Investigating the Validity of Quantum Master Equations

A Thesis

submitted to
Indian Institute of Science Education and Research Pune
in partial fulfillment of the requirements for the
BS-MS Dual Degree Programme

by

Akash Trivedi

Indian Institute of Science Education and Research Pune
Dr. Homi Bhabha Road,
Pashan, Pune 411008, INDIA.

April 2022

Supervisor: Abhishek Dhar

Certificate

This is to certify that this dissertation entitled Investigating the Validity of Quantum Master Equations towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune, represents work carried out by Akash Trivedi at the International Centre for Theoretical Sciences, Bangalore under the supervision of Abhishek Dhar, Professor, Department of Physics, during the academic year 2021-22.

Akash Trivedi

Abhishek Dhar

Abhishek Dhar

Committee:

Abhishek Dhar

Bijay Agarwalla

Sreejith GJ

This thesis is dedicated to the unusually remarkable, challenging and enriching year that I have lived till the date.

Declaration

I hereby declare that the matter embodied in the report entitled Investing the Validity of Quantum Master Equations are the results of the work carried out by me at the Department of Physics, International Centre for Theoretical Sciences, Bangalore, under the supervision of Professor Abhishek Dhar and the same has not been submitted elsewhere for any other degree.

Akash Trivedi

Abhishek Dhar

Abhishek Dhar

Acknowledgements

I want to thank my supervisor, Professor Abhishek Dhar, for providing the fantastic opportunity to work on this project. Your guidance has been truly enlightening. I am incredibly grateful to Prof. Bijay Agarwalla, Prof. Sanjib Sabhapandit, Prof. Manas Kulkarni and Prof. Anupam Kundu for their constant guidance and the amazing brain-storming sessions that we had every week in the past year. I really can not thank you enough for your time and patience. This experience has not only enriched my understanding of the subject but has also provided me with a remarkable experience in scientific research.

I am sincerely thankful to Prof. Bijay Agarwalla. He has been guiding me since my second year at IISER. He has always been there to talk about any academic as well as non-academic issues. A big thanks for all the opportunities for semester projects, summer projects and, of course, the journal club discussions. I would like to thank all my batchmates at IISER, especially Aditya Kolhatkar, Ritwick Ghosh, Rushikesh Patil and Sabarenath JP. You all have been a constant source of inspiration and kind teachers to answer the silliest of questions throughout my academic journey at IISER. Finally, I can't forget to thank my family and school friends for their constant support and wishes.

I want to acknowledge the Long Term Visiting Students Program of ICTS, which funded my project and allowed me to use the excellent resources at ICTS. Special thanks to the people of ICTS, who have been extremely helpful in all manners. I would also like to acknowledge the Kishore Vaigyanik Protsahan Yojana (KVPY) and the Infosys Foundation Scholarship for funding my studies and their support for research in natural sciences.

Abstract

From well-established subjects like electronics to modern subjects like quantum technology, every field dealing with the physics of nanoscale uses the formalism of open quantum systems. The master equation formalism is one of the most widely used approaches in studying open quantum systems. In this approach, the dynamics of the reduced density matrix of the system is governed by an integro-differential equation called the master equation. There are multiple approximations—Born, Markov and Secular approximations—that go into deriving a master equation. This thesis aims to provide a thorough analysis of these approximations and improve the understanding of the regime(s) of validity master equations. We do this by studying a model system using both the Markovian and the Non-Markovian versions of the master equation within the Born approximation. We then compare these results with *exact* results obtained by using the Langevin equation approach, which is an exact approach.

After understanding the motivation to take up this study in the introduction section, we will briefly describe our methodology followed in undertaking this study. In chapter 1, we will introduce the model and understand the reasons behind choosing a Rubin bath for this study. In chapter 2, we solve our model system using the exact Langevin approach and learn about some physical properties of the quantum Brownian motion. In the next chapter, we study the same setup using different master equations. We then compare these two approaches in detail in chapter 4. We also present some additional studies to understand the conclusions that we obtained from the comparison. In chapter 5, we provide a prescription to perform the Born-Markov approximation in the Langevin equation formalism. Finally, we conclude the thesis and discuss the work that we are planning to do in the future.

Contents

Abstract **xi**

Introduction **1**

Methodology **5**

1 The Model and Bath Properties **7**

1.1 The Model 7

1.2 Spectral Density of the Bath 8

1.3 Kernels 10

Appendix **17**

1.A Simplifying $\gamma(0)$ 17

2 Langevin Equation Approach **19**

2.1 Deriving the Langevin Equation 20

2.2 Solving the Langevin Equation 21

2.3 Analysing the Solutions 25

2.4 A Discussion on the Weak Coupling Limit 36

2.5 Limitations of the Langevin Equation Approach 37

Appendix **38**

2.A Solving the Bath Equations . . . 38

2.B Leibniz Route vs Integration by Parts Route . . . 38

3 Master Equation Approach **42**

3.1 Born Master Equation (BME) . . . 44

3.2 Born semi-Markov Master Equation (BSMME) . . . 50

3.3 Born Markov Master Equation (BMME) . . . 59

Appendix **62**

3.A Detailed Calculations . . . 62

4 Comparisons between Both Approaches **66**

4.1 Comparing the Homogeneous Parts . . . 66

4.2 Free Particle Limit of a Bounded Particle . . . 68

4.3 Comparing BME and BSMME using the Ohmic Bath . . . 72

5 Born-Markov Approximations in the Langevin Approach **75**

5.1 Born Approximation . . . 76

5.2 semi-Markov Approximation . . . 79

5.3 Summary Table . . . 81

Appendix **82**

5.A Detailed Calculations . . . 82

Conclusions and Future Plans **85**

List of Figures

1.1 Setup of the Problem. 7

2.3.1 Free Particle: $\langle x^2 \rangle_t$ vs t 30

2.3.2 Free Particle: $\langle x^2 \rangle_t$ vs t - Different Temperatures. 31

2.3.3 Free Particle: $\ln(\langle x^2 \rangle_t)$ vs $\ln(t)$ - Different Temperatures. 32

2.3.4 Free Particle: $\ln(\langle x^2 \rangle_t)$ vs $\ln(t)$ - Different Parameters. 32

2.3.5 Bounded Particle: Fits for $\langle x^2 \rangle_t$ vs t as $t \to 0$. 34

2.3.6 Bounded Particle: $\langle x^2 \rangle_t$ vs t. 35

2.3.7 Bounded Particle: $\langle x^2 \rangle_t$ vs t - Different Temperatures. 35

3.1.1 Bounded Particle: Comparison of approaches at $T = 0$. 49

3.1.2 Bounded Particle: Comparison of approaches at $T \to \infty$. 50

3.1.3 Free Particle: Comparison of approaches for Different Temperatures. 51

4.1.1 Bounded Particle: Comparison of Different Approaches - Homogeneous Part. . . . 67

4.1.2 Free Particle: Comparison of Different Approaches - Homogeneous Part. 67

4.1.3 Free Particle: Homogeneous Part - Different Parameters. 68

4.2.1 Bounded Particle: Comparison of Different Approaches in the Limit $\hbar\omega_0 <<$ $\hbar\gamma << \hbar\omega_p << k_B T$ 69

4.2.2 Bounded Particle: Comparison of Different Approaches in the Limit $k_BT << \hbar\omega_0 << \hbar\gamma << \hbar\omega_p$ 70

4.2.3 Bounded Particle: Comparison of Different Approaches in the Limit $\omega_0 << \gamma << \omega_p$ as $t \to 0$ 71

4.2.4 Bounded Particle: Comparison of Different Approaches in the Limit $\hbar\omega_0 << \hbar\gamma << \hbar\omega_p$ - Homogeneous Parts 71

Introduction

Brief Background and Motivation

The natural way of understanding anything has a very similar structure in every discipline. We start from understanding some overwhelmingly simplified models and then keep building layers of complexities on the existing knowledge and machinery to model the real world at the end. The subject of open quantum systems is one such layer to the knowledge of closed system dynamics, which studies the evolution of a system under its own Hamiltonian. Closed system dynamics is useful for studying systems that have no interaction with any other system. The subject of open quantum systems incorporates the effect of other systems lying in the vicinity of the system of our interest.

We start our description by dividing the universe into two parts: the system and the environment. We then aim to understand the effect of the environment on the system. We commonly model the environment as a "bath", which has a large number of degrees of freedom compared to the system. The bath is usually taken to be in the equilibrium state at some temperature β and a chemical potential μ. We generally take a quantum bath, i.e. the particles of the bath are indistinguishable. The system can be anything that we want to study. Usually, a Boson, a Fermion or a spin (or even a chain of any of these) serves as a good model system. We learn some exclusive phenomena like dissipation and decoherence by studying these paradigmatic models of open quantum systems.

The formalism of open quantum systems has found great importance in both theoretical and experimental understanding in various fields like photonics, condensed matter physics and mesoscopic physics ([21]). It also plays a crucial role in understanding the meaning of quantum measurements. The fields of quantum thermodynamics and quantum optics heavily uses the formalism of open quantum systems ([24], [6]). The cutting-edge experimental facilities have made it possible to control and study many quantum systems in various regimes of parameters. Hence, it is very important to have a tractable and consistent theoretical framework to study open quantum systems.

There are multiple formalisms to study the dynamics of open systems, such as the path integral approach, the Langevin equation approach, the Green's function approach (NEGF) and the master equation approach ([13], [11]). The bath has humongous degrees of freedom, and our system usually interacts with a much smaller number of degrees of freedom of the bath. It is not practical (and possible) to keep track of all the degrees of freedom when we study the dynamics. That is the primary reason why exact approaches like the Langevin and the path integral approach has very limited applicability. To capture the relevant degrees of freedom and make our analysis tractable, we perform various approximations. The master equation approach is the most widely used formalism, and it does a number of such approximations.

In the master equation formalism, one studies the differential equation governing the dynamics of the reduced density matrix of the system. If the system-bath coupling is weak, one can do a "Born approximation". It is a perturbative approximation and gives the **Born Master Equation**. Further, if the bath obeys some nice properties, which we will discuss in chapter 3, we can do a "Markov approximation". The **Born-Markov Master Equation** or the **Redfield Equation** is local in time and much simpler to solve. The Lindblad form of dynamics has been studied extensively in various contexts. A master equation describing an open system, i.e. the Redfield equation can also be reduced to the **Lindblad form** if we can perform the "secular approximation" on top of the Born-Markov approximation. There are a bunch of different types of Lindblad equations like the local Lindblad, global Lindblad, universal Lindblad ([19], [18]), etc. All these master equations have their own regimes of applicability.

The Lindblad master equations are proven to always preserve the positivity of a density matrix. But, recently it has been shown that it can fail to preserve conservation laws ([25], [23]) or can fail to predict correct thermalisation ([15], [23]). The Redfield equation can overcome this limitations ([22]), but it is known to have violated positivity ([3], [10]). Even we will witness such an instance in chapter 3. Existence of such limitations arising from the underlying approximation was one of the motivations behind investigating the approximations in deriving the master equation and reach a complete understanding of the regime(s) of their validity.

The master equation approach is used in studying a plethora of systems. Once we derive the master equation, we often hope that it gives some valuable insights even about regimes where it violates the approximations that went into deriving it. We will witness such an instance in chapter 4. To investigate and understand such possibilities was another motivation behind taking up this study.

Outline of the thesis

In this project, the central idea was to apply the master equation approach to a simple model system and compare the results to *exact* results obtained by using other methods—particularly, the Langevin dynamics approach—on the same system. This systematic comparison will clarify the regimes of applicability of the master equation approach for more complicated systems where the exact solutions are more difficult to obtain.

Our model system is a Brownian particle connected to a Bosonic bath. This model has served as the workhorse for many studies that are done using the formalism of open quantum systems. It has found its application in describing phenomena like transport and magnetism ([2]). Despite being studied extensively ([16], [17], [9]), there have been limited number of studies on comparing the master equation approach to the exact approaches. Some of the relevant earlier works are ([4], [19], [20]).

We have compared the dynamics of moments obtained from the exact Langevin equation, Born and Born-Markov master equations at all times for various baths, potentials and temperature regimes. In the process, we will absorb some obvious and some really shocking results. Alongside, we will rediscover most of the basic features of quantum Brownian motion. One take away that I would like you all to have is the importance of model systems in physics. It is astonishing that a model made up of balls and spring yields similar equations of motion as a suspended particle in a fluid, i.e. a classical Brownian particle.

The plan of the thesis is as follows: we will start by understanding the model and discuss some features of the bath that will be useful throughout the thesis. We will understand why we particularly chose Rubin bath for our study. We will also understand the features that a bath requires to serve as a Markovian bath. In chapter 2, we will solve and analyse the problem using the exact Langevin approach. We will discuss about a discrepancy in the literature that we found during our review. We will also derive something we call **a general sum rule**. We hope that it can be useful in future studies. In that chapter, you must see the beautiful figure 2.3.1; it depicts the behaviour of a Brownian particle for a finite temperature. It has a simultaneous presence of low temperature and high temperature behaviour in it. We will conclude that chapter by improving our understanding of the weak coupling limit and limitations of the Langevin approach.

In chapter 3, we will solve and analyse the problem using different master equations. We will clearly state and justify the Born and the Markov approximation. Actually, we will perform what we call a "**semi-Markov approximation**", which is slightly different from the traditional Markov approximation that we see in textbooks. We will learn about the benefits of semi-Markov approximation over the traditional Markov approximation. We will then discuss the very well-known divergence problems for an Ohmic bath and how our study suggests that one can avoid this problem by using a Drude bath with a large cutoff. **The results in this chapter are full of surprises.** We will see that a Born semi-Markov approximation works but only a Born approximation does not work for a certain regime. We will also see how Born semi-Markov approximation can work even for zero temperatures, where it was not supposed to work. We will discover that as opposed to the popular belief that the master equation works only for large times, it can work perfectly even for transients.

In chapter 4, we will try to complete the whole comparison. We will study the bounded Brownian particle in the "free particle limit" to understand results in previous chapters. The study shown in the last section of this chapter will serve as the icing on the cake to dismantle our traditional understanding of these approximations. Here, we show that **using Markovian kernels in the Born-approximated master equation is not equivalent to using Markovian kernels in Born Markov-approximated master equation**. This is surprising because if we use Markovian kenrels, the Markov approximation is supposed to become an exact statement and two approaches should have matched.

In chapter 5, we have prescribed the Born and Markov approximation in Langevin equation formalism. This study further clarifies the meaning of these approximations. Finally, we will conclude the work and discuss about our future plans.

Methodology

I will first describe the scope of our work. As I have mentioned earlier, we have compared three different approaches: Langevin approach, Born master equation and the Born semi-Markov master equation. We have done this comparison for all temperatures, for all times and for two different external potentials. For the ease of calculations, we will separate the comparison of temperature-dependent “inhomogeneous parts” of solutions from the temperature-independent “homogeneous parts”.

For solving the problem using the Langevin approach, we will solve for $x(t)$ of the system from the Langevin equation, which is an ordinary second order inhomogeneous differential equation. We will analytically reduce our problem to solving a non-trivial integral. We will do this integral numerically and get our results in terms of plots. To assist ourselves in understanding these plots, we will also analyse the integral analytically in various asymptotic limits.

For solving the problem using the master equation approach, we will obtain a system of differential equations governing the dynamics of moments. These equations become algebraic set of equations in the Laplace space. We will solve them and then numerically find their inverse Laplace transforms. We will again do some analytical expansions in the Laplace space to understand the numerical results better.

We will now list general conventions that are used in this thesis alongside some other relevant information that has been used repeatedly in the thesis.

- Unless stated otherwise, suffix “S” stands for the system and “B” for the bath. The suffix “I” will be used for representing the operators in the interaction picture.

- **Fourier Transforms**: For any function $f(t)$, its Fourier transform is represented by $\hat{f}(\omega)$:

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} dte^{i\omega t} f(t), \quad f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} d\omega e^{-i\omega t} \hat{f}(\omega) \tag{1}$$

- **Laplace Transforms**: For any function $f(t)$, its Laplace transform is represented by $\tilde{f}(z)$:

$$\tilde{f}(z) = \int_0^\infty dt e^{-zt} f(t) \tag{2}$$

- **Numerical Conventions**: In all our numerical studies, we have set $\hbar = k_B = M = 1$. We have used certain set of parameters throughout the thesis. We have shown microscopic parameters like mk and k' in all figures. Each set of microscopic parameters corresponds to macroscopic parameters like γ and ω_p. The table below provides a list of all used microscopic parameters and corresponding macroscopic parameters.

mk	k'	γ	ω_p	mk	k'	γ	ω_p
0.050	5.0	0.112	22.361	0.001	200.0	0.016	6324.555
0.050	20.0	0.112	89.443	0.040	200.0	0.1	1000.0
0.005	5.0	0.035	70.711	400.0	20000.0	10.0	1000.0

Table 1: *List of parameters used for numerical study.*

We will also list frequently used functions and its Laplace transforms:

$f(t)$	$\tilde{f}(z)$	$f(t)$	$\tilde{f}(z)$
e^{-ct}	$\frac{1}{z+c}$	$tg(t)$	$-\frac{d\tilde{g}(z)}{dz}$
$\frac{dg(t)}{dt}$	$z\tilde{g}(z) - g(0)$	$\frac{d^2g(t)}{d^2t}$	$z^2\tilde{g}(z) - zg(0) - \dot{g}(0)$
$g * h(t) = \int_0^t d\tau g(t-\tau)h(\tau)$	$\tilde{g}(z)\tilde{h}(z)$	$\int_0^t d\tau g(\tau)$	$\frac{\tilde{g}(z)}{z}$
$\sin(at)$	$\frac{a}{z^2+a^2}$	$\cos(at)$	$\frac{z}{z^2+a^2}$
$\delta(t)$	$\frac{1}{2}$	$e^{-ct}g(t)$	$\tilde{g}(z+c)$
t^n	$\frac{n!}{z^{n+1}}$	$\ln(t)$	$-\frac{\gamma_E + \ln(z)}{z}$
$\frac{25 - 12(\gamma_E + \ln(t))}{288} t^4$	$\frac{\ln(z)}{z^5}$	$(1 - \gamma_E - \ln(t))t$	$\frac{\ln(z)}{z^2}$

Table 2: *Laplace transforms that are used in the thesis.*

Chapter 1

The Model and Bath Properties

In this chapter, we will understand the model system that we have used. We will also analyse various properties of the bath. The quantities that we define in this chapter will be used repeatedly in this thesis.

1.1 The Model

A Boson attached to a Bosonic bath with certain types of coupling serves as the model of a quantum Brownian particle. This model yields the same equations of motion as one obtains from the phenomenological description of Brownian motion. In this section, we will understand the setup of the problem.

