 >$  or higher orders appear in the evolution equation (7.11) for the expectation value  $< p >$ . This is reassuring, because when  $< p >$  goes to zero, these terms would start to dominate in the Eq. (7.11) after long enough times. To see the cancellation explicitly we evaluate their contribution as

$$\begin{aligned}\frac{d}{dt} < p > &= -\frac{1}{2} \sum_q |B(q)|^2 q^2 \text{Tr}[p(p^2 \rho + \rho p^2 - e^{iqx} p \rho p e^{-iqx})] \\ &= -\sum_q |B(q)|^2 q^2 \text{Tr}[p(p - e^{iqx} p e^{-iqx}) p \rho] \\ &= -\sum_q |B(q)|^2 q^3 \text{Tr}(p^2 \rho) = 0 ,\end{aligned}\quad (8.12)$$

because of the symmetry of  $B(q)$ .

The Gallis result, thus reconciles our results with the Lindblad form. It also gives exactly the correct linear damping in the equation of motion for  $< p >$ , which is a requirement for the Brownian motion theory. It can also be seen to give no contribution to the equation of motion for  $< x >$  as is required.

The Gallis form of the Master Equation does, however, not satisfy the requirements (3.4) for the second moments exactly. Already the damping rate of  $< p^2 >$  was seen to contain a correction term in Eq.(8.8). This does not, however cause any complications. Likewise the equation for  $< (xp + px) >$  is found to be damped at the rate  $\gamma$  in accordance with (3.4). However, the second moment of the position derives a rate of change

from (8.2) which becomes

$$\frac{d}{dt} < x^2 > = \frac{\beta}{8m^2} \sum_q \overline{V_q^2} q^2 = \frac{\beta}{8} \frac{\gamma}{m} \geq 0 . \quad (8.13)$$

This contributes a diffusive motion to  $< x^2 >$ , which is small in the high temperature limit.

One can easily see that the presence of the term (8.13) does cause some difficulties. If we look at the harmonic oscillator case, the equations (3.4) possess the steady state solution

$$\begin{aligned}< (xp + px) > = 0 \\ \frac{< p^2 >}{2m} &= \frac{1}{2} kT = \frac{1}{2} m \Omega^2 < x^2 > ,\end{aligned}\quad (8.14)$$

which agrees with the equipartition and the virial results. With the term (8.13), however, the only steady

state solution possible violates the virial theorem and the classical equipartition for the oscillator. If these are enforced, no steady state solution is possible.

We have found that the Gallis result gives a Master Equation in the Lindblad form and provides the correct equations for the first moments of the dynamical variables. The second moments are, however, not entirely correct, and, in particular, the diffusive increase of the second moment of the position variable leads to unwanted physical consequences; this either violates some simple physical relations or destroys the behaviour at large times for any temperature. For high temperatures this problem will occur at later times only.

## IX. Discussion of validity

At many points in the derivations above, I have remarked on the possible validity of the ensuing results. It would be desirable to identify exactly those situations where the results hold, but unambiguous conclusions seem hard to obtain. In this section I will try to present the various cases where it seems likely that a Brownian motion description may be approximately adequate.

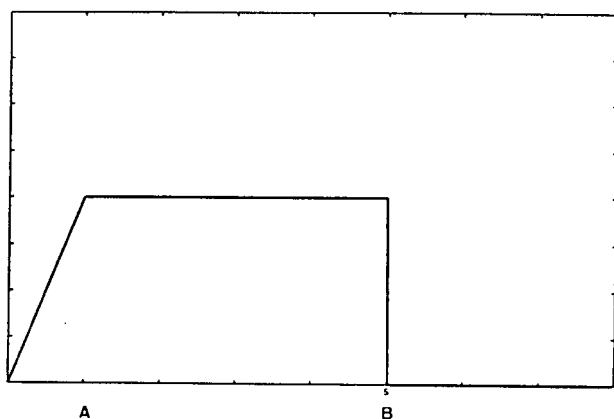


Figure 1. The figure shows the simple form of the reservoir spectral density  $A(\omega)$  assumed in this paper. The spectrum is linear up to the frequency  $\omega = A$  and stays constant after that. The cut-off is at the value  $\omega = B \gg A$ . In a physical reservoir we expect the elementary excitations to give structure to the spectrum in the range  $A - B$ .

The properties of the reservoir are all contained in the spectral density function  $A(\omega)$ . We have shown that this has to be linear in  $\omega$  near zero, and we assume

that it has an upper cut-off  $B$  determining the reservoir correlation time  $\tau_c$ . For the sake of the arguments, we consider the simplest analytical form satisfying these requirements, viz. that in Fig. 1. The spectrum rises linearly to some value  $\omega = A$ , after which it stays constant up to the cut-off  $\omega = B \gg A$ . In real physical systems the behaviour near  $A$  must be smooth and there will appear some structure in the region  $A < \omega < B$ .

Most physical properties are determined from a comparison between the energy of the motion, let us characterize this by some typical largest frequency  $\Omega$ , and the behaviour of the reservoir fluctuations described by the function (II.11)

$$d(\omega) = \frac{1}{2} \coth\left(\frac{\beta\omega}{2}\right) A(\omega). \quad (9.1)$$

In addition to the parameters  $A, B$  and  $\Omega$ , we also have the additional thermal parameter  $kT$ ; the physical behaviour depends on the relations between these.