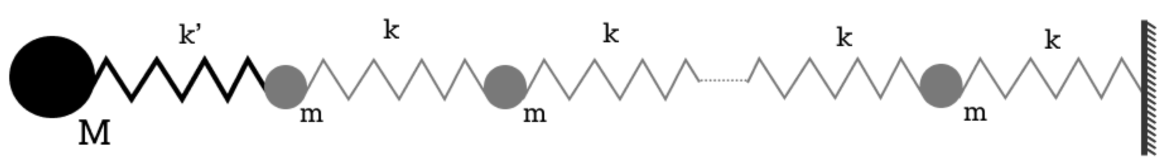


Figure 1.1: *Setup of the Problem.*

Our system is a particle with mass M, coordinate x and momentum p. It is placed in a potential $V(x)$. It is coupled to a Rubin bath, as shown in the figure 1.1. A Rubin bath is a one-dimensional chain with N number of particles of mass m each. Let n label these particles with x_n and p_n being the position and momentum, respectively. Particle 1 is attached to the system with coupling k', and bath particles are attached to each other with strength k. The Hamiltonian of the full system is

$$H = \frac{p^2}{2M} + V(x) + \sum_{n=1}^{N} \left(\frac{p_n^2}{2m} + \frac{k}{2} (x_n - x_{n+1})^2 \right) + \frac{k'}{2} (x - x_1)^2$$

where $x_{N+1} = 0$. We can break the Hamiltonian into a more convenient form by clubbing all the system coordinates and calling it a system Hamiltonian H_S. The bath Hamiltonian H_B comprises all bath coordinates, and the interaction Hamiltonian $\hat{H}_I$ has all terms which have both system and the bath coordinates:

$$H_S = \frac{p^2}{2M} + V(x) + \frac{k'}{2} x^2; \quad H_B = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \frac{k}{2} (x_n - x_{n+1})^2 + \frac{k'}{2} x_1^2; \quad \hat{H}_{SB} = -k' x x_1 \tag{1.1}$$

We will now write the bath Hamiltonian in the diagonalised form by writing it in its normal mode basis. In the matrix notation, we have $H_B = \mathbf{p}^T m^{-1} \mathbf{p}/2 + \mathbf{x}^T \phi \mathbf{x}/2$, where $\mathbf{x} = (x_1, x_2, ..., x_n)$ and $\mathbf{p} = (p_1, p_2, ..., p_n)$, and ϕ is the force matrix. We then do a linear transformation $\mathbf{X} = m^{1/2} U \mathbf{x}$ and $\mathbf{P} = m^{-1/2} U \mathbf{p}$, where U is an orthogonal transformation which diagonalises force matrix: $U \phi U^T = m \Omega^2$. $\Omega^2 = \{\Omega_s^2\}$ (with s ranging from 1 to N) is the diagonal matrix with entries being the square of bath eigenfrequencies.

We know that $\mathbf{x} = m^{-1/2} U^{-1} \mathbf{X}$, this implies $x_i = m^{-1/2} U_{ji} X_j$ (summation implied). Using this, we can write the equation 1.1 in the normal mode coordinates:

$$\begin{aligned} H_B &= \sum_{s=1}^{N} \frac{P_s^2}{2} + \frac{\Omega_s^2 X_s^2}{2} = \sum_s \hbar \Omega_s \left(b_s^\dagger b_s + \frac{1}{2} \right); \quad b_s = \sqrt{\frac{\Omega_s}{2\hbar}} \left[X_s + i \frac{P_s}{\Omega_s} \right] \\ \hat{H}_{SB} &= -x \sum_{s=1}^{N} C_s X_s \equiv -x B; \quad C_s = m^{-1/2} k' U_{s1}; \quad B = \sum_s C_s \sqrt{\frac{\hbar}{2\Omega_s}} (b_s + b_s^\dagger) \end{aligned} \tag{1.2}$$

b_s is the annihilation operator of the s^{th} bath mode. It follows the usual bosonic commutation relation: $[b_s, b_{s'}^\dagger] = \delta_{ss'}$ and $[b_s, b_{s'}] = 0 = [b_s^\dagger, b_{s'}^\dagger]$.

1.2 Spectral Density of the Bath

The spectral density of a bath is a crucial quantity that carries information about the effect of a bath on the system. It gives information about the strength with which each of the normal modes of the bath interacts with the system. As we go along, we will see that the spectral density will be required to calculate many important quantities. The definition of spectral density is

$$\Gamma(\omega) \equiv \sum_s \frac{\pi C_s^2}{2\omega}[\delta(\omega - \Omega_s) + \delta(\omega + \Omega_s)] \tag{1.3}$$

The above expression can be simplified using the eigenfunctions of the bath. For the Rubin bath, we can get ([8])

$$\Gamma(\omega) = \begin{cases} \frac{\gamma_0 \omega \sqrt{1 - \frac{m\omega^2}{4k}}}{1+\omega^2\tau^2}, & \text{if } \omega \leq 2\sqrt{\frac{k}{m}} \\ 0, & \text{otherwise} \end{cases}, \quad \gamma_0 = \sqrt{mk}, \quad \tau = \sqrt{1 - \frac{k'}{k}} \frac{\gamma_0}{k'} \tag{1.4}$$

Let us now analyse this quantity by taking some limits.

Drude Limit: Let a be the equilibrium distance between two bath oscillators. Then, we can go to the continuum limit by taking the limits $m \to 0$ and $a \to 0$, keeping the mass density $\sigma = m/a$ constant. We should also take the limit $k \to \infty$, keeping Young's modulus ka constant. In that case, the spectral density will become

$$\Gamma(\omega) = \gamma_0 \omega \frac{\omega_p^2}{\omega^2 + \omega_p^2}; \quad \gamma_0 = \sqrt{mk}, \quad \omega_p = \frac{k'}{\gamma_0} \tag{1.5}$$

Here, ω_p is the so-called Lorentz-Drude cutoff. This expression of spectral density is exactly the same as that of a Drude bath.

Ohmic Limit: On top of the Drude limit, go to the limit $k' \to \infty \equiv \omega_p \to \infty$; the spectral density becomes:

$$\Gamma(\omega) = \gamma_0 \omega; \quad \gamma_0 = \sqrt{mk} \tag{1.6}$$

This spectral density is the same as that of an Ohmic bath. The Drude and the Ohmic bath are very commonly used in the literature. So, the choice of a Rubin bath also allows us to study these other baths. We will be working in the Drude limit in our study.

As we shall see in the chapter 3 that the Markovian approximation works best for an Ohmic bath. But, here, we show that the Ohmic limit corresponds to a large k' limit, in fact, $k' \to \infty$. In the introduction, I argued that the Born approximation is a perturbative expansion in the interaction Hamiltonian. So, the Born approximation seems to require that k' should be small, whereas the Markovian approximation seems to require that k' should be large. So, will the Born-Markov approximation work for this model? — Spoiler alert — it does. To find out the reason, you will need to wait till section 2.4.

1.3 Kernels

In this section, we will define multiple quantities which might look a bit incoherent. As of now, you can just accept these definitions. We will see these quantities arising naturally in our study once we start analysing our system. In fact, in the master equation formalism, these kernels are all that we require from the bath to determine the effect of the bath on the dynamics of the system. We will define and analyse the dissipation, damping and noise kernels. To define these kernels, we first need to define the "random force term", $\eta(t)$. We define $\eta(t)$ in terms of B that we had in the equation 1.2:

$$\begin{aligned}\eta(t) &= e^{iH_Bt}Be^{-iH_Bt} \\ &= \sum_s C_s\sqrt{\frac{\hbar}{2\Omega_s}}(e^{i\Omega_s t}b_s^\dagger + e^{-i\Omega_s t}b_s) = \sum_s C_s\left(X_s(0)\cos(\Omega_s t) + \frac{P_s(0)}{\Omega_s}\sin(\Omega_s t)\right)\end{aligned} \tag{1.7}$$

It is very clear from this definition that $\langle\eta(t)\rangle_{th} = 0$ (since $\langle b_s\rangle_{th} = 0$). Now, we can define the dissipation kernel, $\Sigma(\tau)$:

$$\begin{aligned}\Sigma(\tau) &= \frac{i}{\hbar}\langle[\eta(\tau),\eta(0)]\rangle_B, \quad \{\text{Trace is with respect to the initial bath density matrix } \rho_B.\} \\ &= \sum_{s,s'} C_sC_{s'}\frac{i}{2\sqrt{\Omega_s\Omega_{s'}}}\left\langle[e^{i\Omega_s\tau}b_s^\dagger + e^{-i\Omega_s\tau}b_s, b_{s'}^\dagger + b_{s'}]\right\rangle_B \\ &= \sum_{s,s'} C_sC_{s'}\frac{i}{2\sqrt{\Omega_s\Omega_{s'}}}\left(e^{i\Omega_s\tau}\langle[b_s^\dagger, b_{s'}]\rangle_{th} + e^{-i\Omega_s\tau}\langle[b_s, b_{s'}^\dagger]\rangle_{th}\right) \\ &= \sum_s \frac{C_s^2}{\Omega_s}\sin(\Omega_s\tau)\end{aligned} \tag{1.8}$$

where in the third line, ρ_B is taken as $\rho_{th} = \frac{e^{-\beta H_B}}{Z}$, the equilibrium state at temperature β. Similarly, we can also derive an expression for the noise kernel, $D_1(\tau)$:

$$D_1(\tau) = \langle\{\eta(\tau),\eta(0)\}\rangle_{th} = \hbar\sum_s \frac{C_s^2}{\Omega_s}\cos(\Omega_s\tau)\coth\left(\frac{\beta\hbar\Omega_s}{2}\right) \tag{1.9}$$

We can also relate the kernels to the spectral density $\Gamma(\omega)$ (equation 1.3) as

$$\begin{aligned}\Sigma(\tau) &= \sum_s \frac{C_s^2}{\Omega_s}\sin(\Omega_s\tau) \equiv \frac{2}{\pi}\int_{-\infty}^{\infty} d\omega\Gamma(\omega)\theta(\omega)\sin(\omega\tau) \\ D_1(\tau) &= \hbar\sum_s \frac{C_s^2}{\Omega_s}\cos(\Omega_s\tau)\coth\left(\frac{\beta\hbar\Omega_s}{2}\right) \equiv \frac{2\hbar}{\pi}\int_{-\infty}^{\infty} d\omega\Gamma(\omega)\theta(\omega)\cos(\omega\tau)\coth\left(\frac{\beta\hbar\omega}{2}\right)\end{aligned} \tag{1.10}$$

Finally, let us define the damping kernel $\gamma(t)$ and its relation to the dissipation kernel:

$$\gamma(\tau) = \sum_s \frac{C_s^2}{\Omega_s^2}\cos(\Omega_s\tau) \equiv \frac{2}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\Gamma(\omega)}{\omega}\theta(\omega)\cos(\omega\tau); \quad \Sigma(t) = -\frac{d\gamma(t)}{dt} \tag{1.11}$$

We will be using these kernels in the Laplace space as well. We will take z as the Laplace parameter in this thesis. All functions in the Laplace space will have a *tilde* over it. The relation between these two kernels in the Laplace space:

$$\Sigma(t) = -\frac{d\gamma(t)}{dt} \implies \tilde{\Sigma}(z) = -z\tilde{\gamma}(z) + \gamma(0) = -z\tilde{\gamma}(z) + k' \tag{1.12}$$

where we have used the fact that $\gamma(0) = k'$. This has been shown in the appendix 1.A. Let us evaluate these kernels for baths that we are going to use. We will be using the specified form of the spectral densities that we defined in the previous section.

1.3.1 Drude Limit: Time-Space

We will use $\Gamma(\omega) = \gamma_0\omega\frac{\omega_p^2}{\omega^2+\omega_p^2}$, where $\omega_p = k'/\gamma_0$. We will derive an expression for $\Sigma(\tau)$ and $D_1(\tau)$ for this spectral density. Use equation 1.10 and let $\tau > 0$:

$$\begin{aligned}
\Sigma(\tau) &= \frac{2}{\pi}\int_0^{\infty} d\omega \sin(\omega\tau)\gamma_0\omega\frac{\omega_p^2}{\omega^2+\omega_p^2} \\
&= \frac{2\gamma_0\omega_p^2}{\pi}\frac{1}{2}\int_{-\infty}^{\infty} d\omega \sin(\omega\tau)\frac{\omega}{\omega^2+\omega_p^2} \\
&= \frac{2\gamma_0\omega_p^2}{\pi}\frac{1}{4i}\int_{-\infty}^{\infty} d\omega \left[\frac{e^{i\omega\tau}\omega}{(\omega - i\omega_p)(\omega+i\omega_p)} - \frac{e^{-i\omega\tau}\omega}{(\omega - i\omega_p)(\omega+i\omega_p)}\right] \\
&= \frac{2\gamma_0\omega_p^2}{\pi}\frac{1}{4i}\left[\frac{(2\pi i)e^{-\omega_p\tau}(i\omega_p)}{2i\omega_p} - \frac{(-2\pi i)e^{-\omega_p\tau}(-i\omega_p)}{-2i\omega_p}\right] \\
&= \gamma_0\omega_p^2 e^{-\omega_p\tau};\ \text{Similarly, for } \tau < 0 : \Sigma(\tau) = -\gamma_0\omega_p^2 e^{\omega_p\tau}
\end{aligned} \tag{1.13}$$

In the second line, we have changed the integration limit from $\{0 \to \infty\}$ to $\{-\infty \to \infty\}$ as the integrand is an even function. The integration is done using Cauchy's residue theorem. Finally:

$$\Sigma(\tau) = \text{sign}(\tau)\gamma_0\omega_p^2 e^{-\omega_p|\tau|} \tag{1.14}$$

Similarly, we can evaluate:

$$\gamma(\tau) = 2\int_0^{\infty} d\omega \cos(\omega\tau)\frac{\gamma_0}{\pi}\frac{\omega_p^2}{\omega^2+\omega_p^2} = \gamma_0\omega_p e^{-\omega_p|\tau|} \tag{1.15}$$

Now, let us move towards the noise kernel. We will need:

$$\coth\left(\frac{\hbar\omega}{2k_BT}\right) = \frac{2k_BT}{\hbar\omega}\sum_{n=-\infty}^{\infty}\frac{1}{1+(\nu_n/\omega)^2}; \quad \nu_n = \frac{2\pi n k_B T}{\hbar} \tag{1.16}$$

ν_n are called Matsubara frequencies. Use equation 1.10 and assume $\tau > 0$:

$$\begin{aligned}
D_1(\tau) &= 2\hbar\int_0^{\infty} d\omega\cos(\omega\tau)\frac{\gamma_0}{\pi}\omega\frac{\omega_p^2}{\omega^2+\omega_p^2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\\
&= \frac{4\gamma_0 k_BT\omega_p^2}{\pi}\sum_{n=-\infty}^{\infty}\frac{1}{2}\int_{-\infty}^{\infty}d\omega\cos(\omega\tau)\frac{1}{\omega^2+\omega_p^2}\frac{\omega^2}{\omega^2+\nu_n^2}\\
&= \frac{4\gamma_0 k_BT\omega_p^2}{\pi}\sum_{n=-\infty}^{\infty}\frac{1}{4}\int_{-\infty}^{\infty}d\omega\left[\frac{e^{i\omega\tau}\omega^2}{(\omega^2+\omega_p^2)(\omega^2+\nu_n^2)}+\frac{e^{-i\omega\tau}\omega^2}{(\omega^2+\omega_p^2)(\omega^2+\nu_n^2)}\right]\\
&= \frac{2\gamma_0 k_BT\omega_p^2}{\pi}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}d\omega\frac{e^{i\omega\tau}\omega^2}{(\omega+i\omega_p)(\omega-i\omega_p)(\omega-i\nu_n)(\omega+i\nu_n)}\\
&= \frac{2\gamma_0 k_BT\omega_p^2}{\pi}\left(\sum_{n=-\infty}^{0}(2\pi i)\left[\frac{e^{-\omega_p\tau}(-\omega_p^2)}{(2i\omega_p)(\nu_n^2-\omega_p^2)}+\frac{e^{\nu_n\tau}(-\nu_n^2)}{(-2i\nu_n)(\omega_p^2-\nu_n^2)}\right]\right.\\
&\qquad\qquad\left.+\sum_{n=0}^{\infty}(2\pi i)\left[\frac{e^{-\omega_p\tau}(-\omega_p^2)}{(2i\omega_p)(\nu_n^2-\omega_p^2)}+\frac{e^{-\nu_n\tau}(-\nu_n^2)}{(2i\nu_n)(\omega_p^2-\nu_n^2)}\right]\right)\\
&= 2\gamma_0 k_BT\omega_p^2\sum_{n=-\infty}^{\infty}\frac{\omega_p e^{-\omega_p\tau}-|\nu_n|e^{-|\nu_n|\tau}}{\omega_p^2-\nu_n^2};\ \text{Similarly, for } \tau<0:\\
D_1(\tau) &= 2\gamma_0 k_BT\omega_p^2\sum_{n=-\infty}^{\infty}\frac{\omega_p e^{\omega_p\tau}-|\nu_n|e^{|\nu_n|\tau}}{\omega_p^2-\nu_n^2}
\end{aligned} \tag{1.17}$$

To obtain the fourth step from the third, we do a variable change $\omega \to -\omega$ in the second part of the integrand, and we will see it equal to the first part of the integrand, and hence we can merge them absorbing a factor of 2. It is again Cauchy's residue theorem in the fifth step. For $n > 0$ and $n < 0$, we encounter different poles, and so the sum is split. Finally:

$$D_1(\tau) = 2\gamma_0 k_BT\omega_p^2\sum_{n=-\infty}^{\infty}\frac{\omega_p e^{-\omega_p|\tau|}-|\nu_n|e^{-|\nu_n||\tau|}}{\omega_p^2-\nu_n^2}; \quad \nu_n = \frac{2\pi n k_BT}{\hbar} \tag{1.18}$$

We will now look at this kernel for various temperature limits.

High Temperature Limit: $k_BT >> \hbar\omega_p$. This implies that $\nu_n >> \omega_p$ for $n > 0$. Hence, we will split the $n = 0$ part of the sum:

$$\begin{aligned}
D_1(\tau) &= 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|} + 4\gamma_0 k_B T\omega_p^2 \sum_{n=1}^{\infty} \frac{\omega_p e^{-\omega_p|\tau|} - |\nu_n| e^{-|\nu_n||\tau|}}{\omega_p^2 - \nu_n^2} \\
&\approx 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|} - 4\gamma_0 k_B T\omega_p^2 \sum_{n=1}^{\infty} \frac{\omega_p e^{-\omega_p|\tau|}}{\nu_n^2} \\
&= 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|} \left(1 - \frac{1}{3}\left(\frac{\hbar\omega_p}{2k_B T}\right)^2\right) \approx 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|} \equiv D_1^{\infty}(\tau)
\end{aligned}$$

where we have used the fact that $\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$.

We can get the same form of $D_1(\tau)$ even if we put $\coth(\hbar\beta\omega/2) \approx 2/(\beta\hbar\omega)$ in the equation 1.10 and then perform the integral.

$$\begin{aligned}
D_1^{\infty}(\tau) &= \frac{2\hbar}{\pi}\int_0^{\infty} d\omega \frac{\gamma_0\omega_p^2\omega}{\omega^2+\omega_p^2}\cos(\omega\tau)\frac{2}{\beta\hbar\omega} \\
&= \frac{4\gamma_0\omega_p^2 k_B T}{\pi}\int_0^{\infty} d\omega \frac{\cos(\omega\tau)}{\omega^2+\omega_p^2} = 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|}
\end{aligned} \tag{1.19}$$

This calculation can be taken as a heuristic to approximate $\coth(\hbar\beta\omega/2) \approx 2/(\beta\hbar\omega)$ in the limit $k_B T >> \hbar\omega_p$ in our future analysis. For numerical studies, we will take $T = 10000$ whenever we want to work in this limit.

Zero Temperature Limit: We can also write the sum (1.18) in the form

$$D_1(\tau) = 2\gamma_0 k_B T\omega_p e^{-\omega_p|\tau|} + \frac{2\hbar\gamma_0\omega_p^2}{\pi}\sum_{n=1}^{\infty} hf(nh); \quad f(x) = \frac{\omega_p e^{-\omega_p|\tau|} - xe^{-x|\tau|}}{\omega_p^2 - x^2}, \quad h = \frac{2\pi k_B T}{\hbar} \tag{1.20}$$

For small h (i.e. small T), we know that $\sum_{n=1}^{N} hf(a+nh)$ is bounded between $\int_a^b dx f(x)$ and $\int_{a+h}^{b+h} dx f(x)$ with $b = a + Nh$. For our case, $a = 0$ and $b = \infty$. In the limit $h \to 0$, all three definitions converge to the same value. So, for the zero temperature case ($h = 0$):

$$\begin{aligned}
D_1(\tau) &= \frac{2\hbar\gamma_0\omega_p^2}{\pi}\int_0^{\infty} dx \frac{\omega_p e^{-\omega_p|\tau|} - xe^{-x|\tau|}}{\omega_p^2 - x^2} \\
&= \frac{2\hbar\gamma_0\omega_p^2}{\pi}\left[\sinh(\omega_p\tau)\mathrm{Shi}(\omega_p\tau) - \cosh(\omega_p\tau)\mathrm{Chi}(\omega_p\tau)\right] \equiv D_1^0(\tau)
\end{aligned} \tag{1.21}$$

We call it $D_1^0(\tau)$[1].

[1] $\mathrm{Chi}(t) = \gamma_E + \ln(t) + \int_0^t dx \frac{(\cosh(x)-1)}{x}$, γ_E being the Euler's constant and $\mathrm{Shi}(t) = \int_0^t dx \frac{\sinh(x)}{x}$.

1.3.2 Drude Limit: Laplace Space

$\Sigma(t)$ and $\gamma(t)$ are trivial to write in the Laplace space using basic Laplace transforms. We will do Laplace transform of equations 1.14 and 1.15 using table 2:

$$\tilde{\Sigma}(z) = \frac{\gamma_0 \omega_p^2}{z + \omega_p}, \quad \tilde{\gamma}(z) = \frac{\gamma_0 \omega_p}{z + \omega_p} \tag{1.22}$$

The noise kernel is not so trivial. But, interestingly using the basic definition (equation 1.10) of the noise kernel, we can easily perform the Laplace transform:

$$\begin{aligned}\tilde{D}_1(z) &= 2\hbar \int_0^\infty d\omega \frac{z}{z^2+\omega^2} \frac{\gamma_0 \omega}{\pi} \frac{\omega_p^2}{\omega^2+\omega_p^2} \coth\left(\frac{\hbar\omega}{2k_BT}\right) \\ &= \frac{2\hbar z \gamma_0 \omega_p^2}{\pi} \int_0^\infty d\omega \frac{\omega}{(z^2+\omega^2)(\omega^2+\omega_p^2)} \coth\left(\frac{\hbar\omega}{2k_BT}\right)\end{aligned} \tag{1.23}$$

In the high temperature limit, $k_BT >> \hbar\omega_p$, we again put $\coth(\hbar\beta\omega/2) \approx 2/(\beta\hbar\omega)$. For zero temperatures, we will use $\lim_{T\to 0} \omega \coth\left(\frac{\hbar\omega}{2k_BT}\right) = |\omega|$ to simplify the above equation:

$$\begin{aligned}\tilde{D}_1^\infty(z) &= \frac{2\hbar z \gamma_0 \omega_p^2}{\pi} \int_0^\infty d\omega \frac{\omega}{(z^2+\omega^2)(\omega^2+\omega_p^2)} \frac{2k_BT}{\hbar\omega} = \frac{2\gamma_0 k_BT \omega_p}{\omega_p + z}, \text{ and} \\ \tilde{D}_1^0(z) &= \frac{2\hbar z \gamma_0 \omega_p^2}{\pi} \int_0^\infty d\omega \frac{|\omega|}{(z^2+\omega^2)(\omega^2+\omega_p^2)} = \frac{2\hbar\gamma_0\omega_p^2}{\pi} z \frac{\ln(\omega_p) - \ln(z)}{\omega_p^2 - z^2}\end{aligned} \tag{1.24}$$

For arbitrary temperature (use the expansion of $\coth$ as given in equation 1.16):

$$\begin{aligned}\tilde{D}_1(z) &= \frac{2\hbar z \gamma_0 \omega_p^2}{\pi} \int_0^\infty d\omega \frac{\omega}{(z^2+\omega^2)(\omega^2+\omega_p^2)} \frac{2k_BT}{\hbar} \sum_{n=-\infty}^{\infty} \frac{\omega}{\omega^2+\nu_n^2} \\ &= \frac{2\gamma_0 k_BT\omega_p}{\omega_p+z} + \frac{8k_BTz\gamma_0\omega_p^2}{\pi} \sum_{n=1}^\infty \int_0^\infty d\omega \frac{\omega^2}{(z^2+\omega^2)(\omega^2+\omega_p^2)(\omega^2+\nu_n^2)} \\ &= \tilde{D}_1^\infty(z) + \frac{4k_BTz\gamma_0\omega_p^2}{\omega_p+z} \sum_{n=1}^\infty \frac{1}{(z+\nu_n)(\nu_n+\omega_p)} \\ &= \tilde{D}_1^\infty(z) + \frac{2\hbar\gamma_0\omega_p^2}{\pi} \frac{z}{\omega_p^2 - z^2} \left[\Psi\left(1 + \frac{\hbar\omega_p}{2\pi k_BT}\right) - \Psi\left(1 + \frac{\hbar z}{2\pi k_BT}\right)\right] \\ &= \tilde{D}_1^\infty(z) + \frac{\tilde{D}_1^0(z)}{\ln(\omega_p) - \ln(z)} \left[\Psi\left(1 + \frac{\hbar\omega_p}{2\pi k_BT}\right) - \Psi\left(1 + \frac{\hbar z}{2\pi k_BT}\right)\right]\end{aligned} \tag{1.25}$$

$\Psi(x)$ is the DiGamma function. It correctly reduces to the $\tilde{D}_1^\infty(z)$ and $\tilde{D}_1^0(z)$ in the limit $T \to \infty$ and $T \to 0$, respectively since $\Psi(1+x) \to \gamma_E$ as $x \to 0$ (or large T) and $\Psi(1+x) \to \ln(x)$ as $x \to \infty$ (or zero T).

1.3.3 Ohmic Limit

Here, we have $\Gamma(\omega) = \gamma_0 \omega$. We will again use equation 1.10 to get the dissipation kernel:

$$\begin{aligned} \Sigma(\tau) &= \frac{2}{\pi}\int_0^\infty d\omega \sin(\omega\tau)\gamma_0\omega = \frac{2\gamma_0}{\pi}\int_0^\infty d\omega\, \omega \sin(\omega\tau) = -2\gamma_0 \frac{d}{d\tau}\delta(\tau) \\ \implies \tilde{\Sigma}(z) &= -\gamma_0 z + 2\gamma_0\delta(0) \end{aligned} \tag{1.26}$$

Damping kernel $\gamma(\tau)$[2]:

$$\gamma(\tau) = \frac{2\gamma_0}{\pi}\int_0^\infty d\omega \cos(\omega\tau) = 2\gamma_0\delta(\tau) \implies \tilde{\gamma}(z) = \gamma_0 \tag{1.27}$$

Noise kernel:

$$D_1(\tau) = \frac{2\hbar}{\pi}\int_0^\infty d\omega \cos(\omega\tau)\gamma_0\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right) \tag{1.28}$$

High Temperature Limit: The limit in which we can approximate $\coth(\hbar\beta\omega/2) \approx 2/(\beta\hbar\omega)$ is worth giving a consideration. For the Ohmic case, the temperature-dependent energy scale should be higher than all the frequencies that we are integrating over, i.e. $k_B T >> \hbar\omega \in \{0, \infty\}$. This is, of course, a regime of theoretical interest. But, this approximation has been used quite commonly in the literature where the bath has an Ohmic type of spectral density for a large chunk of its normal modes. The most practical thing to do for avoiding this problem is to introduce a hard cut-off ω_d, such that $\Gamma(\omega) = 0$ for $\omega > \omega_d$.

However, **Only in this limit**, i.e. $k_B T >> \hbar\omega \in \{0, \infty\}$. $D_1(\tau) \approx 4\gamma_0 k_B T \delta(\tau)$. So, when we consider this "high temperature" limit and an Ohmic bath, we obtain both damping and noise kernels as delta functions. As we shall see, when both these kernels are delta functions, the evolution of the system at some time t will solely depend on the state of the system at time t (and not on what it was at some time $t' < t$). This is what is called as the "Markovian limit". In this Markovian limit, equations of a quantum Brownian particle reduce to that of a classical Brownian particle subjected to white noise ([5], [1]).

[2]For any function $f(x)$, we have

$$\begin{aligned} \int_0^\infty f(x)\delta(x)dx &= \int_0^\infty \frac{f(x)+f(-x)}{2}\delta(x)dx + \int_0^\infty \frac{f(x)-f(-x)}{2}\delta(x)dx \\ &= \frac{1}{2}\int_{-\infty}^\infty \frac{f(x)+f(-x)}{2}\delta(x)dx + 0 = \frac{f(0)}{2} \end{aligned}$$

The first part is an even function and hence, we get a factor of $1/2$ by changing the limit from $\{0 \text{ to } \infty\}$ to $\{-\infty \text{ to } \infty\}$. The second part is an odd function and an odd function is zero at $x = 0$. Also, $\delta(x) = 0$ for $x \neq 0$. So, the integrand and hence the integration is zero. This justifies $\mathcal{L}(\delta(t)) = \frac{1}{2}$.

In Laplace space, $\tilde{D}_1^\infty(z) = 2\gamma_0 k_B T$. For zero temperature:

$$\begin{aligned} D_1^0(\tau) &= \frac{2\hbar\gamma_0}{\pi}\int_0^\infty d\omega\cos(\omega\tau)\omega \\ \implies \tilde{D}_1^0(z) &= \frac{2\hbar\gamma_0 z}{\pi}\int_0^\infty d\omega\frac{\omega}{z^2+\omega^2} = \lim_{\omega_p\to\infty}\frac{2\hbar\gamma_0 z}{\pi}[\ln(\omega_p)-\ln(z)] \end{aligned} \tag{1.29}$$

Time Translational Symmetry of Kernels

Observe the following:

$$\begin{aligned} \langle\eta(t-t')\eta(0)\rangle_{th} &= \frac{1}{Z}\text{tr}\left\{e^{iH_B(t-t')}Be^{-iH_B(t-t')}Be^{-\beta H_B}\right\} \\ &= \frac{1}{Z}\text{tr}\left\{e^{iH_Bt}Be^{-iH_Bt}e^{iH_Bt'}Be^{-\beta H_B}e^{-iH_Bt'}\right\} \\ &= \frac{1}{Z}\text{tr}\left\{e^{iH_Bt}Be^{-iH_Bt}e^{iH_Bt'}Be^{-iH_Bt'}e^{-\beta H_B}\right\} \\ &= \langle\eta(t)\eta(t')\rangle_{th} \end{aligned} \tag{1.30}$$

where I have used the cyclic property of trace in line 2. This equation helps us in proving that

$$\begin{aligned} \Sigma(t-t') &= \frac{i}{\hbar}\langle[\eta(t-t'),\eta(0)]\rangle_{th} = \frac{i}{\hbar}\langle[\eta(t),\eta(t')]\rangle_{th} \\ D_1(t-t') &= \langle\{\eta(t-t'),\eta(0)\}\rangle_{th} = \langle\{\eta(t),\eta(t')\}\rangle_{th} \end{aligned} \tag{1.31}$$

This is, of course, a very well-known result for the equilibrium states. I have shown it here for the sack of completeness.

Appendix

1.A Simplifying $\gamma(0)$

We have $\gamma(0) = \sum_s \frac{C_s^2}{\Omega_s^2}$ (from equation 1.11). From equation 1.2, we have $C_s = m^{-1/2}k'U_{s1}$ and $m\Omega^2 = U\phi U^T$. So:

$$\sum_s \frac{C_s^2}{\Omega_s^2} = k'^2 \sum_s \frac{U_{s1}U_{s1}}{m\Omega_s^2} = k'^2 \sum_s U_{1s}^T (m\Omega^2)_{ss}^{-1} U_{s1} = k'^2 [U^T (m\Omega^2)^{-1} U]_{11} = k'^2 [\phi^{-1}]_{11} \quad (1.32)$$

Now, let us observe ϕ, we wrote $\frac{\mathbf{x}^T\phi\mathbf{x}}{2} = \frac{k'}{2}x_1^2 + \frac{k}{2}x_N^2 + \frac{k}{2}\sum_{n=1}^{N-1}(x_n - x_{n+1})^2$ and $\mathbf{x} = \{x_1, x_2, ...x_n\}$. So, we have a $N \times N$ matrix with $\phi_{ij} = \frac{\partial^2}{\partial x_i \partial x_j}\left(\frac{\mathbf{x}^T\phi\mathbf{x}}{2}\right)$:

$$\phi = \begin{pmatrix} k+k' & -k & 0 & ... & 0 \\ -k & 2k & -k & ... & 0 \\ 0 & -k & 2k & ... & 0 \\ . & . & . & ... & . \\ 0 & 0 & 0 & ... & 2k \end{pmatrix}_{N\times N} , \quad \text{adjoint}(\phi_{11}) = \begin{vmatrix} 2k & -k & 0 & ... & 0 \\ -k & 2k & -k & ... & 0 \\ 0 & -k & 2k & ... & 0 \\ . & . & . & ... & . \\ 0 & 0 & 0 & ... & 2k \end{vmatrix}_{(N-1)\times(N-1)} \quad (1.33)$$

Now, we are interested in $[\phi^{-1}]_{11}$.

Calculating $[\phi^{-1}]_{11}$:

We will focus on finding the determinant of $\phi = |\phi|$. Let $D_N = |\phi_{N\times N}|$. It is easy to see that $D_1 = k + k'$, $D_2 = 2kD_1 - k^2$, $D_3 = 2kD_2 - k^2 D_1$ and so on. In general, it is easy to see that $D_N = 2kD_{N-1} - k^2 D_{N-2}$. This is also means that $D_0 = 1$. Now, let us try to play with this recursion relation:

$$\begin{aligned} D_N = k(2D_{N-1} - kD_{N-2}) = k^2(3D_{N-2} - 2kD_{N-3}) &= k^3(4D_{N-3} - 3kD_{N-4}) = \\ ... &= k^{N-1}(ND_1 - (N-1)kD_0) \\ &= k^{N-1}(k + Nk') \end{aligned} \tag{1.34}$$

Now, $[\phi^{-1}]_{11} = \frac{\text{adjoint}(\phi_{11})}{D_N}$. Adjoint$(\phi_{11})$ is determinant of a matrix that can be obtained from a $(N-1) \times (N-1)$-ϕ matrix with $k' = k$ (see equation 1.33). So, its determinant is just D_{N-1} with $k = k'$ and so, adjoint$(\phi_{11}) = Nk^{N-1}$ and hence $[\phi^{-1}]_{11} = \frac{N}{k+Nk'}$.

In the limit $N \to \infty$, we get $[\phi^{-1}]_{11} \to \frac{1}{k'}$ and hence $\gamma(0) = \sum_s \frac{C_s^2}{\Omega_s^2} = k'$.

Chapter 2

Langevin Equation Approach

In this chapter, we will study the dynamics of the system that we described in the previous chapter using the Langevin equation approach. We will learn to derive the Langevin equation, ways to solve it and then try to understand why its applicability is limited to very simple systems. This is an exact approach with very reasonable approximations.

One of the approximation that we do is that the initial state of the entire setup is in a product state, i.e. $\rho(0) = \rho_S(0) \otimes \rho_B(0)$. This is something that is totally in our control when we do an experiment, and it is possible to prepare this initial state experimentally. It is possible to carry out this study even without this approximation ([12]), but it will complicate the study without bringing much of new insights. So, we will accept this approximation and try to see what we can learn about the system.

Another assumption is to take the number of bath particles $N \to \infty$. It is essential if we want our system to thermalise. It avoids the Poincare recurrences in the dynamics of the system. In numerical studies, we often see this recurrence due to the finite size of the bath. But, the theoretical results that we predict agree with the numerical results till the time up to which the finite-size effects are not relevant. Increasing the bath size often leads to agreement of these theoretical results for larger times. So, there will exist some time t^*, after which we can't trust the results predicted by this approximation. For most practical purposes, t^* is insanely large, and we can safely take this approximation.

In this chapter, the study is done in the Heisenberg picture. We will not have any suffix for it for the clarity of notations.

2.1 Deriving the Langevin Equation

We start by writing the Heisenberg equation of motion for the system and the bath coordinates and momenta. We will use the Hamiltonian that we defined in equations 1.1 and 1.2. For system operators:

$$\begin{aligned}
\dot{x}(t) &= \frac{i}{\hbar}[H, x(t)] = \frac{i}{\hbar}[H_S, x(t)] = \frac{p(t)}{M} \\
\dot{p}(t) &= \frac{i}{\hbar}[H, p(t)] = \frac{i}{\hbar}[H_S + \hat{H}_I, p(t)] = \frac{i}{\hbar}[V(x), p(t)] + \frac{i}{\hbar}[\hat{H}_I, p(t)] = -V_c'(x(t)) + \sum_s C_s X_s(t)
\end{aligned} \tag{2.1}$$

Here, $V_c(x) = V(x) + \frac{k'}{2}x^2$. Similarly, for the bath:

$$\begin{aligned}
\dot{X}_s(t) &= \frac{i}{\hbar}[H, X_s(t)] = \frac{i}{\hbar}[H_B, X_s(t)] = P_s(t) \\
\dot{P}_s(t) &= \frac{i}{\hbar}[H, P_s(t)] = \frac{i}{\hbar}[H_B + \hat{H}_I, P_s(t)] = \frac{i}{\hbar}[V_B(x), P_s(t)] + \frac{i}{\hbar}[\hat{H}_I, P_s(t)] = -\Omega_s^2 X_s(t) + C_s x(t)
\end{aligned} \tag{2.2}$$

Here, $V_B(x) = \sum_s \frac{\Omega_s^2 X_s^2}{2}$. It is straightforward to evaluate $\ddot{x}(t)$ and $\ddot{X}_s(t)$ using equations 2.1 and 2.2:

$$M\ddot{x}(t) + V_c'(x(t)) - \sum_s C_s X_s(t) = 0, \quad \ddot{X}_s(t) + \Omega_s^2 X_s(t) - C_s x(t) = 0. \tag{2.3}$$

The next step is to solve the bath equation of motion treating $C_s x(t)$ as an inhomogeneous term. The bath equation can be solved exactly (refer to appendix 2.A):

$$\begin{aligned}
X_s(t) &= \sqrt{\frac{\hbar}{2\Omega_s}}(e^{i\Omega_s t}b_s^\dagger + e^{-i\Omega_s t}b_s) + \frac{C_s}{\Omega_s}\int_0^t dt_1 x(t_1)\sin[\Omega_s(t-t_1)] \\
&= X_s(0)\cos(\Omega_s t) + \frac{P_s(0)}{\Omega_s}\sin(\Omega_s t) + \frac{C_s}{\Omega_s}\int_0^t dt_1 x(t_1)\sin[\Omega_s(t-t_1)]
\end{aligned} \tag{2.4}$$

Substitute it into the first equation of 2.3 to get the **Langevin equation**:

$$\boxed{M\ddot{x}(t) + V_c'(x(t)) - \int_0^t dt_1 x(t_1)\Sigma(t-t_1) = \eta(t)} \tag{2.5}$$

where,

$$\eta(t) = \sum_s C_s \left(X_s(0)\cos(\Omega_s t) + \frac{P_s(0)}{\Omega_s}\sin(\Omega_s t) \right), \quad \Sigma(t) = \sum_s \frac{C_s^2}{\Omega_s}\sin(\Omega_s \tau) \tag{2.6}$$

These expressions are precisely the same as how we defined them in equations 1.7 and 1.10 in the previous chapter. Also, by comparing equations 2.3 and 2.5, it is clear that

$$\int_0^t dt_1 x(t_1)\Sigma(t-t_1) + \eta(t) = \sum_s C_s X_s(t) = B(t) \tag{2.7}$$

where we have used the definition of $B(t)$ from the Hamiltonian 1.2.