In Fig. 2, we see the function  $d(\omega)$  for the cases  $kT = A$ ,  $kT = \frac{1}{2}A$ ,  $kT = \frac{1}{3}A$  and  $\frac{1}{20}A$ . We can see that for  $kT \geq A$ , no flat region for  $\omega > A$  exists; the behaviour is dominated by the thermal factor in (9.1). Because of the cancellation of the frequency dependence near zero, there always exists a linear regime for

$$\omega \simeq kT \leq A. \quad (9.2)$$

Fig. 3 demonstrates this in the low frequency region for the case  $kT = \frac{1}{6}A$ . The flat region is well below the value  $A$ , and the behaviour is very smooth near zero frequencies.

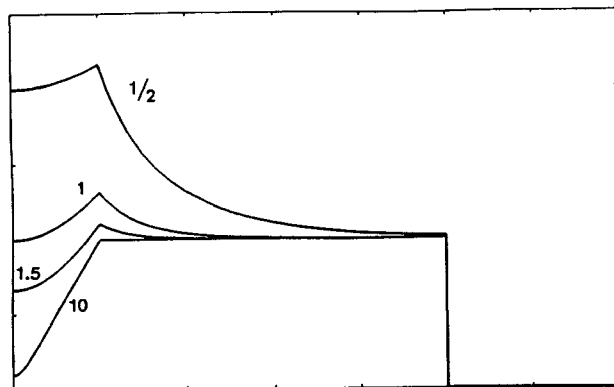


Figure 2. This shows the thermal fluctuation spectrum of the reservoir  $d(\omega)$ . It consists of the spectral density shown in Fig. 1 multiplied with the thermal factor as in Eq. (9.1). The parameter labelling the curves is  $(\beta A/2)$ .

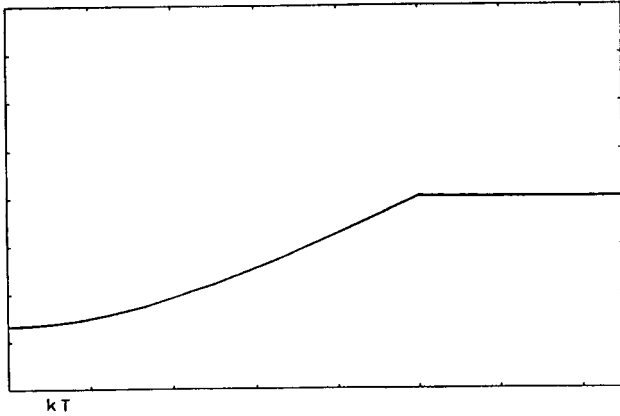


Figure 3. The fluctuation spectrum  $d(\omega)$  is shown for the special case  $(\beta A/2) = 3$ . This represents a typical case when the thermal energy  $kT$  (indicated in the picture) is much less than the linear part of the spectrum  $\omega < A$ . The low frequency region offers a rather invariant response to low energy excitations.

The fluctuations of the reservoir guarantee that the kinetic energy does not fall below the thermal one. In all physical cases we expect that

$$\Omega \geq kT . \quad (9.3)$$

We obtain the first region of validity of the derivations in this paper

$$kT \leq \Omega < A . \quad (9.4)$$

This is, indeed, the slow motion limit discussed in Sec. V, where the fluctuation-dissipation theorem takes the classical form (5.13). A relevant question is now whether we can have quantum effects from the motion and still retain the classical description of the reservoir effects?

The curvature of the potential function  $V(x)$  is taken to be characterized by a length scale  $a$ , and the de Broglie wave length  $\lambda$  is of the order  $(m\Omega)^{-1/2}$ . Quantum effects are then seen if the wave packet is less than  $a$  which is less than  $\lambda$  (see e.g. Ref.[39]). The quantum uncertainty energy is then

$$E_0 \geq \frac{1}{ma^2} > \frac{1}{m\lambda^2} \simeq \Omega . \quad (9.5)$$

Thus the spread in energy is larger than the energy itself, and the validity of our derivations hold only if the condition (9.4) is replaced by the stronger condition

$$\Omega \leq E_0 < A . \quad (9-6)$$

On the other hand, replacing  $\Omega$  by  $kT$  according to (9.3) we enter a situation where the Brownian motion time evolution has been found to lead to difficulties for short times, as has been pointed out by Ambegaokar<sup>[40]</sup> and Munroe and Gardiner<sup>[45]</sup>. The possibility to observe Brownian motion behaviour retaining quantum effects appears to be unlikely even if no conclusive proof has been given one way or the other.

In the region  $kT \simeq A$ , the whole spectral region is rather flat; the cusps in Fig. 2 are unphysical and we expect them to smear out in any realistic system. Then it seems that the Brownian motion models have a very wide range of validity

$$kT \simeq A \leq Q \ll B . \quad (9.7)$$

Starting at any energy well below  $B$ , the system should damp according to the Brownian motion behaviour all the way down to its final equilibrium energy. In this case there seems to be no reason to assume that the conservative evolution could not contain quantum features. In the region (9.7) all cases seem realizable.

Finally, we have to consider the case  $kT > A$ . Then the smooth region can be found only below  $\omega = A$ , but because we have the frequency spectrum of the motion constrained by the condition (9.3), the motion will always see the rapidly changing part of the spectrum, see Fig. 2. If we have the linear region extending all the way up to the cut-off, then the whole region becomes smoothly varying. However, then the thermal energy spectrum extends beyond the cut-off  $B$ , and we have no right to assume that the dissipative behaviour becomes universal.

The above conditions have been discussed under the assumption that the spectrum of the motion extends from its upper limit  $\Omega$  closely towards zero. This follows for many potentials, but for the case treated in Sec.VI, the spectrum of the motion contains only the single frequency  $\Omega_0$  for all energies. Thus the system probes the fluctuation spectrum at this single frequency only. The spectral density appears flat locally, and the results derived in Sec. VI hold. In this case the rotating wave form of the Master Equation gives a good description. The motion of a harmonic oscillator may thus be damped as a Brownian motion for any frequency  $\Omega_O$  well below the cut-off  $B$ . No restrictions

seem to be necessary, and the general form (6.14) of the fluctuation-dissipation relation may be needed.

When the frequency of the oscillator is changed, the dissipative parameters remain the same only if we stay on a flat portion of the fluctuation spectrum. If the spectrum has rapidly varying structures, we will find rapidly varying dissipative parameters. Then universality can be found only close to zero frequencies when the Brownian motion behaviour is classical, and the energy approaches its final equilibrium value smoothly. This implies that many oscillator states can participate even close to the equilibrium, which implies

$$\Omega_0 \ll kT . \quad (9.8)$$

Then the motion behaves nearly classically.

If the coupling function  $V(x)$  to the reservoir is not of the Langevin type (4.5), the spectral components entering the proto-master equation (4.6) will contain integer multiples of  $\Omega_0$ . However, only such components need be included which make up the excitation energy  $E$  of the system. Thus the condition (9.3) is replaced by the condition

$$N\Omega_0 \simeq E \geq kT . \quad (9.9)$$

Towards the end of the damping process in any binding potential the dynamic behaviour will appear harmonic. Thus the final stages will be found to be Brownian if the curvature of the potential is such that the case (9.8) ensues; then the evolution is universal but the dissipative behaviour is classical. A universal dissipative evolution from a quantum regime to the final thermal equilibrium can be seen only in the case (9.7). Then all energies see the same dissipative parameters during the whole history.

For unbound motion, the parameter characterizing the energy scale is less self-evident. For a particle acted on by a constant force  $F$  (like a gravitational attraction), the steady state kinetic energy is

$$E_{\text{kin}} = \frac{F^2}{m\gamma^2} . \quad (9.10)$$

This is added to the thermal fluctuation energy, and these determine the maximum frequency of the evolution  $\Omega$ . Thus, the Brownian motion description can be found valid in any of the cases (9.4) or (9.7). The free particle case can be discussed along similar lines.

One main approximation underlies all our work here; we have assumed that the Master Equation is Markovian. This takes it for granted that all time evolution of the system, including that induced by the reservoir, takes times much exceeding the correlation time  $\tau_c$ . In the notation of the present paper this implies that

$$kT \leq |\Omega + i\gamma| \ll B . \quad (9.11)$$

The diffusion correlation function  $D(\tau)$  acts like a delta function, when the Fourier transform of the fluctuation spectral density  $d(\omega)$  is well localized in time. This seems to occur independently of  $kT$  in our model, and a large  $B$  seems to be the only necessary assumption. The Markovian nature of the damping term is manifest under even less stringent conditions. I want to stress that I utilize no quantum Langevin equation, and hence the correlations of the Langevin force is of no concern here.

My conclusion is that, as long as  $B$  is large enough, the Fokker-Planck form of the dissipative mechanism may be valid as a universal description of the damping for many different situations. Especially the low temperature limit and the quantum form of the fluctuation-dissipation theorem can be compatible with a Fokker-Planck form of the dissipative time evolution for the Wigner function.

## X. Conclusions and relations to other works

The damping becomes linear in the momentum  $p$  because the Master Equation contains a term proportional to

$$\dot{V}(x) \propto \dot{x} \propto p . \quad (10.1)$$

The spectral density  $A(\omega)$  is an odd function; for small values of  $\omega$  this is found to imply linearity in the time derivative. The fact that  $A(\omega)$  is odd follows because we have coupled the system to a Hermitean operator of the reservoir. It is, of course, possible that some other odd power dominates; in that case no Brownian motion behaviour can be seen.

Our method of derivation originates already in the work by Wangsness and Bloch<sup>[2]</sup>, who put down the basic criteria for its validity; in our notation

$$t \gg \tau_c, \quad \Omega \ll B. \quad (10.2)$$

This allows the dynamic evolution to be nonperturbative because we can follow it to times such that  $\Omega t \gg 1$ .