2.1.1 Resolving a Discrepancy in the Literature

At this point, I would like to point out one discrepancy that I have observed in the literature and its resolution. Many authors simplify equation 2.5 further and write it in terms of $\gamma(t)$ (defined in equation 1.11). There are two ways of doing it:

1. Use Leibniz rule (as done in [5]).
2. Use integration by parts (as done in [7]).

We want to point out that for the case of an Ohmic bath, upon solving the obtained differential equation, the Leibniz route will give the incorrect answer. In contrast, the by-parts route will provide the correct answer (we compare it against the solution obtained directly by solving equation 2.5). This mistake has been seen even in texts like [5]. For smoother baths, both approaches give the same result. The solutions are shown in detail in the appendix 2.B.

2.2 Solving the Langevin Equation

Let us try to solve the Langevin equation 2.5. We will work with two potentials: Quadratic potential ($V(x) = \frac{1}{2}M\omega_0^2 x^2$) and a free particle ($V(x) = 0$).

2.2.1 Quadratic Potential

For $V(x) = \frac{1}{2}M\omega_0^2 x^2$, the Langevin equation 2.5 becomes:

$$\ddot{x}(t) + \frac{k'}{M}x(t) + \omega_0^2 x(t) - \frac{1}{M}\int_0^t dt_1 x(t_1)\Sigma(t-t_1) = \frac{1}{M}\eta(t) \tag{2.8}$$

Let us first solve the homogeneous part of it (putting $\eta(t) = 0$): Let $g_1(t)$ and $g_2(t)$ are two of its *fundamental solutions* such that $g_1(0) = 1$, $\dot{g}_1(0) = 0$ and $g_2(0) = 0$ and $\dot{g}_2(0) = 1$[1].

[1] Let $y_1(t)$ and $y_2(t)$ are two solutions of a second order differential equation. Since any linear combination of them is also a solution, define $g_1(t) = g_{11}y_1(t) + g_{12}y_2(t)$ and $g_2(t) = g_{21}y_1(t) + g_{22}y_2(t)$ such that $g_{11} = \frac{\dot{y}_2(0)}{\Lambda}$, $g_{12} = -\frac{\dot{y}_1(0)}{\Lambda}$, $g_{21} = -\frac{y_2(0)}{\Lambda}$, $g_{22} = \frac{y_1(0)}{\Lambda}$, where $\Lambda = y_1(0)\dot{y}_2(0) - y_2(0)\dot{y}_1(0)$.

Taking the Laplace transform of the equation 2.8:

$$z^2\tilde{x}(z) - zx_1(0) - \dot{x}_1(0) + \left(\omega_0^2 + \frac{k'}{M}\right)\tilde{x}_1(z) - \frac{\tilde{x}_1(z)\tilde{\Sigma}(z)}{M} = 0 \tag{2.9}$$

This gives (depending on initial conditions):

$$\tilde{g}_1(z) = \frac{z}{z^2 + \omega_0^2 + \frac{z}{M}\tilde{\gamma}(z)}, \quad \tilde{g}_2(z) = \frac{1}{z^2 + \omega_0^2 + \frac{z}{M}\tilde{\gamma}(z)} \tag{2.10}$$

where we have used $\tilde{\Sigma}(z) = -z\tilde{\gamma}(z) + k'$ (see equation 1.12). Since $g_2(0) = 0$, we can also conclude that $\tilde{g}_1(z) = z\tilde{g}_2(z) - g_2(0) \implies \dot{g}_2(t) = g_1(t)$. Let us call $g_2(t) \equiv g(t)$. Because of the nature of $g_1(t)$ and $g_2(t)$, the homogeneous solution will be $x^h(t) = \dot{g}(t)x(0) + g(t)\dot{x}(0)$. Let $c(t)$ be a specific solution of the inhomogeneous equation. It satisfies

$$\ddot{c}(t) + \frac{k'}{M}c(t) + \omega_0^2 c(t) - \frac{1}{M}\int_0^t dt_1 c(t_1)\Sigma(t - t_1) = \frac{1}{M}\eta(t); \quad c(0) = 0,\ \dot{c}(0) = 0$$

Take the Laplace transform, and we obtain

$$\tilde{c}(z) = \frac{\tilde{\eta}(z)\tilde{g}(z)}{M} \implies c(t) = \frac{1}{M}\int_0^t dt_1 g(t - t_1)\eta(t_1)$$

where we have used the convolution property of the inverse Laplace transforms. Finally, the solution of Langevin equation is:

$$x(t) = \dot{g}(t)x(0) + g(t)\dot{x}(0) + \frac{1}{M}\int_0^t dt_1 g(t - t_1)\eta(t_1) \quad \text{with} \quad \tilde{g}(z) = \frac{1}{z^2 + \omega_0^2 + \frac{z}{M}\tilde{\gamma}(z)}$$

So, now we need to find this $g(t)$ for various parameters and temperatures.

Finding $g(t)$

For the Drude bath, we have $\tilde{\gamma}(z) = \frac{\gamma_0\omega_p}{z+\omega_p}$ (section 1.3). So,

$$\tilde{g}(z) = \frac{z + \omega_p}{z^3 + \omega_p z^2 + (\omega_0^2 + 2\gamma\omega_p)\, z + \omega_0^2\omega_p}; \quad \gamma = \frac{\gamma_0}{2M} \tag{2.11}$$

It is trivial to analytically find the inverse Laplace transform of $\tilde{g}(z)$ if we can find the roots of its denominator. It is not very insightful if we do it for arbitrary values of parameters. So, let us find the inverse Laplace transform in various limits of our interest.

1. In the limit $\gamma << \omega_0 << \omega_p$, roots of the denominator are $z = -\gamma \pm i\omega_r$ ($\omega_r = \sqrt{\omega_0^2 - \gamma^2}$) and $z = -\omega_p$. That gives $\tilde{g}(z) = \frac{1}{\omega_0^2 + (z+\gamma)^2} \approx \frac{1}{z^2+\omega_0^2+2z\gamma}$.

2. In the limit $\omega_0 << \gamma << \omega_p$, roots of the denominator are $z = -\frac{\omega_0^2}{2\gamma}$, $z = -2\gamma$ and $z = -\omega_p$. That gives $\tilde{g}(z) = \frac{2\gamma}{(z+2\gamma)(\omega_0^2+2\gamma z)}$.

Finding the inverse Laplace transform:

$$\begin{aligned} g(t) &= e^{-\gamma t}\frac{\sin(\omega_r t)}{\omega_r}, \text{ in the limit } \gamma << \omega_0 << \omega_p \\ g(t) &= \frac{2\gamma\left(e^{-2\gamma t} - e^{-(\omega_0^2/2\gamma)t}\right)}{\omega_0^2 - (2\gamma)^2}, \text{ in the limit } \omega_0 << \gamma << \omega_p \end{aligned} \tag{2.12}$$

For the Ohmic bath, $\tilde{\gamma}(z) = \gamma_0$. So, we obtain

$$\tilde{g}(z) = \frac{1}{z^2 + \omega_0^2 + 2z\gamma} \implies g(t) = e^{-\gamma t}\frac{\sin(\omega_r t)}{\omega_r}, \text{ assuming } \omega_0 > \gamma \tag{2.13}$$

Hence, $g(t)$ for an Ohmic bath and a Drude bath with a large cutoff are the same.

2.2.2 Free Particle

Solving for $V(x) = 0$ is equivalent to putting $\omega_0 = 0$ in the above analysis. The solution will still be of the form

$$x(t) = \dot{g}(t)x(0) + g(t)\dot{x}(0) + \frac{1}{M}\int_0^t dt_1 g(t-t_1)\eta(t_1) \quad \text{with} \quad \tilde{g}(z) = \frac{1}{z^2 + \frac{z}{M}\tilde{\gamma}(z)}$$

For the Drude bath, we use $\tilde{\gamma}(z) = \frac{\gamma_0\omega_p}{z+\omega_p}$ and then finding the inverse Laplace transform using partial fractions of the resultant function, we get:

$$g(t) = \frac{1}{2\gamma} + e^{-\frac{\omega_p t}{2}}\left[\left(1 - \frac{\omega_p}{4\gamma}\right)\frac{\sinh\left(\omega_p^r t/2\right)}{\omega_p^r/2} - \frac{1}{2\gamma}\cosh\left(\omega_p^r t/2\right)\right]; \quad \omega_p^r = \sqrt{\omega_p^2 - 8\gamma\omega_p} \tag{2.14}$$

Similarly for the Ohmic bath, we obtain:

$$x(t) = \dot{g}(t)x(0) + g(t)\dot{x}(0) + \frac{1}{M}\int_0^t dt_1 g(t-t_1)\eta(t_1), \quad g(t) = \frac{1 - e^{-2\gamma t}}{2\gamma} \tag{2.15}$$

We obtain the equation 2.15 even if we take $\gamma << \omega_p$ limit of equation 2.14. So, again a Drude bath with a large cutoff yields the same $g(t)$ as an Ohmic bath.

2.2.3 A General Sum Rule!

We have seen that the general solution of the Langevin equation is of the form:

$$x(t) = \dot{g}(t)x(0) + \frac{g(t)}{M}p(0) + \frac{1}{M}\int_0^t dt_1 g(t-t_1)\eta(t_1)$$
$$p(t) = M\ddot{g}(t)x(0) + \dot{g}(t)p(0) + \int_0^t dt_1 \dot{g}(t-t_1)\eta(t_1)$$

Using this, we can investigate $\langle[x(t),p(t)]\rangle$:

$$\langle[x(t),p(t)]\rangle = (\dot{g}^2(t) - g(t)\ddot{g}(t))\langle[x(0),p(0)]\rangle + \frac{1}{M}\int_0^t\int_0^t dsds' g(t-s)\dot{g}(t-s')\langle[\eta(s),\eta(s')]\rangle \tag{2.16}$$

Now, for any time t, we should get $\langle[x(t),p(t)]\rangle = i\hbar$. At $t=0$, it is obviously true since $\dot{g}(0)=1$ and $g(0)=0$. We can also see it in the limit $t\to\infty$. In this limit, the first term of equation 2.16 will always go to zero (for free particle $g(t)$ might be non-zero, but $\dot{g}(t)$ and $\ddot{g}(t)$ will always be zero). To evaluate the second term, we will need to use:

$$\langle[\eta(s),\eta(s')]\rangle = -i\hbar\Sigma(s-s') = -\frac{2i\hbar}{\pi}\int_0^\infty d\omega\Gamma(\omega)\sin(\omega(s-s')) = -\frac{\hbar}{\pi}\int_{-\infty}^\infty d\omega\Gamma(\omega)e^{i\omega(s-s')}$$

where we have used the fact that $\Gamma(\omega)$ is an odd function[2]. Define $g^r(t) = g(t)\theta(t)$. This also implies $\dot{g}^r(t) = \dot{g}(t)\theta(t)$ (since $g(0)=0$). Now, equation 2.16 in $t\to\infty$ limit becomes:

$$\begin{aligned}
\langle[x,p]\rangle_\infty &= -\frac{\hbar}{M\pi}\int_{-\infty}^\infty d\omega\Gamma(\omega)\int_0^\infty\int_0^\infty dsds' g(t-s)\dot{g}(t-s')e^{i\omega(s-s')} \\
&= -\frac{\hbar}{M\pi}\int_{-\infty}^\infty d\omega\Gamma(\omega)\int_{-\infty}^\infty ds g^r(t-s)e^{-i\omega(t-s)}\int_{-\infty}^\infty ds'\dot{g}^r(t-s')e^{i\omega(t-s')} \\
&= -\frac{\hbar}{M\pi}\int_{-\infty}^\infty d\omega\Gamma(\omega)\hat{g}^r(-\omega)[-i\omega\hat{g}^r(\omega)] \\
&= \frac{i\hbar}{M\pi}\int_{-\infty}^\infty d\omega\Gamma(\omega)\hat{g}^r(-\omega)\omega\hat{g}^r(\omega) = (i\hbar)\int_{-\infty}^\infty\frac{d\omega}{M\pi}\omega\hat{g}^r(\omega)\Gamma(\omega)\hat{g}^r(-\omega) = i\hbar
\end{aligned} \tag{2.17}$$

where, $\hat{g}^r(\omega)$ is the Fourier transform of $g^r(t)$. In the last line, we have used the sum rule ([14]):

$$\frac{2}{M}\int_{-\infty}^\infty\frac{d\omega}{2\pi}\omega\hat{g}^r(\omega)\Gamma(\omega)\hat{g}^r(-\omega) = 1$$

The commutation (equation 2.16) must be true even at arbitrary times, which gives us a general sum rule:

$$\boxed{1 = \dot{g}^2(t) - g(t)\ddot{g}(t) - \frac{1}{M}\int_0^t\int_0^t d\tau d\tau' g(\tau)\dot{g}(\tau')\Sigma(\tau'-\tau)} \tag{2.18}$$

[2]It is clear from the definition in equation 1.3.

2.3 Analysing the Solutions

To compare the solutions with multiple approaches, we will study the first and second moments of the system. From the general form of $x(t)$ that we have obtained in the previous section, it is easy to write general expressions for all the first and second moments:

$$\begin{aligned}
\langle x\rangle_t &= \dot{g}(t)\langle x\rangle_0 + \frac{g(t)}{M}\langle p\rangle_0 + \frac{1}{M}\int_0^t ds g(t-s)\langle\eta(s)\rangle \\
\langle p\rangle_t &= M\ddot{g}(t)\langle x\rangle_0 + \dot{g}(t)\langle p\rangle_0 + \int_0^t ds\dot{g}(t-s)\langle\eta(s)\rangle \\
\langle x^2\rangle_t &= \dot{g}^2(t)\langle x^2\rangle_0 + \frac{g^2(t)}{M^2}\langle p^2\rangle_0 + \frac{\dot{g}(t)g(t)}{M}\langle xp+px\rangle_0 \\
&\quad + \frac{1}{2M^2}\int_0^t\int_0^t dsds' g(t-s)g(t-s')\langle\{\eta(s),\eta(s')\}\rangle \\
\langle p^2\rangle_t &= M^2\ddot{g}^2(t)\langle x^2\rangle_0 + \dot{g}^2(t)\langle p^2\rangle_0 + M\ddot{g}(t)\dot{g}(t)\langle xp+px\rangle_0 \\
&\quad + \int_0^t\int_0^t dsds'\dot{g}(t-s)\dot{g}(t-s')\frac{\langle\{\eta(s),\eta(s')\}\rangle}{2} \\
\langle xp+px\rangle_t &= 2M\dot{g}(t)\ddot{g}(t)\langle x^2\rangle_0 + \frac{2g(t)\dot{g}(t)}{M}\langle p^2\rangle_0 + (\dot{g}(t)\dot{g}(t) + g(t)\ddot{g}(t))\langle xp+px\rangle_0 \\
&\quad + \frac{1}{M}\int_0^t\int_0^t dsds' g(t-s)\dot{g}(t-s')\langle\{\eta(s),\eta(s')\}\rangle
\end{aligned} \tag{2.19}$$

Here, $\langle A_S\rangle_t = \text{tr}\{A_S(t)\otimes I_B(t)\ \rho(0)\} = \text{tr}_S\{A_S(t)\rho_S(0)\}$, where we have used the fact that the initial state of system and bath was uncorrelated.

In the above expressions, we will call the integral terms (last term in each expression) as the **inhomogeneous part** of the moment. The rest of the terms are called the **homogeneous parts**. So, once we know $g(t)$, we can fully determine the homogeneous parts. It is crucial to note that all the temperature dependence lies in the inhomogeneous parts (through the noise kernel). We have made this distinction to make the comparison and analysis easy. Additionally, note that the first moments are fully homogeneous (since $\langle\eta(t)\rangle = 0$).

The homogeneous parts are easy to obtain since we have already obtained $g(t)$, and we will directly compare them against the results from the master equation results in the section 4.1. However, we can make a quick and intuitive interpretation about the homogeneous parts: for a free particle, observe that $g^2(t) \sim t^2$ and $\dot{g}^2(t) \sim 1$ for small times (refer to the equation 2.45). This gives the initial ballistic growth in $\langle x^2\rangle \sim \frac{\langle p^2\rangle_0 t^2}{M^2}$. This is expected since it roughly means that the distribution is growing with speed roughly $\sim \langle p\rangle_0/M$. This is what the system would have done in the absence of a bath. Since the effect of the bath would be negligible at such small times, we get these closed system dynamics. In fact, we will see in the next section that the inhomogeneous part grows as $\sim t^4$ in this limit, which is subleading for small times. Slowly, the inhomogeneous parts of the solutions will take over, and this homogeneous part will dampen out.

We will now analyse the inhomogeneous parts of the second moments. We will only focus on $\langle x^2 \rangle_t$ for our comparisons. Analysis of other moments can be done in a similar fashion.

2.3.1 Inhomogeneous Part of $\langle x^2 \rangle_t$ for a Free Particle

We will use a Drude bath. Recall from equation 2.19 that the inhomogeneous part of $\langle x^2 \rangle_t$ is:

$$
\begin{aligned}
\langle x^2 \rangle_t &= \frac{1}{2M^2} \int_0^t \int_0^t d\tau d\tau' g(\tau) g(\tau') D_1(\tau - \tau') \\
&= \frac{2\hbar}{2M^2\pi} \int_0^\infty d\omega \Gamma(\omega) \coth\left(\frac{\hbar\beta\omega}{2}\right) \int_0^t \int_0^t d\tau d\tau' g(\tau) g(\tau') \cos(\omega(\tau - \tau')) \\
&= \frac{\gamma_0 \hbar \omega_p^2}{\pi M^2} \int_0^\infty d\omega \frac{\omega}{\omega^2 + \omega_p^2} \coth\left(\frac{\hbar\beta\omega}{2}\right) f(\omega, t)
\end{aligned} \tag{2.20}
$$

where we have used the definition of noise kernel from equation 1.10 and the explicit form of the spectral density for a Drude bath from equation 1.5. We have also defined the function $f(\omega, t)$:

$$
f(\omega, t) = \int_0^t \int_0^t d\tau d\tau' g(\tau) g(\tau') \cos(\omega(\tau - \tau')) \tag{2.21}
$$

In principle, equation 2.20 is all that we need to evaluate numerically to get the behaviour of $\langle x^2 \rangle_t$ at any time. We have shown these plots in this chapter. However, if we want to know the behaviour in terms of the microscopic parameters of our model, then we need to do further analytical study.