In this work we have chosen to couple the reservoir to a function of position  $V(x)$ . Ford et al.<sup>[16]</sup> point out that such a Hamiltonian may not have a lower bound; for a harmonic oscillator they show the flaw to be corrected by a suitable renormalization of the energy. It implies the introduction of counter terms canceling our (5.5). This is possible to achieve by a canonical transformation, but the physical meaning of the different couplings are not identical.

Which coupling function is chosen, i.e. do we use functions of  $x$  or  $p = m\dot{x}$ , is not irrelevant. If the coupling to the reservoir is through a Hermitean operator, for long times the density matrix tends to become diagonal in the representation of the eigenstates of that operator. Physically it is highly significant whether the density matrix becomes diagonal in the momentum or position representation. By choosing a potential  $V(x)$  we force spatial quantum correlations to die out with time, which has been used to justify localization of the particles in real space. In the Dynamical Reduction Program<sup>[20–21]</sup>, this effect is postulated to be a real universal mechanism to constrain quantum systems to show classical behaviour.

For harmonic oscillator systems, we can choose to perform the rotating-wave-approximation as discussed in Refs. [6] and [16]. Physically the damping behaviour of the system is seen to be the same, because of the symmetry between  $x$  and  $p$  in the phase plane of the harmonic oscillator. The relaxation rate can be distributed at will between the components owing to their rapid interchange at the oscillator frequency. With the rotating-wave approximation the Master Equation is much easier to justify and seems to lead to a much less controversial time evolution. For a quantized electromagnetic mode, this is the natural representation of the Master Equation.

The work by Ford et al.<sup>[16]</sup> does stress the need for a universal description of dissipation in the same spirit that I have tried to implement in the present paper. They want their description to be ‘independent of the

potential  $V$  and dependent only on the the parameters characterizing the coupling to the reservoir’.

Many treatments suggest that the classical-looking Brownian motion Fokker-Planck equation can hold only in the high temperature limit. Caldeira and Leggett<sup>[11]</sup> explicitly require that

$$kT > B. \quad (10.3)$$

The same limit is considered e.g. by Hakim and Ambegaokar<sup>[12]</sup> and Haake and Reibold<sup>[42]</sup>. The situation seems to be in conflict with our physical picture of a universal reservoir. Near equilibrium, the excitation energy of the system must be at least of the order  $kT$ , and then the frequency spectrum of the motion would extend beyond the reservoir cut-off  $B$ . In this case dissipative behaviour cannot be fully universal. A generic reservoir approach can exist only if the cut-off  $B$  can be taken to be the largest frequency parameter of the system. Thus I have assumed that all dynamic evolution must be confined to lower frequencies as Eq.(9.11) says. This condition agrees with that assumed by Wangsness and Bloch (10.2).

Unruh and Zurek<sup>[19]</sup> point out that the formal derivation seems to require (10.3) also in their model. However, they prove numerically that when  $B$  grows to infinity the quantum corrections are negligible except for very short initial times. Then the initial state is changed by violent transients, which wipe out much of the initial quantum coherence.

The fact that the Brownian motion Master Equation cannot be applied to short times is obvious from its derivation; we have to observe the system over many correlation times  $t \gg \tau_c$ . The difficulties at the early stages of the evolution have been discussed by Ambegaokar<sup>[40]</sup> and Diosi<sup>[41]</sup>. A detailed investigation is carried out by Haake and Reibold<sup>[42]</sup>, who conclude that the Master Equation may be used for times such that

$$t \times kT \simeq 1, \quad (10.4)$$

but the dissipative parameters are then time dependent; this agrees with the conclusion arrived at by Paz et al.<sup>[43]</sup>. In the present work, the dissipative parameters turn out to be constant but, in any case, it is clear that the equation should be taken as an asymptotic

behaviour approaching equilibrium. For short times there will be large initial transients<sup>[19]</sup> which are called 'slips' by Haake and collaborators; see [42] and references therein. Thus we cannot recover the correct initial state from the later stages of the time evolution but only the state at the end of the transient region where the Master Equation becomes valid. The present derivation may give corrections to the simple Markovian behaviour, but these are expected to be of the orders  $(kT/B)$  and  $(A/B)$  only. For a large cut-off, they are negligible. They affect the exact form of the approach to equilibrium, but they will not endanger the Markovian character of the evolution.

In the limit of weak damping,  $\gamma \rightarrow 0$ , the Brownian motion Master Equation seems to follow in all treatments; see e.g. Caldeira and Leggett<sup>[11]</sup> and Haake and Reibold<sup>[42]</sup>. The latter work also shows that the overdamped case does not display the same kind of universality. It is not clear that our Born-Markov approach excludes the overdamped case. If we are in a universal region, it should be possible to let the oscillational frequency of the harmonic motion go continuously to zero passing through the overdamped region. This must be possible if we expect to describe also the case of a free or constantly accelerated particle. For the low energy limit, these cases are, however, expected to behave in the classical way. The result of the derivation presented in this paper does not seem to depend on the ratio  $(\gamma/B)$  as long as the relation (9.11) is satisfied.

In the harmonic oscillator case treated in Sec. VI I found that the Master Equation contains terms of the form  $[x, [p, \rho]]$ , which give a mixed derivative  $(\partial^2/\partial x \partial p)$  in the equation for the Wigner function. The term is proportional to  $\beta$  and disappears in the high temperature limit or for the slow motion case treated in Sec. V. Haake and Reibold<sup>[42]</sup> point out that this term does give a nonpositive diffusion matrix. Diosi<sup>[41]</sup> corrects the situation by adding a term  $[p, [p, \rho]]$  which gives diffusion in position space, i.e. terms in  $(\partial^2/\partial x^2)$ . I have already explained why such terms seem to be unphysical. They give reservoir action on the equations for the moments of  $x$ , which have no interpretation in terms of physical Langevin forces and lead to incessant heating.

I have connected the Phenomenological Master Equation to the Lindblad form through the work of

Gallis<sup>[34]</sup>. His treatment does give rise to some problems, including the possibility of uncontrolled heating. We have also been unable to use the Lindblad formulation to perform a numerical simulation. Convergence problems have prevented us from obtaining consistent results. Why the phenomenological description of the physically so well understood case of Brownian motion should turn out to be this difficult to fit into the presumably generic Lindblad treatment is still a great mystery.

In this paper I have introduced the reservoir approximation by decree. The Born-Markov approximation is assumed valid, and I have postulated the existence of reservoirs for which this holds true. Subsequently I have found a variety of situations where a dissipative Master Equation can give a behaviour that copies the classical Brownian motion. Especially, I have suggested that both the low temperature quantum limit and the overdamped oscillator limit may be described by a quantum Brownian motion. These conclusions disagree with some results derived from analytically soluble models. Why is this so?

One possible answer is that the reservoir behaviour is not realizable in these limiting cases. Then no conditions can justify the Born-Markov derivation, and only the classical limit holds. This may be so for soluble oscillator models, but I have envisaged the reservoir as forced to be steadily renewed at an extremely fast rate. The reservoir presupposes its own heat bath. Then the instantaneous destruction of all correlations imposed by the interaction can be justified. This seems like an infinite regress, but it is not excluded by any logical inconsistency, and it may, in fact, correspond closely to the situation prevailing in real reservoirs.

I thus suggest the possibility that reservoirs composed of independent oscillators may lead to different conclusions from those cases where real heat baths are responsible for the dissipative effects. These are vast entities with infinitely fast phase relaxation and superior ability to exchange energy without reaction. If this is true, it may offer the ultimate explanation for the universality of dissipative behaviour in viscous media. Whether such behaviour can be combined with quantum features of the dynamical time evolution is not finally answered by my calculations. It may, however,

be within experimental reach in short pulse laser investigations of molecular dynamics.

### Acknowledgements

I want to thank J.Dalibard and Y.Castin for showing me how to find a Lindblad form for the friction Master Equation. I also want to thank S.Barnett, M.Collett, L.Diosi, C.Gardiner, F.Haake, B.Munroe, and I.Percival, for instructive and helpful discussions of their results. During Seminars and Workshops, many other scientists, too numerous to mention, have presented useful comments and questions concerning my attempts to understand the linear friction in Quantum Theory. I am indebted to them all.

### Appendix I: Derivation of Master Equation

In this Appendix we shall present a derivation of the proto-master equation (4.6). We start from the Hamiltonian in Eq.(4.1) and go to the interaction picture with respect to the system and reservoir degrees of freedom. For the total density matrix of the coupled systems  $\rho_{\text{tot}}$  we then obtain the interaction picture reservoir-system operator

$$\rho_{SR} = \exp[+i(H + H_R)t]\rho_{\text{tot}} \exp[-i(H + H_R)t] \quad (I.1)$$

Just like in the classical kinetic theory, this is the first in a hierarchy of coupled equations for the correlations functions. In order to truncate the hierarchy, we have to decouple the system of equations at some point. The simplest is the second order Born approximation, where dissipative terms are included only to second order in  $\lambda$ . This allows us to factorize the density operator on the right hand side of (I.7) into

The equation of motion for this operator becomes

$$i\dot{\rho}_{SR} = \lambda[V(t)\Gamma(t)\rho_{SR}] \quad (I.2)$$

where the operators

$$V(t) = \exp(iHt)V \exp(-iHt)$$

$$\Gamma(t) = \exp(iH_R t)\Gamma \exp(-iH_R t) \quad (I.3)$$

are Heisenberg operators for the uncoupled systems.

Introducing the reduced density operator for the system of interest alone

$$\rho = \text{Tr}_R \rho_{SR} , \quad (I.4)$$

we obtain for it from (I.2) the equation of motion

$$\dot{\rho}(t) = -i\lambda[V(t)\varphi(t, t) - \varphi(t, t)V(t)]. \quad (I.5)$$