Let us put $M = 1$. We will do our analysis in the limit $\gamma << \omega_p$ (reason will be clarified later). We need to use $g(t) = \frac{1 - e^{-\gamma_0 t}}{\gamma_0}$ (equation 2.15) in equation 2.21 to get:

$$
f(\omega, t) = \frac{2\gamma_0^2(1 - \cos(\omega t)) - 2\omega\gamma_0 \sin(\omega t)(1 - e^{-\gamma_0 t}) + \omega^2(1 - e^{-\gamma_0 t})^2}{\gamma_0^2 \omega^2 (\omega^2 + \gamma_0^2)} \tag{2.22}
$$

High Temperature Limit

In the limit $k_BT >> \hbar\omega_p$, we put $\coth(\hbar\beta\omega/2) \approx 2/(\hbar\beta\omega)$ in the integral 2.20. This integral can performed exactly to obtain:

$$\begin{aligned}\langle x^2\rangle_t = &\frac{2\gamma_0^3(1-e^{-\omega_p t}) - \omega_p^2\gamma_0(1-e^{-\gamma_0 t})^2 + 2\omega_p\gamma_0^2(1-\gamma_0 t - e^{-\gamma_0 t} - e^{-\omega_p t} + e^{-(\omega_p+\gamma_0)t})}{\beta\omega_p\gamma_0^2(\omega_p^2-\gamma_0^2)} \\ &- \frac{\omega_p^3(3-2\gamma_0 t + e^{-2\gamma_0 t} - 4e^{-\gamma_0 t})}{\beta\omega_p\gamma_0^2(\omega_p^2-\gamma_0^2)}\end{aligned} \tag{2.23}$$

We can expand this expression in time to get (we put back M by dimensional analysis):

$$\begin{aligned}&\textbf{Long time limit}: \ \langle x^2\rangle_t = 2\frac{k_BT}{\gamma_0}t - \frac{k_BT(3\omega_p^2+8\omega_p\gamma+8\gamma^2)}{4M\omega_p\gamma^2(\omega_p+2\gamma)} \to 2\frac{k_BT}{\gamma_0}t - \frac{3k_BT}{4M\gamma^2} \text{ as } \omega_p >> \gamma \\ &\textbf{Short time limit}: \langle x^2\rangle_t = k'\frac{k_BT}{4M^2}t^4 + \mathcal{O}(t^5)\end{aligned} \tag{2.24}$$

Let us understand these results. At large times, a free particle behaves as $\sim 2Dt$, where $D = \frac{k_BT}{\gamma_0}$. This is the well-known diffusive behaviour of a Brownian particle, and D is called the Stokes-Einstein coefficient. If we investigate $\langle p^2\rangle$, it would be Mk_BT, which suggests the equipartition theorem. We can study all the different features of a Brownian particle through this model. The constant $\left(\frac{3k_BT}{4M\gamma^2}\right)$ seems to depend very complexly on bath properties.

At small times, we see a t^4 behaviour with a coefficient of $k'\frac{k_BT}{4M^2}$. As we discussed earlier, the homogeneous contribution $\sim t^2$ will be dominant in this regime. t^4 behaviour is bath-specific behaviour. For an Ohmic bath, we get $\sim t^3$ ([5]). One way to understand this is to realise write $k'\frac{k_BT}{4M^2} = \frac{1}{4}\frac{k'}{M}\frac{k_BT}{M}t^4$. $\frac{k'}{M}$ is a natural frequency scale since the system is coupled to the bath with the coupling k'. $\frac{k_BT}{M}$ is coming from the bath as an estimation of $\langle v^2\rangle$.

Heuristic Argument: This behaviour stems from the noise term in the Langevin equation. Let us justify it for the free particle. Recall the Langevin equation for a free particle:

$$M\ddot{x}(t) + k'x(t) - \int_0^t dt_1 x(t_1)\Sigma(t-t_1) = \eta(t) \tag{2.25}$$

We can write this equation in terms of the damping kernel $\gamma(t)$ using equation 2.48:

$$M\ddot{x}(t) + \int_0^t dt_1 \dot{x}(t_1)\gamma(t-t_1) = \eta(t) - \gamma(t)x(0) \tag{2.26}$$

We will take the limit $t \to 0$ of the above equation. Recall that $\gamma(t) = \gamma_0\omega_p e^{-\omega_p|t|}$ for a Drude bath. Hence, in the limit $t \to 0$, we can approximate $\gamma(t) \approx \gamma_0\omega_p = k'$. So, in the limit $t \to 0$:

$$M\ddot{x}(t) = \eta(t) - k'x(0) \implies \dot{x}(t) = \frac{1}{M}\int_0^t dt_1\eta(t_1) - \frac{k'x(0)t}{M} \tag{2.27}$$

Let us now find the $\langle x^2\rangle_t$:

$$\begin{aligned}\langle x^2\rangle_t &= \int_0^t\int_0^t dt_1dt_2\langle\dot{x}(t_1)\dot{x}(t_2)\rangle \\ &= \frac{1}{M^2}\int_0^t\int_0^t dt_1dt_2\int_0^{t_1}dt_3\int_0^{t_2}dt_4\langle\eta(t_3)\eta(t_4)\rangle + \frac{k'^2x^2(0)}{M^2}\int_0^t\int_0^t dt_1dt_2t_1t_2\end{aligned} \tag{2.28}$$

For a Drude bath, we know that $\langle\eta(t_1)\eta(t_2)\rangle \sim \gamma_0\omega_p e^{-\omega_p(t_1-t_2)}$. For small t, both t_1 and t_2 will be small and hence $\langle\eta(t_1)\eta(t_2)\rangle \sim \gamma_0\omega_p = k'$. Putting this, we easily get a t^4. For an Ohmic bath, $\langle\eta(t_1)\eta(t_2)\rangle \sim \delta(t_1 - t_2)$. Hence, we get a t^3 from this heuristic.

Zero Temperature Limit

Here, we will use $\omega\coth(\hbar\beta\omega/2) \to |\omega|$ in simplifying the integral 2.20. Unlike the high temperature case, this integral is now difficult to do exactly. However, the integral can be performed in asymptotic limits. Let us start with the long time limit (we put $e^{-\gamma_0 t} \to 0$ in the expression 2.22):

$$\begin{aligned}\langle x^2\rangle_t &\approx \frac{\hbar\omega_p^2}{\pi\gamma_0}\int_0^\infty d\omega\frac{\omega^2 - 2\omega\gamma_0\sin(\omega t) + 2\gamma_0^2(1-\cos(\omega t))}{\omega(\omega^2+\omega_p^2)(\omega^2+\gamma_0^2)} \\ &= \frac{\hbar\omega_p^2}{\pi\gamma_0}\left(I_1(t) - 2\gamma_0 I_2(t) + \frac{2\gamma_0^2}{\omega_p^2-\gamma_0^2}I_3(t)\right)\end{aligned} \tag{2.29}$$

where we have defined

$$\begin{aligned}I_1(t) &= \int_0^\infty d\omega\frac{\omega}{(\omega^2+\omega_p^2)(\omega^2+\gamma_0^2)} = \frac{\ln(\omega_p/\gamma_0)}{\omega_p^2-\gamma_0^2} \\ I_2(t) &= \int_0^\infty d\omega\frac{\sin(\omega t)}{(\omega^2+\omega_p^2)(\omega^2+\gamma_0^2)} \\ I_3(t) &= (\omega_p^2-\gamma_0^2)\int_0^\infty d\omega\frac{1-\cos(\omega t)}{\omega(\omega^2+\omega_p^2)(\omega^2+\gamma_0^2)} = \int_0^\infty d\omega\frac{1-\cos(\omega t)}{\omega}\left(\frac{1}{\omega^2+\gamma_0^2} - \frac{1}{\omega^2+\omega_p^2}\right)\end{aligned} \tag{2.30}$$

$I_2(t)$ and $I_3(t)$ can be done analytically. Please note that these are not simple contour integrals, and doing them for more complicated systems can be highly tedious. For our setup, it has a complicated expression in terms of exponential integrals, Ei. Anyway, we are only interested in asymptotic behaviour:

$$I_2(t\to\infty) = \frac{1}{\omega_p^2\gamma_0^2 t} \to 0, \quad I_3(t\to\infty) = \left[\frac{\gamma_E + \ln(\gamma_0 t)}{\gamma_0^2} - \frac{\gamma_E + \ln(\omega_p t)}{\omega_p^2}\right] \tag{2.31}$$

Putting this, we get

$$\begin{aligned}\langle x^2\rangle_t &\approx \frac{\hbar\omega_p^2}{\pi\gamma_0}\frac{\ln(\omega_p/\gamma_0)}{\omega_p^2-\gamma_0^2} + \frac{2\hbar\gamma_0\omega_p^2}{\pi(\omega_p^2-\gamma_0^2)}\left[\frac{\gamma_E+\ln(\gamma_0 t)}{\gamma_0^2} - \frac{\gamma_E+\ln(\omega_p t)}{\omega_p^2}\right] \\ &= \frac{2\hbar}{\pi\gamma_0}\left(\gamma_E+\ln(t)+\frac{\omega_p^2\ln(\gamma_0)-\gamma_0^2\ln(\omega_p)}{\omega_p^2-\gamma_0^2}+\frac{\omega_p^2\ln(\omega_p/\gamma_0)}{2(\omega_p^2-\gamma_0^2)}\right) \\ &= \frac{2\hbar}{\pi\gamma_0}\left(\ln(t)+\gamma_E+\frac{\omega_p^2\ln(\gamma_0)}{2(\omega_p^2-\gamma_0^2)}+\frac{(\omega_p^2-2\gamma_0^2)\ln(\omega_p)}{2(\omega_p^2-\gamma_0^2)}\right) \equiv \frac{2\hbar}{\pi\gamma_0}\left(\ln(t)+\text{constant}\right)\end{aligned} \tag{2.32}$$

On the other hand, for very small times, we will replace

$$1-e^{-\gamma_0 t} \approx \gamma_0 t - \frac{(\gamma_0 t)^2}{2} + \frac{(\gamma_0 t)^3}{6} \equiv I(t)$$

to get (from equation 2.20):

$$\begin{aligned}\langle x^2\rangle_t &\approx \frac{\hbar\omega_p^2}{\pi\gamma_0}\int_0^\infty d\omega\frac{\omega^2 I^2(t)-2\omega\gamma_0\sin(\omega t)I(t)+2\gamma_0^2(1-\cos(\omega t))}{\omega(\omega^2+\omega_p^2)(\omega^2+\gamma_0^2)} \\ &\approx \frac{\hbar\omega_p^2}{\pi\gamma_0}\left[I^2(t)I_1(t)-2\gamma_0 I_2(t)I(t)+\frac{2\gamma_0^2}{\omega_p^2-\gamma_0^2}I_3(t)\right] \\ &\approx \frac{\hbar\omega_p^2\gamma_0 t^4}{48\pi(\omega_p^2-\gamma_0^2)}\left[(\omega_p^2-\gamma_0^2)(21-12\gamma_E)-12\omega_p^2\ln(\omega_p t)+12\gamma_0^2\ln(\gamma_0 t)\right]+\mathcal{O}(t^5)\end{aligned} \tag{2.33}$$

where we have used the small time limit results of $I_2(t)$ and $I_3(t)$:

$$\begin{aligned}I_2(t\to 0) &= \frac{1}{\omega_p^2-\gamma_0^2}\left[\ln\left(\frac{\omega_p}{\gamma_0}\right)t+\frac{t^3}{36}\left[(\omega_p^2-\gamma_0^2)(6\gamma_E-11)+6\omega_p^2\ln(\omega_p t)-6\gamma_0^2\ln(\gamma_0 t)\right]\right]+\mathcal{O}(t^5) \\ I_3(t\to 0) &= \left[\frac{t^2}{2}\ln\left(\frac{\omega_p}{\gamma_0}\right)+\frac{t^4}{288}\left[(\omega_p^2-\gamma_0^2)(12\gamma_E-25)+12\omega_p^2\ln(\omega_p t)-12\gamma_0^2\ln(\gamma_0 t)\right]\right]+\mathcal{O}(t^6)\end{aligned} \tag{2.34}$$

Summarising equations 2.32 and 2.33 (we have incorporated M back):

$$\begin{aligned}&\textbf{Long time limit}: \langle x^2\rangle_t = \frac{2\hbar}{\pi\gamma_0}\left(\ln\left(\sqrt{\frac{k'}{M}}t\right)+\gamma_E\right), \text{ in the limit } \gamma_0 << \omega_p \\ &\textbf{Short time limit}: \langle x^2\rangle_t = \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7-4\gamma_E-4\ln(\omega_p t)\right], \text{ in the limit } \gamma_0 << \omega_p\end{aligned} \tag{2.35}$$

All these predictions have been verified against the exact numerical data for various parameters. Let us understand these results. At large times, it is the subdiffusive behaviour $\sim \ln(t)$. This originates from the zero-point fluctuations of the bath ([5]). Since the temperature of the bath is zero, only zero-point modes of the bath interact with the system. The constant is $\sqrt{k'/M}$. Since the system is connected to the bath with the coupling k', $\sqrt{k'/M}$ is a natural frequency scale of the system. For small times, we again have a sub-dominant t^4 behaviour (compared to the homogeneous part).

Intermediate Temperatures

At any arbitrary temperature, the initial dynamics is exactly same as the zero temperature dynamics. After some time, we see a crossover to the behaviour as $\sim 2\frac{k_B T}{\gamma_0}t + \text{constant}$[3], which is akin to what we obtain for high temperature limit. The crossover time t^* must be a complicated function of different parameters. However, it definitely increases as we increase β. You can see this phenomena in figure 2.3.1.

We will now try to understand why the small-time behaviour is the same as the zero temperature case. Take the integral 2.20. Let us convert the integral into a dimensionless parameter $z = \omega t$.

$$= \frac{\gamma_0 \hbar \omega_p^2}{\pi M^2} \int_0^\infty dz \frac{z}{z^2 + \omega_p^2 t^2} \coth\left(\frac{\hbar \beta z}{2t}\right) f(z,t) \tag{2.36}$$

For small times, we can approximate $\coth\left(\frac{\hbar\beta z}{2t}\right) \sim 1$, which as same as taking $\beta \to 0$. So mathematically speaking, both the limits have the same effect on the integral, and hence the results are the same.

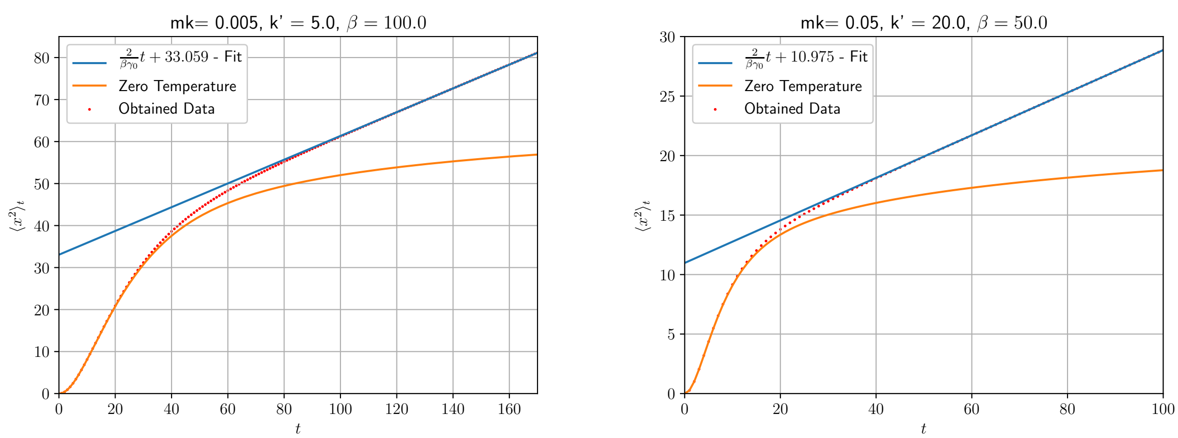


Figure 2.3.1: *Inhomogeneous part of $\langle x^2 \rangle_t$ vs t for different temperatures in the limit $\gamma << \omega_p$.*

In the figure 2.3.2, we have plotted $\langle x^2 \rangle_t$ for different temperatures with other parameters fixed. Two figures represent a linear and log-linear plot of the same. In the figure 2.3.3, you can see a log-log plot of it. From these three plots, we can identify four distinct behaviours and regions:

- Initial $\sim t^4$ (from 0 to $\sim \frac{1}{\omega_p}$).

[3] the constant is not $-\frac{k_B T(3\omega_p^2 + 4\omega_p\gamma_0 + 2\gamma_0^2)}{\omega_p \gamma_0^2(\omega_p + \gamma_0)}$. See figure 2.3.1. The constant terms are positive. On the other hand, $-\frac{k_B T(3\omega_p^2 + 4\omega_p\gamma_0 + 2\gamma_0^2)}{\omega_p \gamma_0^2(\omega_p + \gamma_0)}$ is negative

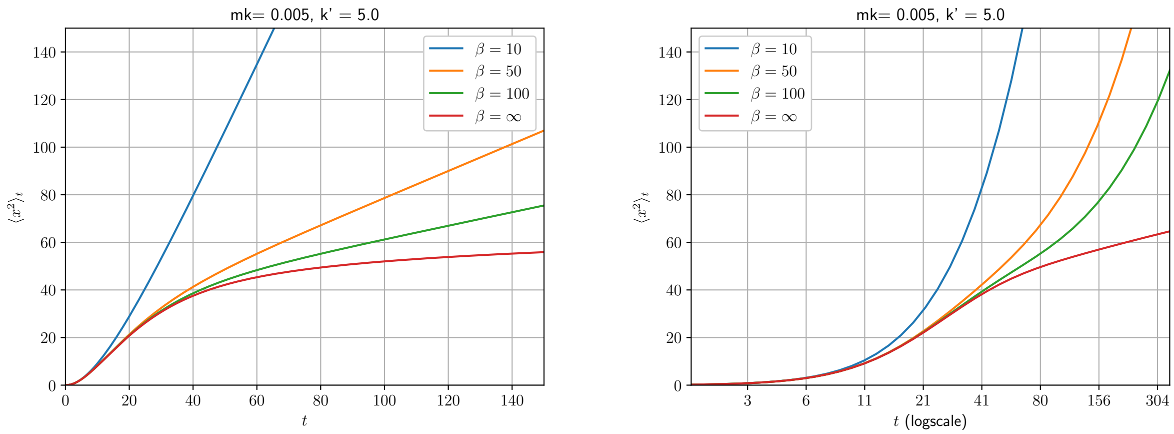


Figure 2.3.2: *Comparison of inhomogeneous part of $\langle x^2 \rangle_t$ for different temperatures in the limit $\gamma << \omega_p$.*

- Polynomial (clear from figure 2.3.3, from $\sim \frac{1}{\omega_p}$ to $\sim \frac{1}{\gamma}$).
- Logarithmic (from $\sim \frac{1}{\gamma}$ to $\sim \frac{1}{k_B T}$).
- Linear (from $\sim \frac{1}{k_B T}$ to ∞).