Here the influence of the reservoir is through the system operator

$$\varphi(t, t') = \text{Tr}_R[\rho_{SR}(t)\Gamma(t')] . \quad (I.6)$$

This, in its turn, is found to obey the equation of motion

$$\frac{d}{dt}\varphi(t, t') = i\lambda[\text{Tr}_R(\rho_{SR}(t)\Gamma(t)\Gamma(t'))V(t) - V(t)\text{Tr}_R(\rho_{SR}(t)\Gamma(t')\Gamma(t))] \quad (I.7)$$

$$\rho_{SR}(t) \approx \rho(t)\sigma_0 , \quad (I.8)$$

where  $\rho(t)$  is given by (I.4) and  $\sigma_0$  is the reservoir density matrix. According to our assumptions in Sec. III, the reservoir acts as a bath and  $\sigma_0$  can be assumed to stay clamped at its initial form; in the calculations we are assuming the reservoir to be in thermal equilibrium. With this assumption, we can solve the equation (I.7) in the form

$$\varphi(t, t') = i\lambda \int_0^t dt'' (K(t'', t')\rho(t'')V(t'') - K(t', t'')V(t'')\rho(t'')) \quad (I.9)$$

where we have introduced the reservoir correlation function

$$K(t, t') = Tr_R[\sigma_0 \Gamma(t) \Gamma(t')] . \quad (I.10)$$

Because the reservoir density matrix is stationary

$$[\sigma_0, H_R] = 0 , \quad (I.11)$$

the correlation function (I.10) has the translational invariance

$$K(t_1, t_2) = K(t_1 - T, t_2 - T) = K(t_1 - t_2) . \quad (I.12)$$

An essential part of our assumption that the reservoir forms an infinite bath is that its correlations decay so fast that we can assume the time evolution for the system of interest to become Markovian. This implies

$$K(t_1 - t_2) \rho(t_1) \approx K(t_1 - t_2) \rho(t_2) , \quad (I.13)$$

because  $K(t_1 - t_2) \approx 0$  for  $|t_1 - t_2| > \tau_c$ .

With these assumptions we insert Eq.(I.9) into (I.5) and obtain the equation

$$\begin{aligned} \dot{\rho} = & -\lambda^2 \left[ \rho(t) \int_0^t d\tau K(t - \tau, t) V(t - \tau) V(t) \right. \\ & - \int_0^t d\tau K(t - \tau, t) V(t) \rho(t) V(t - \tau) - \int_0^t d\tau K(t, t - \tau) V(t - \tau) \rho(t) V(t) \\ & \left. + \int_0^t d\tau K(t, t - \tau) V(t) V(t - \tau) \rho(t) \right] \end{aligned} \quad (I.14)$$

It is advantageous to split the correlation function by writing

$$[K(t - \tau, t)] = D(\tau) + \frac{1}{2} \varphi(\tau) = [K(t, t - \tau)]^* \quad (I.15)$$

Here we have introduced the fluctuation part

$$D(\tau) = \frac{1}{2} Tr_R[\sigma_0 (\Gamma(t - \tau) \Gamma(t) + \Gamma(t) \Gamma(t - \tau))] \quad (I.16)$$

and the linear response function

$$\varphi(\tau) = -i Tr_R(\sigma_0 [\Gamma(t - \tau), \Gamma(t)]_-) \quad (I.17)$$

$$= i(\langle \Gamma(\tau) \Gamma(0) \rangle - \langle \Gamma(0) \Gamma(\tau) \rangle) .$$

It is easily seen that, because  $\Gamma$  is Hermitean, the response function is an odd function of its argument

$$\varphi(-\tau) = -\varphi(\tau) . \quad (I.18)$$

In terms of the functions introduced, we can write the proto- masterequation in the form

$$\begin{aligned} \dot{\rho} = & -\lambda^2 \int_0^t d\tau D(\tau) [\rho V(t - \tau) V(t) + V(t) V(t - \tau) \rho - V(t) \rho V(t - \tau) - V(t - \tau) \rho V(t)] \\ & - \frac{i\lambda^2}{2} \int_{-\infty}^t d\tau \chi(\tau) [\rho V(t - \tau) V(t) - V(t) V(t - \tau) \rho - V(t - \tau) \rho V(t - \tau) + V(t - \tau) \rho V(t)] ; \end{aligned} \quad (I.19)$$

here  $\rho$  is taken at the time  $t$  everywhere. The linear response part is written in terms of the retarded susceptibility

$$\chi(t) = \Theta(t)\varphi(t) , \quad (I.20)$$

where  $\Theta(t)$  is the step function which disappears for negative times.

## Appendix II. The spectral theory

Utilizing the detailed balance condition

$$k_+(\omega) = e^{\beta\omega} k_-(\omega) , \quad (II.3)$$

which holds if the reservoir density matrix  $\sigma_0$  represents a canonical distribution, we find

$$\begin{aligned} k_+(\omega) &= \frac{e^{\beta\omega}}{e^{\beta\omega} - 1} A(\omega) \\ k_-(\omega) &= \frac{1}{e^{\beta\omega} - 1} A(\omega) \end{aligned} \quad (II.4)$$

The Fourier transform of the retarded susceptibility is given by

$$\begin{aligned} \chi(\omega) &= \int_0^{+\infty} e^{i\omega t} \varphi(t) dt \\ &= \int_{-\infty}^{+\infty} e^{i\omega t} \chi(t) dt . \end{aligned} \quad (II.5)$$

Because  $\chi(\omega)$  is analytic in the upper  $\omega$  half plane, we can evaluate the integral in (II.5) for  $\omega + i\epsilon$  and obtain

$$\chi(\omega) = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega' - \omega - i\epsilon} \equiv \chi' + i\chi'' . \quad (II.6)$$