The transition time between behaviour is not exactly the inverse of the various characteristic time scales, but they are of the same order of magnitude. Also, the transitions are very smooth and not abrupt. We have ensured this order of timescales since the underlying regime that we are working with is $\omega_p >> \gamma$. The polynomial behaviour is usually t^2 ([19]). But, it needs a further analytical study.

Let us understand this more: As $T \to 0$, we don't see the linear behaviour at all, and the subdiffusive logarithmic behaviour prevails till $t \to \infty$. On the contrary, as $T \to \infty$, we see the linear behaviour straightaway. However, practically we can only have some finite temperature, and hence we will always see the initial t^4 behaviour. This kind of division of various behaviour depending on various time scales of the system requires further work in different regimes.

Figures 2.3.1 and 2.3.2 compare the behaviour at different temperatures for a fixed set of parameters. We can also study the behaviour for different parameters at a fixed temperature. So, figure 2.3.4 shows the behaviour for $\langle x^2 \rangle_t$ for a fixed zero temperature but for different parameters.

From figures 2.3.1 and 2.3.2, it is clear that as temperature increases, the crossover time decreases. From the figure 2.3.4, we learn that the system equilibrates much slower as we decrease $mk \sim \gamma$. We will use this fact in the section 2.4.

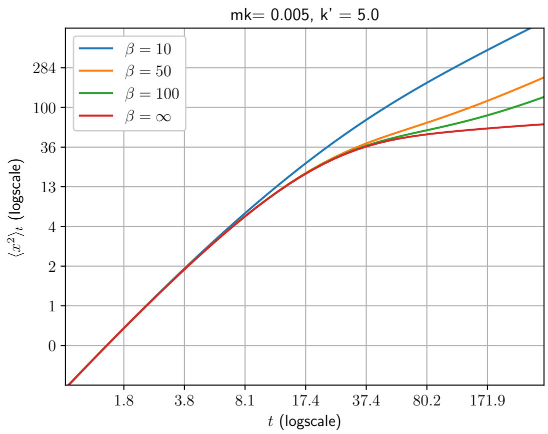


Figure 2.3.3: *Log-log plot of inhomogeneous part of $\langle x^2 \rangle_t$ vs t for different temperatures in the limit $\gamma << \omega_p$.*

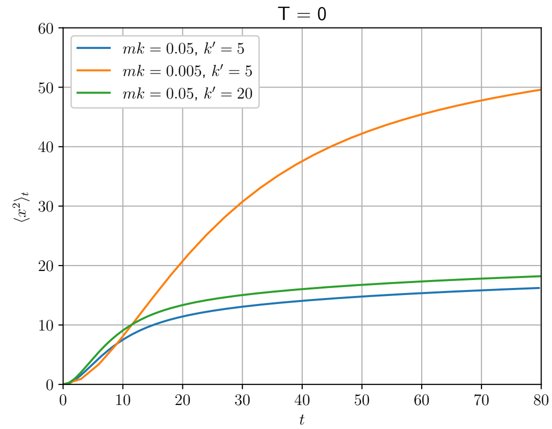


Figure 2.3.4: *Comparison of inhomogeneous part of $\langle x^2 \rangle_t$ vs t for different parameters at $T = 0$.*

2.3.2 Inhomogeneous Part of $\langle x^2 \rangle_t$ for a Bounded Particle

Let us now do the same exercise for a bounded particle. We will use a Drude bath. Recall the equation 2.20:

$$\langle x^2 \rangle_t = \frac{\gamma_0 \hbar \omega_p^2}{\pi M^2} \int_0^\infty d\omega \frac{\omega}{\omega^2 + \omega_p^2} \coth\left(\frac{\hbar\beta\omega}{2}\right) f(\omega, t) \tag{2.37}$$

For bounded particle, we will do our analysis in the limit $\gamma << \omega_0 << \omega_p$. So, we will use $g(t) = e^{-\gamma t} \frac{\sin(\omega_r t)}{\omega_r}$ and get:

$$\begin{aligned} f(\omega, t) = & \frac{2\omega_r^2 + e^{-2\gamma t}[\omega_0^2 + \omega^2 + (\omega_0^2 - 2\gamma^2 - \omega^2)\cos(2\omega_r t) + 2\gamma\omega_r \sin(2\omega_r t)]}{2\omega_r^2(\omega^4 + 2\omega^2(2\gamma^2 - \omega_0^2) + \omega_0^4)} \\ & - \frac{2e^{-\gamma t}[\omega_r \cos(\omega_r t)\cos(\omega t) + \sin(\omega_r t)(\gamma \cos(\omega t) + \omega \sin(\omega t))]}{\omega_r(\omega^4 + 2\omega^2(2\gamma^2 - \omega_0^2) + \omega_0^4)} \end{aligned} \tag{2.38}$$

We will again divide our studies into three cases based on the temperature.

High Temperature Limit

In the limit $k_B T >> \hbar\omega_p$, we again put $\coth(\hbar\beta\omega/2) \approx 2/(\hbar\beta\omega)$. We will just be studying the asymptotic behaviour. To obtain long time behaviour, we put the exponential terms in $f(\omega, t)$ to zero. Then, equation 2.37 becomes:

$$\langle x^2 \rangle_t = \frac{4\gamma\omega_p^2}{\pi\beta M} \int_0^\infty d\omega \frac{1}{(\omega^2+\omega_p^2)(\omega^4+2\omega^2(2\gamma^2-\omega_0^2)+\omega_0^4)}$$

If we further use the fact that $\omega_0 >> \gamma$, we can easily find the roots of the denominator. Roots of the equation $\omega^4+2\omega^2(2\gamma^2-\omega_0^2)+\omega_0^4$ in the limit $\omega_0 >> \gamma$ are $\pm\omega_0 \pm i\gamma$. We can then perform the integral to get:

$$\textbf{Long time limit}: \quad \langle x^2 \rangle_t = \frac{k_B T \omega_p(\omega_p+2\gamma)}{M\left(\gamma^2+\omega_0^2\right)\left((\gamma+\omega_p)^2+\omega_0^2\right)} \rightarrow \frac{k_B T}{M\omega_0^2}, \text{ as } \omega_p >> \omega_0 >> \gamma \tag{2.39}$$

The value saturates at $\frac{k_B T}{M\omega_0^2}$, which is the same as that of an independent oscillator equilibrated at temperature T.

For short time, an analysis similar to equation 2.33 can be done. However, we can plot the numerical data for very small times and fit it. See figure 2.3.5, for very small times, the fit is $A_\infty t^4$. The parameters we have used are $mk = 0.05$, $k' = 5$, $\omega_0 = 1.5$, $M = 1$. For this set of parameters, we can find the following quantity:

$$k'\frac{k_B T}{4M^2} = 12500 \sim A_\infty$$

This is roughly same as the fit parameter A_∞ (figure 2.3.5) and hence, we can conclude that:

$$\textbf{Short time limit}: \langle x^2 \rangle_t = k'\frac{k_B T}{4M^2}t^4 + \mathcal{O}(t^5) \tag{2.40}$$

This behaviour is precisely similar to that of a free particle. This could happen because, at very small times, the trap would not have shown its impact. For instance, the behaviour of the free particle and the bounded particle would have been the same even if the bath was not there.

Zero Temperature Limit

We use $\omega\coth(\hbar\beta\omega/2) = |\omega|$. For long-time limit, we do the same thing of putting the exponentials in $f(\omega, t)$ to zero and then equation 2.37 becomes:

$$\langle x^2 \rangle_t = \frac{2\hbar\gamma\omega_p^2}{\pi M} \int_0^\infty d\omega \frac{\omega}{(\omega^2+\omega_p^2)(\omega^4+2\omega^2(2\gamma^2-\omega_0^2)+\omega_0^4)}$$

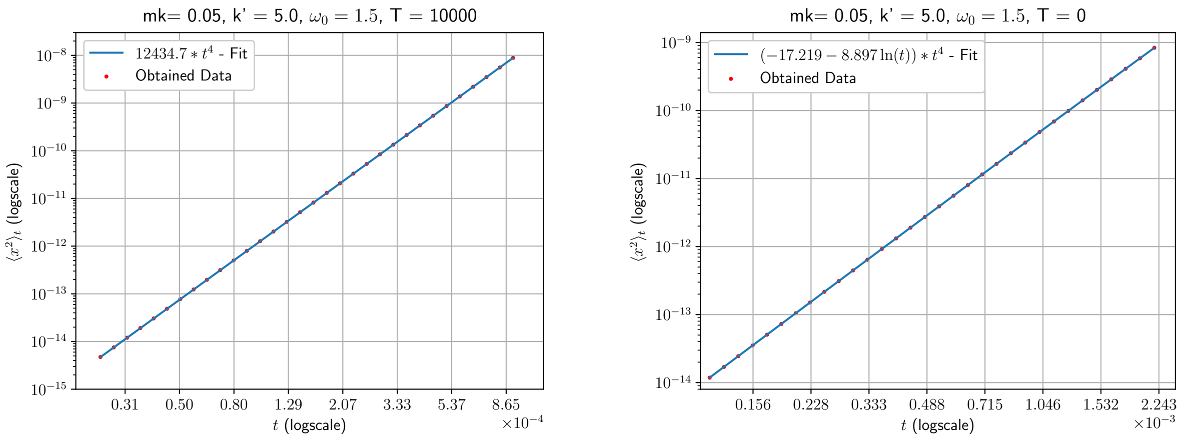


Figure 2.3.5: *Fitting the inhomogeneous part of $\langle x^2 \rangle_t$ vs t at small times for a bounded particle in the limits $\hbar\gamma << \hbar\omega_0 << \hbar\omega_p << k_B T$ and $k_B T << \hbar\gamma << \hbar\omega_0 << \hbar\omega_p$.*

Again the use of inequality $\omega_0 >> \gamma$ makes the evaluation of the integral easy, and we get:

$$\begin{aligned}\langle x^2 \rangle_{t\to\infty} &= \frac{\hbar\omega_p^2 \left[(\omega_p^2 + \omega_0^2 - \gamma^2)\pi - 2\gamma^2 \cot^{-1}\left(\frac{2\gamma\omega_0}{\omega_0^2 - \gamma^2}\right)\right]}{4M\pi\omega_0 \left((\gamma + \omega_p)^2 + \omega_0^2\right)\left((\gamma - \omega_p)^2 + \omega_0^2\right)} \\ &\quad + \frac{\hbar\omega_p^2 \left[(\omega_p^2 + \omega_0^2)\tan^{-1}\left(\frac{\omega_0^2 - \gamma^2}{2\gamma\omega_0}\right) + 2\gamma\omega_0 \ln\left(\frac{\omega_0^2 + \gamma^2}{\omega_p^2}\right)\right]}{2M\pi\omega_0 \left((\gamma + \omega_p)^2 + \omega_0^2\right)\left((\gamma - \omega_p)^2 + \omega_0^2\right)} \\ &\to \frac{\hbar}{2M\omega_0}, \text{ using } \omega_p >> \omega_0 >> \gamma\end{aligned} \tag{2.41}$$

which is again the same behaviour as an isolated oscillator.

For short time, an analysis similar to equation 2.33 can be done. However, we can plot the numerical data for very small times and fit it. See figure 2.3.5, for very small times, the fit is $[A_0 + B_0 \ln(t)]t^4$. The parameters we have used are $mk = 0.05$, $k' = 5$, $\omega_0 = 1.5$, $M = 1$. For this parameters, the following quantities are:

$$\frac{\hbar\omega_p^2\gamma_0[7 - 4(\gamma_E + \ln(\omega_p))]}{16\pi M^2} = -17.212 = A_0, \quad \frac{\hbar\omega_p^2\gamma_0}{4\pi M^2} = 8.897 = B_0$$

These numbers are exactly same as the fit parameters (figure 2.3.5) and hence, we can conclude that:

$$\textbf{Short time limit}: \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7 - 4\gamma_E - 4\ln(\omega_p t)\right] \tag{2.42}$$

This is once again similar to the result of a free particle.

Intermediate Temperature

For arbitrary temperature, we have plotted the numerical results in figure 2.3.2. For large times, we can easily see from the fit that it saturates to $\sim \frac{\hbar}{2M\omega_0} \coth\left(\frac{\hbar\omega_0}{2k_BT}\right)$. This is same as the result of an independent equilibrated oscillator. Let me clarify it a bit: Say $Z_S(\beta)$ is the canonical partition function corresponding to the system Hamiltonian H_S. Now, if we find $\langle x^2 \rangle$ using the partition function $Z_S(\beta)$ then it would be same as $\frac{\hbar}{2M\omega_0} \coth\left(\frac{\hbar\omega_0}{2k_BT}\right)$.

Initially, it coincides with zero temperature behaviour (same as what we saw for the free particle case). The crossover time t^* again seems to depend complexly on all the parameters. However, it certainly increases with β. The figure 2.3.7 shows plots for different temperatures with other parameters fixed. We also observe oscillations in the transients (see figure 2.3.7). It is because of

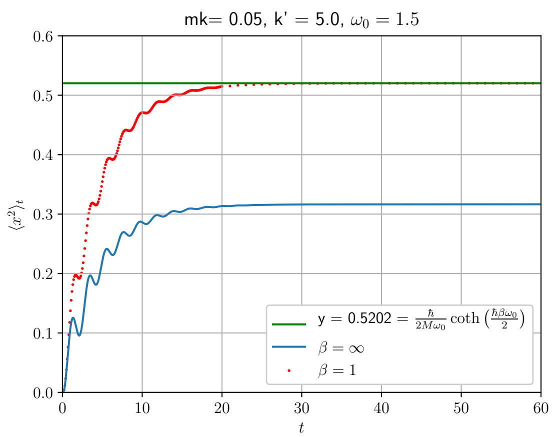


Figure 2.3.6: *Inhomogeneous part of $\langle x^2 \rangle_t$ vs t for a bounded particle in the limit $\gamma << \omega_0 << \omega_p$.*

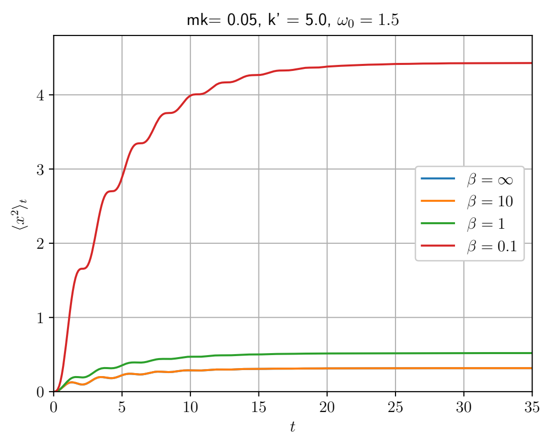


Figure 2.3.7: *Comparison of the inhomogeneous part of $\langle x^2 \rangle_t$ vs t for a bounded particle in the limits $\gamma << \omega_0 << \omega_p$ for different temperatures. Note that $\beta = 10$ and $\beta = \infty$ almost coincides.*

the $\sin(2\omega_r t)$ and $\cos(2\omega_r t)$ in $f(\omega, t)$ (equation 2.38). If we observe the frequency of oscillations, it is nearly π/ω_r.

2.4 A Discussion on the Weak Coupling Limit

Let us decode why we chose $\omega_p >> \omega_0 >> \gamma$ for the bounded particle and $\omega_p >> \gamma$ for the free particle case. From all the results, it is clear that the results in this limit are similar to that of an independent oscillator or a free particle thermalised at temperature β[4]. This motivates us to believe that $\omega_p >> \omega_0 >> \gamma$ is weak coupling limit. Now, let us re-write this in terms of the microscopic parameters: $\omega_p >> \gamma$ is equivalent to $2Mk' >> mk$ (see equation 1.5). So, **the weak coupling limit is not a small k' limit!** This is surprising since the interaction is $\sim \frac{k'}{2}x^2$.

We can observe one more thing: As we decrease $\gamma \sim \sqrt{mk}$, the system relaxes slower (refer to figure 2.3.1). So, γ has the information of coupling strength (the larger the coupling, the faster it equilibrates). This information is rooted in the spectral density (see equation 1.5): $\Gamma(\omega) \propto \gamma_0 \sim \gamma$. In conclusion, we can't naively guess the weak coupling limit just by gazing at the interaction Hamiltonian. We need to look carefully at the spectral density to make sense of the weak coupling limit in the study of open quantum systems.

But, the weak coupling limit must somehow be related to the interaction Hamiltonian, right? - it definitely is. Look at the interaction Hamiltonian in the normal mode coordinates of the bath (equation 1.2). It has C_s, which is related to the spectral density $\Gamma(\omega)$ (equation 1.3), which in turn is related to γ_0. So, γ_0 controls the strength with which normal modes interact with the system.

We are interested in the weak coupling limit since it is a well-known fact that the master equation approach works best in the weak-coupling limit—the approach that we are going to test.

This discussion also answers one of the questions that we wanted to answer at the beginning of this project. If the Ohmic limit is the infinite k' limit (equation 1.5), which naively looked like a very strong coupling limit, then will the Born-Markov master equation approach fail or work? (since it is well-known that the Born-Markov master equation works best in the weak coupling limit and for the Ohmic bath [5]). The answer is clear - Large k' does not necessarily mean the strong coupling limit and the master equation approach work. But does it work flawlessly? - let us find out in the following chapters.

Typically, the term determining the strength of the interaction, say γ, only appears in the interaction Hamiltonian. In that case, the same term also appears in the spectral density, i.e. $\Gamma(\omega) \sim \gamma$. So,

[4] The momentum modes for the free particle case gives $\langle p^2 \rangle = Mk_BT$, which is the same as that of an independent free particle thermalised at the temperature T. However, for the case of a Brownian particle, $\langle x^2 \rangle$ will not equilibrate to 0 as it does for an independent free particle. This is obvious since the particle is coupled to a bath.

weak coupling has a very clear meaning. However, for this particular model, the k'-term enters the bath as well as the system Hamiltonian (see equation 1.1). As a consequence, the spectral density depends very non-trivially on k' (through ω_p in equation 1.5). So, this entire discussion may turn out to be very model-specific, and further study needs to be done to understand more in this direction.

2.5 Limitations of the Langevin Equation Approach

After this exercise, we might also be able to appreciate the limited applicability of the exact Langevin approach. Analytically, we could only get only the asymptotic results, that too only in very special regimes. Even in this very simple setup, it is hard to find an exact analytical expression of $\langle x^2 \rangle_t$ for arbitrary t at an arbitrary temperature. Finding $f(\omega, t)$ is also a non-trivial task outside the weak coupling regime. So, you can imagine that for a more complicated problem, an exact analytical approach will not take us much far.

Numerically, we were able to do this problem quite comfortably. But, it becomes harder if you try to switch to other regimes than the weak coupling limit (though a completely doable problem). The numerical simulation will become harder as we try to model a more realistic setup, say with a non-trivial $V(x)$, or with multiple particles with some interaction in the system or with a more realistic bath. For a non-quadratic $V(x)$, the very first step of getting a closed-form of $g(t)$ while solving the Langevin equation (equation 2.5) will be a non-trivial task. Even if you get them, finding its inverse Laplace transform will be even more challenging.

There is one more approach called the steady-state Langevin equation approach ([7]) to obtain the exact equilibrium properties of any system. It is applicable to many more problems. But, it will tell only about the equilibrium properties (not even about how it approaches equilibrium!). On the other hand, master equation approaches have much wider applicability, and we will learn about them in the next chapter.

Appendix

2.A Solving the Bath Equations

We want to solve the equation of motion for the bath: $\ddot{X}_s(t) + \Omega_s^2 X_s(t) = C_s x(t)$. The corresponding homogenoeus equation $\ddot{X}_s(t) + \Omega_s^2 X_s(t) = 0$ has a very well-known solution: $X_s^h(t) = X_s(0)\cos(\Omega_s t) + \frac{P_s(0)}{\Omega_s}\sin(\Omega_s t)$. We now need to find a specific solution of the inhomogeneous equation. Let the full solution be $X_s(t) = X_s^h(t) + X_s^I(t)$. Then, we need to solve the equation:

$$\ddot{X}_s^I(t) + \Omega_s^2 X_s^I(t) = C_s x(t); \quad X_s^I(0) = 0,\ \dot{X}_s^I = 0$$

The equation is trivial to solve in the Laplace space:

$$\tilde{X}_s^I(z) = \frac{C_s \tilde{x}(z)}{z^2 + \Omega_s^2} \implies X_s^I(t) = \frac{C_s}{\Omega_s}\int_0^t dt_1 \sin\left(\Omega_s(t-t_1)\right) x(t_1)$$

where we use properties from table 2 to perform the inverse Laplace transform. $X_s(t) = X_s^h(t) + X_s^I(t)$ is same as equation 2.4.

2.B Leibniz Route vs Integration by Parts Route

We will use free particle (i.e. $V(x) = 0$) for simplicity. Equation 2.5 for free particle:

$$M\ddot{x}(t) + k' x(t) - \int_0^t dt_1 x(t_1)\Sigma(t-t_1) = \eta(t) \tag{2.43}$$

2.B.1 Ohmic Bath

Leibniz Route

What is generally done is to write $\Sigma(t-t_1) = -\frac{\partial \gamma(t-t_1)}{\partial t}$[5]. We can then use the following simplification[6]:

$$-\int_0^t dt_1 \Sigma(t-t_1) x(t_1) = \int_0^t dt_1 x(t_1) \frac{\partial}{\partial t}\gamma(t-t_1) = \frac{d}{dt}\left(\int_0^t dt_1 x(t_1)\gamma(t-t_1)\right) - \gamma(0)x(t) \tag{2.44}$$

Using it, equation 2.43 becomes:

$$M\ddot{x}(t) + \frac{d}{dt}\int_0^t dt_1 x(t_1)\gamma(t-t_1) = \eta(t) \implies \ddot{x}(t) + 2\gamma\dot{x}(t) = \frac{1}{M}\eta(t); \quad \gamma \equiv \frac{\gamma_0}{2M} \tag{2.45}$$

where we have used $\gamma(t) = 2\gamma_0\delta(t)$[7] and $\gamma(0) = k'$ (see appendix 1.A). In order to solve it, let us first solve the homogeneous equation (with $\eta(t) = 0$). Let $g_1(t)$ and $g_2(t)$ are two of the *fundamental solutions* of homogeneous equation such that $g_1(0) = 1$, $\dot{g}_1(0) = 0$ and $g_2(0) = 0$, $\dot{g}_2(0) = 1$. We take the Laplace transform of homogeneous equation:

$$\begin{aligned} &z^2\tilde{g}_1(z) - zg_1(0) - \dot{g}_1(0) + 2\gamma(z\tilde{g}_1(z) - g_1(0)) = 0 \implies \tilde{g}_1(z) = \frac{z+2\gamma}{z^2+2z\gamma} = \frac{1}{z}. \\ &\text{And similarly,} \quad \tilde{g}_2(z) = \frac{1}{z^2+2z\gamma}. \end{aligned} \tag{2.46}$$

The full solution will be $x(t) = g_1(t)x(0) + g_2(t)\dot{x}(0) + c(t)$, where $c(t)$ is a specific solution of the inhomogeneous equation. $c(t)$ can be obtained easily (it is the exactly same procedure as we have done in appendix 2.A) and the solution is:

$$x(t) = x(0) + \frac{1-e^{-2\gamma t}}{2\gamma}\dot{x}(0) + \int_0^t dt_1 \frac{1-e^{-2\gamma(t-t_1)}}{2M\gamma}\eta(t_1) \tag{2.47}$$

This solution is different from equation 2.15 that we obtained by solving equation 2.5. We have checked that this problem persists for a bounded particle (i.e. $V(x) = \frac{1}{2}M\omega_0^2 x^2$) as well.

---

[5] If you write $\Sigma(t-t_1) = \sum_s \frac{C_s^2}{\Omega_s}\sin(\Omega_s(t-t_1))$ and $\gamma(t-t_1) = \sum_s \frac{C_s^2}{\Omega_s^2}\cos(\Omega_s(t-t_1))$, it is clear.

[6] using Leibniz rule: $\frac{d}{dt}\left(\int_{a(t)}^{b(t)} f(t,s)ds\right) = f(t,b(t))\frac{d}{dt}b(t) - f(t,a(t))\frac{d}{dt}a(t) + \int_{a(t)}^{b(t)}\frac{\partial}{\partial t}f(t,s)ds$

[7] Please do not confuse between the damping kernel $\gamma(t)$ and the constant $\gamma = \frac{\gamma_0}{2M}$. We will always use an argument whenever we refer to the damping kernel.

By Parts Route

In equation 2.43, we can do integration by parts and simplify the Σ term like this:

$$\begin{aligned} -\int_0^t dt_1 \Sigma(t-t_1)x(t_1) = -\int_0^t d\tau \Sigma(\tau)x(t-\tau) &= \int_0^t d\tau \dot{\gamma}(\tau)x(t-\tau) \\ &= \gamma(t)x(0) - \gamma(0)x(t) - \int_0^t d\tau \frac{dx(t-\tau)}{d\tau}\gamma(\tau) \\ &= \gamma(t)x(0) - \gamma(0)x(t) + \int_0^t dt_1 \dot{x}(t_1)\gamma(t-t_1) \end{aligned} \tag{2.48}$$

We can again use $\gamma(t) = 2\gamma_0\delta(t)$ and $\gamma(0) = k'$ to get:

$$\ddot{x}(t) + 2\gamma\dot{x}(t) = \frac{\eta(t) - 2\gamma_0\delta(t)x(0)}{M}$$

The homogeneous part of this differential equation is exactly same as equation 2.45 and hence $g_1(t)$ and $g_2(t)$ will be same. So, the full solution is:

$$\begin{aligned} x(t) &= x(0) + \frac{1-e^{-2\gamma t}}{2\gamma}\dot{x}(0) + \frac{1}{M}\int_0^t dt_1 g_2(t-t_1)\left(\eta(t_1) - 2\gamma_0\delta(t_1)\right) \\ &= e^{-2\gamma t}x(0) + \frac{1-e^{-2\gamma t}}{2\gamma}\dot{x}(0) + \int_0^t dt_1 \frac{1-e^{-2\gamma(t-t_1)}}{2M\gamma}\eta(t_1) \end{aligned}$$

This solution is the same as equation 2.15 that we obtained by solving equation 2.5.

2.B.2 Free Particle: Drude Bath

Since the integration by parts is fine, let us check the Leibniz route for a smoother bath, i.e. a Drude bath.

Leibniz Route

We will now use $\gamma(t) = \gamma_0\omega_p e^{-\omega_p t}$ in equation 2.45. Let again $g_1(t)$ and $g_2(t)$ are two of the *fundamental solutions* of homogeneous equation. We take Laplace transform of homogeneous equation (use $\tilde{\gamma}(z) = \frac{\gamma_0\omega_p}{z+\omega_p}$):

$$\begin{aligned} &z^2\tilde{g}_1(z) - z\tilde{g}_1(0) - \dot{g}_1(0) + \frac{z}{M}(\tilde{\gamma}(z)\tilde{g}_1(z)) - \lim_{t\to 0}\frac{1}{M}\int_0^t dt_1 x(t_1)\gamma(t-t_1) = 0 \\ &\implies \tilde{g}_1(z) = \frac{1}{z + \frac{2\gamma\omega_p}{z+\omega_p}}, \quad \text{And similarly,} \quad \tilde{g}_2(z) = \frac{1}{z^2 + \frac{2\gamma\omega_p z}{z+\omega_p}}. \end{aligned} \tag{2.49}$$

The full solution will be $x(t) = g_1(t)x(0) + g_2(t)\dot{x}(0) + \frac{1}{M}\int_0^t dt_1 g_2(t-t_1)\eta(t_1)$ with

$$g_1(t) = e^{-\frac{\omega_p t}{2}}\left[\cosh\left(\omega_p^r t/2\right) + \frac{\omega_p}{2}\frac{\sinh\left(\omega_p^r t/2\right)}{\omega_p^r/2}\right]; \quad \omega_p^r = \sqrt{\omega_p^2 - 8\gamma\omega_p}$$
$$g_2(t) = \frac{1}{2\gamma} + e^{-\frac{\omega_p t}{2}}\left[\left(1 - \frac{\omega_p}{4\gamma}\right)\frac{\sinh\left(\omega_p^r t/2\right)}{\omega_p^r/2} - \frac{1}{2\gamma}\cosh\left(\omega_p^r t/2\right)\right] \tag{2.50}$$

This is the same as what we obtained in equation 2.14 that we obtained by solving equation 2.5. We have also done this case with the by-part route, and obviously, it matches the equation 2.14.

Chapter 3

Master Equation Approach

In this chapter, we will learn the quantum master equation approach by solving our problem using this approach. Starting from the Hamiltonian, we will derive a master equation while understanding all the approximations along the way. We will analyse both the Markovian and non-Markovian master equations. Here too, we will assume that the initial state is the product state and the number of bath sites is infinite.

The starting point is to move to the interaction picture. We will put a suffix "I" to everything that is in the interaction picture. Unless stated otherwise, suffixes "S" and "B" will be used for system and bath operators, respectively. Let $\rho_I(t)$ be the full density matrix of the system and the bath in the interaction picture. If H_I is the interaction part of the Hamiltonian in the interaction picture, then we can write the von-Neumann equation (since the evolution of system + bath is unitary):

$$\frac{d}{dt}\rho_I(t) = -\frac{i}{\hbar}[H_I(t), \rho_I(t)]; \quad H_I(t) = e^{iH_0 t}\hat{H}_I e^{-iH_0 t} \tag{3.1}$$

A formal solution to the above equation is

$$\rho_I(t) = \rho_I(0) - \frac{i}{\hbar}\int_0^t dt_1 [H_I(t_1), \rho_I(t_1)] \tag{3.2}$$

If we substitute equation 3.2 into equation 3.1 and then take a partial trace over the bath, we get the crudest form of the master equation:

$$\boxed{\frac{d}{dt}\rho_{SI}(t) = -\frac{i}{\hbar}\mathrm{tr}_B[H_I(t), \rho_I(0)] - \frac{1}{\hbar^2}\int_0^t dt_1\, \mathrm{tr_B}[H_I(t), [H_I(t_1), \rho_I(t_1)]] \qquad (3.3)}$$

where $\rho_{SI}(t) = \mathrm{tr}_B(\rho_I(t))$ is the reduced system density matrix in the interaction picture. From equation 1.2, note that $\hat{H}_I = -x \otimes B$. So, let us write the explicit form of $H_I(t)$:

$$H_I(t) = -e^{iH_0 t}[x \otimes B]e^{-iH_0 t} = -x_I(t) \otimes B_I(t); \quad x_I(t) = e^{iH_S t} x e^{-iH_S t}, \; B_I(t) = e^{iH_B t} B e^{-iH_B t} \tag{3.4}$$

Equation 1.7 tells us that $B_I(t) = \eta(t)$. Let us analyse the first term of equation 3.3:

$$\begin{aligned} -\text{tr}_B[H_I(t), \rho_I(0)] &= \text{tr}_B[x_I(t) \otimes \eta(t), \rho_{SI}(0) \otimes \rho_{BI}(0)] \\ &= \text{tr}_B[x_I(t) \otimes \eta(t), \rho_{SI}(0) \otimes \rho_{th}] \\ &= [x_I(t), \rho_{SI}(0)]\langle \eta(t) \rangle_{th} \\ &= 0. \end{aligned} \tag{3.5}$$

Here, we have used the fact that the initial state of the system + bath is in a product state. We have also used the fact that the bath is in the thermal state (the initial state is the same in any picture).

Since we will only be dealing with a harmonic trap and free particle case, let us write the Hamiltonian explicitly for the trap case:

$$\begin{aligned} &H_S = \frac{p^2}{2M} + \frac{1}{2}(M\omega_0^2 + k')x^2 = \frac{1}{2}M\omega_n^2 x^2; \quad H_B = \sum_{s=1}^{N} \frac{P_s^2}{2} + \frac{\Omega_s^2 X_s^2}{2} = \sum_s \hbar\Omega_s \left(b_s^\dagger b_s + \frac{1}{2}\right) \\ &\hat{H}_{SB} = -x \sum_{s=1}^{N} C_s X_s \equiv -xB; \quad C_s = m^{-1/2} k' U_{s1}; \quad B = \sum_s C_s \sqrt{\frac{\hbar}{2\Omega_s}}(b_s + b_s^\dagger) \end{aligned} \tag{3.6}$$

Using this, now we can explicitly write the equation 3.4:

$$\begin{aligned} x_I(t) &= e^{iH_S t} x e^{-iH_S t} = x(0)\cos(\omega_n t) + \frac{p(0)}{M}\frac{\sin(\omega_n t)}{\omega_n} \\ \eta(t) &= e^{iH_B t} B e^{-iH_B t} = \sum_s C_s \sqrt{\frac{\hbar}{2\Omega_s}}(e^{i\Omega_s t} b_s^\dagger + e^{-i\Omega_s t} b_s) \end{aligned} \tag{3.7}$$

Finally, let us also recall what we need to do to find the expectation value of any operator A in the interaction picture:

$$\frac{d\langle A \rangle_t}{dt} = \text{tr}\{\dot{A}_I(t)\rho_{SI}(t)\} + \text{tr}\{A_I(t)\dot{\rho}_{SI}(t)\} \tag{3.8}$$

Exact Master Equation

We can try to obtain moments from the von-Neumann equation 3.1 itself. It will match with the exact Langevin results. It is just obtaining the Heisenberg equation for moments starting from the interaction picture (instead of the Heisenberg picture in the Langevin method).

3.1 Born Master Equation (BME)

In this section, we will understand the Born approximation. It is a perturbative approximation, i.e. we truncate the master equation to a certain order with respect to certain parameters.

Statement: Put $\rho_I(t) \approx \rho_{SI}(t) \otimes \rho_{BI}(t) = \rho_{SI}(t) \otimes \rho_{th}$ for all times t in the master equation 3.3.

Justification: We have assumed that $\rho_I(0) = \rho_{SI}(0) \otimes \rho_{BI}(0)$. If the interaction between the system and the bath was not present, ρ_I would have always remained in the product state. The interaction will develop correlations between them and so in the weak system-bath coupling, as a perturbative expansion, one can write ([6]): $\rho_I(t) \approx \rho_{SI}(t) \otimes \rho_{BI}(t) + \mathcal{O}(\hat{H}_I)$. Here, $\rho_{SI}(t) = e^{iH_S t}\rho_{SI}(0)e^{-iH_S t}$ and $\rho_{BI}(t) = e^{iH_B t}\rho_{BI}(0)e^{-iH_B t}$ are the evolved reduced density matrices in the interaction picture of the system and the bath, respectively[1].

We want to truncate the master equation to the second order in $\hat{H}_I$. Now, the right hand side of the master equation 3.3 already have two $\hat{H}_I$ making it $\mathcal{O}(\hat{H}_I^2)$. So, we will truncate the ρ_I term to the zeroth order in $\hat{H}_I$ and hence, $\rho_I(t) \approx \rho_{SI}(t) \otimes \rho_{BI}(t)$.

Since H_B and ρ_{th} commute, we can conclude that

$$\rho_{BI}(t) = e^{iH_B t}\rho_{BI}(0)e^{-iH_B t} = e^{iH_B t}\rho_{th}e^{-iH_B t} = \rho_{th}$$

If you find this entire Born approximation hard to digest, I would recommend section 9.1 of reference [5], where a very neat derivation of this approximation is given using something called as the projection operators method. Incorporating this approximation and equation 3.5, let us re-write and simplify the master equation 3.3:

$$\begin{aligned}
\frac{d}{dt}\rho_{SI}(t) &= -\frac{1}{\hbar^2}\int_0^t dt_1\, \mathrm{tr_B}[H_I(t), [H_I(t_1), \rho_{SI}(t_1) \otimes \rho_{th}]] \\
&= -\frac{1}{\hbar^2}\int_0^t dt_1 \Big(\langle \eta(t)\eta(t_1)\rangle_{th}[x_I(t)x_I(t_1)\rho_{SI}(t_1) - x_I(t_1)\rho_{SI}(t_1)x_I(t)] \\
&\qquad\qquad - \langle \eta(t_1)\eta(t)\rangle_{th}[x_I(t)\rho_{SI}(t_1)x_I(t_1) - \rho_{SI}(t_1)x_I(t_1)x_I(t)]\Big) \qquad (3.9) \\
&= -\frac{1}{\hbar^2}\int_0^t dt_1 \Big(\frac{\langle \eta(t)\eta(t_1) - \eta(t_1)\eta(t)\rangle_{th}}{2}[x_I(t), \{x_I(t_1), \rho_{SI}(t_1)\}] \\
&\qquad\qquad + \frac{\langle \eta(t)\eta(t_1) + \eta(t_1)\eta(t)\rangle_{th}}{2}[x_I(t), [x_I(t_1), \rho_{SI}(t_1)]]\Big)
\end{aligned}$$

[1] In general, it might be possible that $e^{iH_S t}\rho_{SI}(0)e^{-iH_S t} \neq \mathrm{tr}_B(\rho_I(t))$ and $e^{iH_B t}\rho_{BI}(0)e^{-iH_B t} \neq \mathrm{tr}_S(\rho_I(t))$. However, it can be shown to be equal in the leading order in the weak interaction limit.

The best way to justify the last line of the manipulation is to expand the expression in the last line, and we can easily see that it gives the expression in the second line.