From this we can extract expressions for the real and imaginary parts of  $\chi$  in the usual way; especially we find

$$\chi''(\omega) = \frac{1}{2} A(\omega) . \quad (II.7)$$

We introduce the Fourier transform of the correlation functions (I.10) for the reservoir variables according to

$$Tr_R(\sigma_0 \Gamma(\pm\tau) \Gamma(0)) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} k_{\pm}(\omega) \quad (II.1)$$

Following the practice in many-body theory, see Ref.[44], we introduce the spectral density

$$A(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} Tr_R(\sigma_0 [\Gamma(\tau), \Gamma(0)]) = k_+(\omega) - k_-(\omega) . \quad (II.2)$$

The sum-rule

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(\omega) = 0 \quad (II.8)$$

follows directly from the definition (II.2). This implies that  $A(\omega)$  is an odd function of  $\omega$ . Consequently, if  $A(\omega)$  can be expanded in a power series in  $\omega$ , it must be of the form

$$A(\omega) = \sum_{i=1}^{\infty} a_i \omega^{2i-1} . \quad (II.9)$$

It also follows that the real part  $\chi'(\omega)$  is an even function of  $\omega$ . Thus we have

$$\chi(-\omega) = \chi(\omega)^* . \quad (II.10)$$

Straightforward considerations show that the Fourier transform of the fluctuation function (I.16) is of the form

$$d(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\tau\omega} D(\tau) = \frac{1}{2} \coth\left(\frac{\beta\omega}{2}\right) A(\omega); \quad (II.11)$$

this is thus an even function of  $(\omega)$ . We also need the half-Fourier transform of this quantity. Applying the

same procedure which lead to the expression (II.6) we obtain

$$\int_0^\infty d\tau D(\tau) e^{i\omega\tau} = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{d(\omega')}{\omega' - \omega - i\epsilon} . \quad (II.12)$$

Finally, I note that there are higher order sum rules, which can be derived from the Heisenberg equation of motion for  $\Gamma$ . After (II.8) the following one is

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega A(\omega) = -Tr_R(\sigma_0[\Gamma, [\Gamma, H_r]]) . \quad (II.13)$$

This sum-rule can be used to determine the spectral band width  $B$  of the reservoir. The reservoir correlation time  $\tau_c$  is proportional to the inverse of this band width.

### Appendix III. Commutator corrections

In Sec.VII we use the proto-master equation (5.9) in the form

$$\dot{\rho} = -\frac{g}{2}[V, [\dot{V}, \rho]] - \frac{g}{\beta}[V, [V, \rho]] . \quad (III.1)$$

Using the expansion (7.1) and the averaging procedure (7.6) we find

$$\overline{[V, [V, \rho]]} = 2 \sum_q \overline{V_q^2} (\rho - e^{iqx} \rho e^{-iqx}) . \quad (III.2)$$

The first term of the right-hand side in (III.1) becomes similarly

$$\overline{[V, [\dot{V}, \rho]]} = \sum_q \overline{V_q^2} \left[ e^{iqx}, \left( \left( \frac{d}{dt} e^{-iqx} \right) \rho + \rho \left( \frac{d}{dt} e^{-iqx} \right) \right) \right] . \quad (III.3)$$

The derivative can be expressed as the limit

$$\left( \frac{d}{dt} e^{-iqx} \right) = \frac{1}{\Delta t} (e^{-iq(x+p \Delta t/m)} - e^{-iqx}) . \quad (III.4)$$

Using the Baker-Hausdorff theorem and the commutator between  $x$  and  $p$ , we can easily derive the expres-

sions

$$\begin{aligned} \left( \frac{d}{dt} e^{-iqx} \right) &= \left( -i \frac{q}{m} \right) e^{-iqx} \left( p - \frac{q}{2} \right) \\ &= \left( -i \frac{q}{m} \right) \left( p + \frac{q}{2} \right) e^{-iqx} \end{aligned} \quad (III.5)$$

Using these expressions in Eq. (III.3)

$$\overline{[V, [\dot{V}, \rho]]} = -\frac{i}{m} \sum_q \overline{V_q^2} \{ q e^{iqx} [\rho, p]_+ e^{-iqx} - q^2 (\rho - e^{iqx} \rho e^{-iqx}) \} . \quad (III.6)$$

Introducing (III.2) and (III.6) into (III.1) we obtain the equation

$$\dot{\rho} = -\frac{g}{2m} \sum_q \overline{V_q^2} q e^{iqx} [\rho, p]_+ e^{-iqx} - \frac{2g}{\beta} \sum_q \overline{V_q^2} \left( 1 - \frac{\beta q^2}{4m} \right) (\rho - e^{iqx} \rho e^{-iqx}) . \quad (III.7)$$

This Master Equation is exactly identical with (7.8) in the smooth potential limit of Eqs. (7.13-14). How-

ever, the diffusion constant (7.15) is replaced by

$$D = g\beta \sum_q \overline{V_q^2} q^2 \left( 1 - \frac{\beta q^2}{4m} \right) . \quad (III.8)$$

The second term in the sum (III.8) comes from the non-

commutativity of  $x$  and  $p$ . It is exactly of the form

$$\frac{q_0^2/2m}{kT} \ll 1 \quad (III.9)$$

also encountered in Eq.(8.11). The influence from the commutators  $[x, p]$  are hence shown not to change the form of the Master Equation derived in Sec. VII. This is natural, because the smooth potential limit used to obtain the Brownian motion results (7.13) and (7.14) gives essentially the classical behaviour as seen from the result (III.8).

## References

1. I.R. Senitzky, Phys. Rev. **119**, 670 (1960).
2. R.K. Wangsness and F. Bloch, Phys. Rev. **89**, 728 (1953).
3. G.W. Ford, M. Kac and P. Mazur, J. Math. Phys. **6**, 504 (1965).
4. G.S. Lindblad, Rep. Math. Phys., **10**, 393 (1976).
5. P. Ullersmaa, Physica, **32**, 27, *ibid* **32**, 56, *ibid* **32**, 74, *ibid* **32**, 90 (1966).
6. G. S. Agarwal, Phys. Rev. A **4**, 739 (1971).
7. F. Haake, *Statistical Treatment of Open Systems*, Vol. 66 of *Springer Tracts in Modern Physics* (Springer, Berlin 1973).
8. G.S. Agarwal, in *Progress in Optics*, Vol. XI, p.1, ed. E. Wolf (North- Holland, 1973).
9. H. Dekker, Phys. Rep. **80**, 1 (1981).
10. H. Grabert *Projection Operator Techniques in Nonequilibrium Statistical Mechanics*, Vol. 95 of *Springer Tracts in Modern Physics* (Springer, Berlin 1982).
11. A.O. Caldeira and A.J. Leggett, Physica, **121A**, 587 (1983).
12. V. Hakim and V. Ambegaokar, Phys.Rev. A, **32**, 423 (1985).
13. H. Grabert, U. Weiss and P. Talkner, Z.Phys. B, **55**, 87, (1984).
14. E. Joos and H.D. Zeh, Z. Phys.B **59**, 223 (1985).
15. G.W. Ford and M. Kac, J. Stat. Phys., **46**, 803 (1987).
16. G.W. Ford, J.T. Lewis and R.F. O'Connell, Phys. Rev. A **37**, 4419 (1988).
17. M.J. Collett, Phys. Rev.A, **38**, 2233 (1988).
18. C.W. Gardiner, IBM J. Res. Develop., **32**, 127 (1988).
19. W.G. Unruh and W.H. Zurek, Phys. Rev. D, **40**, 1071 (1989).
20. G.-C. Ghirardi, A. Rimini and T. Weber, Phys. Rev.D **34**, 470, (1986).
21. G.-C.Ghirardi, P. Perle and A. Rimini, Phys. Rev.A **42**, 78 (1990).
22. L. Diosi, J. Phys. A: Math. Gen. **21**, 2885 (1988); Phys. Rev. A **1165** (1989).
23. N. Gisin and I.C. Percival, J. Phys. A: Math. Gen., **25**, 5677 (1992).
24. N. Gisin and I. C. Percival, J. Phys. A: Math. Gen., **26**, 2233 (1993).
25. N. Gisin and I. C. Percival, J. Phys. A: Math. Gen., **26**, 2245 (1993).
26. W.H. Zurek, Physics Today, October 1991, p.36.
27. B.R. Mollow, Phys. Rev. A **12**, 1919 (1975).
28. H. Carmichael, *An Open Systems Approach to Quantum Optics*, (Springer, 1993).
29. K. Moelmer, Y. Castin and J. Dalibard, J. Opt. Soc. Am. B **10**, 527 (1993).
30. S. Stenholm, Physica Scripta **47**, 724 (1993).
31. G.S. Lindblad, Commun. Math. Phys, **48**, 119, (1976).
32. E.B. Davis, *Quantum Theory of Open Systems*, (Academic, 1976).
33. A. Sandulescu and H. Scutaru, Ann. Phys. (New York), **173**, 277 (1987).
34. M.R. Gallis, Phys. Rev. A **48**, 1028 (1993).
35. B.M. Garraway, K.-A. Suominen and S. Stenholm, Physics World, April 1993, p.46.
36. U. Fano, Phys. Rev. **96**, 869 (1954).
37. R.J. Glauber, in *Quantum Optics and Electronics*, ed. C. DeWitt, A. Blandin and C.Cohen-Tannoudji (Gordon and Breach, 1965).
38. J. Dalibard and Y. Castin, private communication.
39. S. Stenholm, Phys. Rev. A **47**, 2523 (1993).
40. V. Ambegaokar, Ber. Bunsenges. Phys. Chem. **95**, 400 (1991).
41. L. Diosi, Europhysics Lett., **22**, 1 (1993).
42. F. Haake and R. Reibold, Phys. Rev. A **32**, 2462 (1985).
43. J.P. Paz, S. Habib and W.H. Zurek, Phys. Rev. D, **47**, 488 (1993).
44. P.C. Martin, in **Many Body Physics**, (Les Houches 1967), p.37, eds. C. DeWitt and R. Balian (Gordon and Breach, New York, 1968).
45. B. Munroe and C. Gardiner, private communication.