Finally, the **Born master equation** (BME):

$$\frac{d\rho_{SI}(t)}{dt} = \int_0^t dt_1 \Bigg(\frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t_1)\}\right] \\ - \frac{1}{2\hbar^2} D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t_1)]\right] \Bigg) \tag{3.10}$$

To simplify further, we will need to substitute $x_I(t)$ in terms of $x_I(t_1)$ and $p_I(t_1)$, which we can do using equation 3.7:

$$\begin{aligned} x_I(t) &= x_I(t_1)\cos(\omega_n(t-t_1)) + \frac{p_I(t_1)}{M}\frac{\sin(\omega_n(t-t_1))}{\omega_n} \\ p_I(t) &= p_I(t_1)\cos(\omega_n(t-t_1)) - M\omega_n x_I(t_1)\sin(\omega_n(t-t_1)) \end{aligned} \tag{3.11}$$

These expressions are not strictly to order 0 in $\hat{H}_I$ since it contains arbitrary orders of k' through $\cos(\omega_n t)$ and $\sin(\omega_n t)$ $\left(\text{remember } \omega_n = \sqrt{\omega_0^2 + (k'/M)}\right)$. Putting this into equation 3.10 will make it to have arbitrary orders of $\hat{H}_I$. So, we need to truncate equation 3.11 to zeroth order[2]:

$$\begin{aligned} x_I(t) &\approx x_I(t_1)\cos(\omega_0(t-t_1)) + \frac{p_I(t_1)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0} \\ p_I(t) &\approx p_I(t_1)\cos(\omega_0(t-t_1)) - M\omega_0 x_I(t_1)\sin(\omega_0(t-t_1)) \end{aligned} \tag{3.12}$$

We will now write the differential equation for $\langle A\rangle_t$ where A is any system operator. We will need to use equation 3.8 and get:

$$\frac{d\langle A\rangle_t}{dt} = \frac{i}{\hbar}\langle [H_0, A]\rangle_t + \int_0^t dt_1 \Bigg(\frac{i}{2\hbar}\Sigma(t-t_1)\mathrm{tr}_S\left(\{[A_I(t), x_I(t)], x_I(t_1)\}\rho_{SI}(t_1)\right) \\ - \frac{1}{2\hbar^2} D_1(t-t_1)\mathrm{tr}_S\left([[A_I(t), x_I(t)], x_I(t_1)]\rho_{SI}(t_1)\right) \Bigg) \tag{3.13}$$

Let us do all the moments. First moments are easiest and we get (refer to appendix 3.A.1 for explanation):

$$\langle \dot{x}\rangle_t = \frac{\langle p\rangle_t}{M}, \quad \langle \dot{p}\rangle_t = -M\omega_n^2\langle x\rangle_t + \int_0^t dt_1 \langle x\rangle_{t_1}\Sigma(t-t_1) \tag{3.14}$$

[2]Most texts does not justify this step very properly. So, I am not sure if there is any better justification to do this approximation. If we analyse equation 3.10 using 3.11, we get very absurd results. For example, we will find a free particle behaving as a particle bounded in a trap frequency $\sqrt{k'/M}$.

This system of differential equations is the same as what we would obtain from the exact Langevin approach (see equation 5.3). This can also be easily generalised to any other potential $V(x)$ and so:

The dynamics of the first moments is totally unaffected by the Born approximation.

The reason behind it could be that the system-bath correlations that we approximated to be negligible while doing the approximation do not play any role in the dynamics of the first moments.

Let us now look at the second moments (refer to appendix 3.A.1 for details):

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t + \int_0^t dt_1\left[C(t-t_1)\langle xp+px\rangle_{t_1} - 2M\omega_0^2 S(t-t_1)\langle x^2\rangle_{t_1}\right] + h(t), \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t + \int_0^t dt_1\left[2C(t-t_1)\langle x^2\rangle_{t_1} + S(t-t_1)\frac{\langle xp+px\rangle_{t_1}}{M}\right] + \frac{f(t)}{M}
\end{aligned} \tag{3.15}$$

with

$$\begin{aligned}
C(t) &= \Sigma(t)\cos(\omega_0 t), \quad S(t) = \Sigma(t)\frac{\sin(\omega_0 t)}{\omega_0} \\
h(t) &= \int_0^t d\tau\cos(\omega_0\tau)D_1(\tau), \quad f(t) = \int_0^t d\tau\frac{\sin(\omega_0\tau)}{\omega_0}D_1(\tau)
\end{aligned} \tag{3.16}$$

These definitions of $C(t)$, $S(t)$, $h(t)$ and $f(t)$ will be used repeatedly in this thesis.

3.1.1 Solving BME for a Bounded Particle

We will now solve the differential equations 3.15. For that, we need to write them in the Laplace space:

$$\begin{aligned}
z\langle\tilde{x}^2\rangle(z) - \langle x^2\rangle_0 &= \frac{\langle xp\tilde{+}px\rangle(z)}{M} \\
z\langle\tilde{p}^2\rangle(z) - \langle p^2\rangle_0 &= -(M\omega_n^2 - \tilde{C}(z))\langle xp\tilde{+}px\rangle(z) - 2M\omega_0^2\tilde{S}(z)\langle\tilde{x}^2\rangle(z) + \tilde{h}(z) \\
z\langle xp\tilde{+}px\rangle(z) - \langle xp+px\rangle_0 &= \frac{2\langle\tilde{p}^2\rangle(z)}{M} - 2(M\omega_n^2 - \tilde{C}(z))\langle\tilde{x}^2\rangle(z) + \frac{\tilde{S}(z)\langle xp\tilde{+}px\rangle(z)}{M} + \frac{\tilde{f}(z)}{M}
\end{aligned} \tag{3.17}$$

Now, this a system of algebraic equations and it can be solved easily. We will once again focus only on $\langle x^2\rangle$:

$$\langle\tilde{x}^2\rangle(z) = \frac{2\tilde{h}(z) + z\tilde{f}(z) + 2\langle p^2\rangle_0 + Mz\langle xp+px\rangle_0 + M[z(Mz-\tilde{S}(z)) + 2(M\omega_n^2 - \tilde{C}(z))]\langle x^2\rangle_0}{4M\omega_0^2\tilde{S}(z) + Mz^2(Mz-\tilde{S}(z)) + 4Mz(M\omega_n^2 - \tilde{C}(z))} \tag{3.18}$$

with (we use Drude bath, refer to section 1.3):

$$\tilde{C}(z) = \frac{\tilde{\Sigma}(z - i\omega_0) + \tilde{\Sigma}(z + i\omega_0)}{2}, \quad \tilde{S}(z) = \frac{\tilde{\Sigma}(z - i\omega_0) - \tilde{\Sigma}(z + i\omega_0)}{2i\omega_0}, \quad \tilde{\Sigma}(z) = \frac{\gamma_0 \omega_p^2}{z + \omega_p}$$
$$\tilde{h}(z) = \frac{\tilde{D}_1(z - i\omega_0) + \tilde{D}_1(z + i\omega_0)}{2z}, \quad \tilde{f}(z) = \frac{\tilde{D}_1(z - i\omega_0) - \tilde{D}_1(z + i\omega_0)}{2iz\omega_0},$$
$$\tilde{D}_1(z) = \frac{2\hbar\gamma_0\omega_p^2}{\pi}\frac{z\ln(z/\omega_p)}{z^2 - \omega_p^2}; \text{ for zero temperature}, \quad \tilde{D}_1(z) = \frac{2k_BT\gamma_0\omega_p}{z + \omega_p}; \text{ for } k_BT >> \hbar\omega_p \tag{3.19}$$

We have just done the Laplace transforms of expressions in equation 3.36 using the table 2. Please note that in the master equation approach, we have not yet separated the homogeneous and inhomogeneous parts of the solutions. This is relatively easy to do now. All the temperature-dependent part is inhomogeneous, and the rest is homogeneous. We know that temperature enters only through the noise kernel D_1. So:

$$\langle \tilde{x}^2 \rangle^{\text{homo}}(z) = \frac{2\langle p^2 \rangle_0 + Mz\langle xp + px \rangle_0 + M[z(Mz - \tilde{S}(z)) + 2(M\omega_n^2 - \tilde{C}(z))]\langle x^2 \rangle_0}{4M\omega_0^2\tilde{S}(z) + Mz^2(Mz - \tilde{S}(z)) + 4Mz(M\omega_n^2 - \tilde{C}(z))}$$
$$\langle \tilde{x}^2 \rangle^{\text{inhomo}}(z) = \frac{2\tilde{h}(z) + z\tilde{f}(z)}{4M\omega_0^2\tilde{S}(z) + Mz^2(Mz - \tilde{S}(z)) + 4Mz(M\omega_n^2 - \tilde{C}(z))} \tag{3.20}$$

We will analyse the inhomogeneous part in this section, and we will do the homogeneous part in the section 4.1. We performed the inverse Laplace transforms numerically, and the results are plotted in figures 3.1.1 and 3.1.2. The figreff6 shows the result for the zero temperature case, whereas the figure 3.1.2 shows it for the case of very high temperatures: $T = 10000$ (where $k_BT >> \hbar\omega_p$ can be assumed).

Let us try to find the asymptotic results:

1. $k_BT >> \hbar\omega_p$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{k_BT}{M\omega_0^2 z} \implies \langle x^2 \rangle_{t\to\infty} = \frac{k_BT}{M\omega_0^2}$$

2. $k_BT >> \hbar\omega_p$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to k'\frac{6k_BT}{M^2 z^5} \implies \langle x^2 \rangle_{t\to 0} = k'\frac{k_BT}{4M^2}t^4$$

3. $k_BT = 0$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{\hbar}{2M\omega_0 z} \implies \langle x^2 \rangle_{t\to\infty} = \frac{\hbar}{2M\omega_0}$$

4. $k_BT = 0$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2\hbar\omega_p^2\gamma_0}{\pi M^2 z^5}\left[3\ln(z/\omega_p) - 1\right] \implies \langle x^2 \rangle_{t\to 0} = \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7 - 4\gamma_E - 4\ln(\omega_p t)\right]$$

Let's compare this against the corresponding results that we obtained using the exact Langevin approach in the section 2.3.2; we find that the asymptotic results from both the approaches are exactly the same. In fact, figures 3.1.1 and 3.1.2 suggests that Born approximation is exact for **all times** for inhomogeneous parts in the weak coupling regime.

We must remember that all this is happening in the limit $\gamma << \omega_0 << \omega_p$. In fact, figure 3.1.1 clearly tells us the story. In the second figure, the inequality is less stricter as compared to the first figure. We can observe that curves get closer as we make the inequality stricter. The reason for this is pretty clear if we see the asymptotic expression for $\langle x^2 \rangle_t$ from the exact Langevin approach (equations 2.39 and 2.41). They have sub-leading contributions which disappears only when the inequality $\gamma << \omega_0 << \omega_p$ grows infinitely stricter.

3.1.2 Solving BME for a Free Particle

We will just replace ω_0 by 0 (now, $M\omega_n^2 = k'$) in equation 3.18:

$$\langle \tilde{x}^2 \rangle(z) = \frac{2\tilde{h}(z) + z\tilde{f}(z) + 2\langle p^2 \rangle_0 + Mz\langle xp + px \rangle_0 + M[z(Mz - \tilde{S}(z)) + 2(M\omega_n^2 - \tilde{C}(z))]\langle x^2 \rangle_0}{Mz^2(Mz - \tilde{S}(z)) + 4Mz(M\omega_n^2 - \tilde{C}(z))} \tag{3.21}$$

with

$$\tilde{C}(z) = \tilde{\Sigma}(z), \quad \tilde{S}(z) = -\frac{d\tilde{\Sigma}(z)}{dz}, \quad \tilde{\Sigma}(z) = \frac{\gamma_0\omega_p^2}{z + \omega_p}, \quad \tilde{h}(z) = \frac{\tilde{D}_1(z)}{z}, \quad \tilde{f}(z) = -\frac{1}{z}\frac{d\tilde{D}_1(z)}{dz},$$
$$\tilde{D}_1(z) = \frac{2\hbar\gamma_0\omega_p^2}{\pi}\frac{z\ln(z/\omega_p)}{z^2 - \omega_p^2};\ \text{for zero temperature}, \quad \tilde{D}_1(z) = \frac{2k_BT\gamma_0\omega_p}{z + \omega_p};\ \text{for } k_BT >> \hbar\omega_p \tag{3.22}$$

Again, we numerically perform the inverse Laplace transform of the inhomogeneous part, and it is plotted in the figure 3.1.3. Let us try to find the asymptotic results for the inhomogeneous part:

1. $k_BT >> \hbar\omega_p$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{4k_BT}{3Mz^3} \implies \langle x^2 \rangle_{t\to\infty} = \frac{2k_BT}{3M}t^2$$

2. $k_BT >> \hbar\omega_p$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to k'\frac{6k_BT}{M^2z^5} \implies \langle x^2 \rangle_{t\to 0} = k'\frac{k_BT}{4M^2}t^4$$

3. $k_B T = 0$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2\hbar}{3M\pi z^2}\left[1 - \ln(z/\omega_p)\right] \implies \langle x^2 \rangle_{t\to\infty} = \frac{2\hbar t}{3\pi M}\left[\gamma_E + \ln(\omega_p t)\right]$$

4. $k_B T = 0$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2\hbar\omega_p^2\gamma_0}{\pi M^2 z^5}\left[3\ln(z/\omega_p) - 1\right] \implies \langle x^2 \rangle_{t\to 0} = \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7 - 4\gamma_E - 4\ln(\omega_p t)\right]$$

For small times, the results match with what we obtained using the Langevin equations (section 2.3.1). But, at large times, the results are horribly wrong for **any temperature**!

For a free particle, BME works well just for very small times and not for large times. This is contrary to a popular belief that master equations can give correct results for large times and not for small times.

In the weak coupling limit, the Born approximation fails for a free particle (apart from very small times), whereas it works perfectly for a bounded particle (for all times).

We will discuss more on this in the section 4.2. The one-line answer is that for the free particle case, the inequality $\gamma << \omega_0 << \omega_p$ is violated. Satisfying this inequality is the necessary condition for the Born approximation to work.

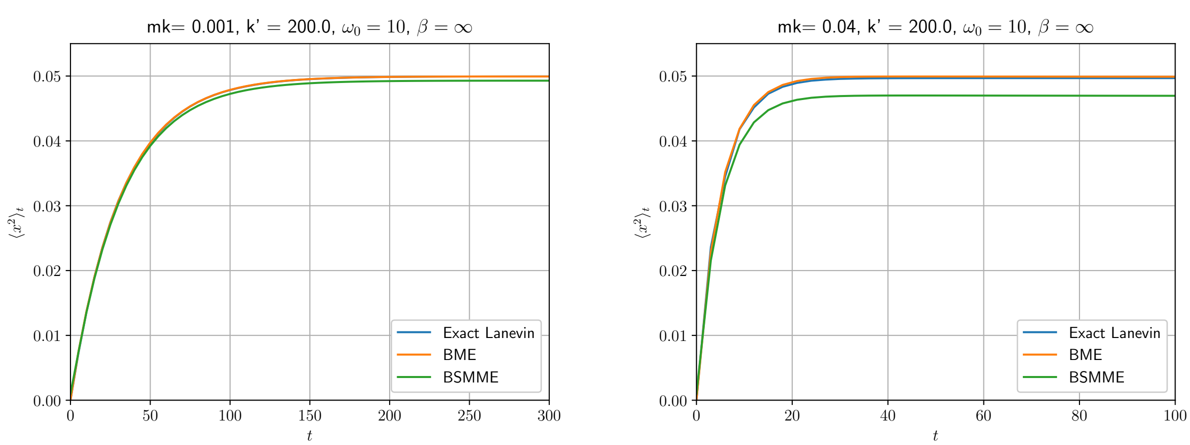


Figure 3.1.1: *Comparison of three approaches for a bounded particle at $T = 0$, but with different parameters in the limit $\gamma << \omega_0 << \omega_p$.*

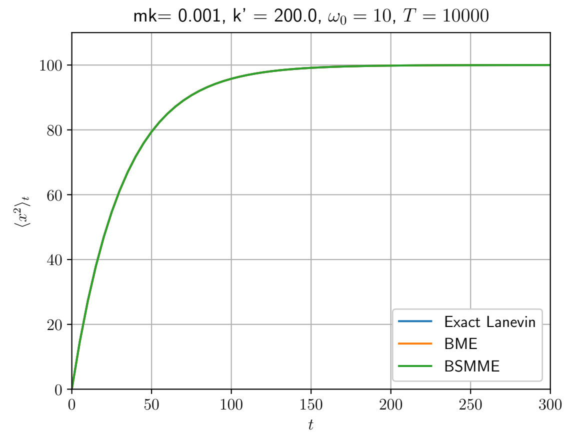


Figure 3.1.2: *Comparison of three approaches for a bounded particle in the limit $\hbar\gamma << \hbar\omega_0 << \hbar\omega_p << K_BT$.*

3.2 Born semi-Markov Master Equation (BSMME)

The Born semi-Markov master equation is obtained by doing a semi-Markov approximation on top of the Born approximation. In this section we will understand the so-called "semi-Markov" approximation. Let us recall the Born master equation 3.10:

$$\frac{d\rho_{SI}(t)}{dt} = \int_0^t dt_1 \left(\frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t_1)\}\right] - \frac{1}{2\hbar^2}D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t_1)]\right] \right) \tag{3.23}$$

semi-Markov approximation: Do $\rho_{SI}(t_1) \rightarrow \rho_{SI}(t)$ in equation 3.23 in the following two steps:

$$\frac{d\rho_{SI}(t)}{dt} \approx \int_0^t dt_1 \left(\frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t)\}\right] - \frac{1}{2\hbar^2}D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t_1)]\right] \right) \tag{3.24a}$$

$$\approx \int_0^t dt_1 \left(\frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t)\}\right] - \frac{1}{2\hbar^2}D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t)]\right] \right) \tag{3.24b}$$

The condition to transit from equation 3.23 to equation 3.24a is $\gamma << \omega_p$ and conditions to transit from equation 3.24a to equation 3.24b is $\gamma << \min\{\omega_p, \nu_1\}$, where $\nu_1 = \frac{2\pi k_B T}{\hbar}$ is the first Matsubara frequency. Note that we are not changing other t_1-dependent variables to t (like $x_I(t_1)$). We will justify this as well.

The **Born semi-Markov master equation**:

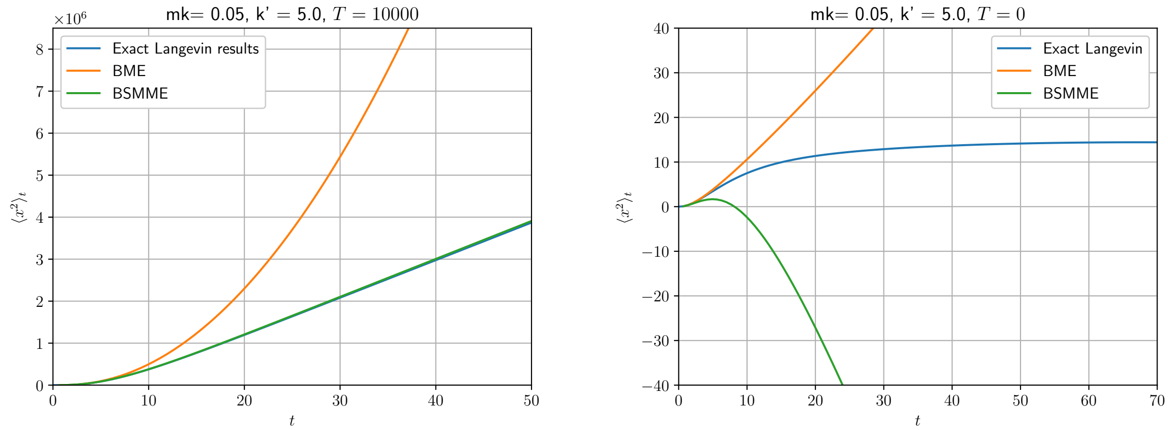


Figure 3.1.3: *Comparison of three approaches for a free particle in the limit $\hbar\gamma << \hbar\omega_p << k_B T$ and $k_B T << \hbar\gamma << \hbar\omega_p$.*

$$\frac{d\rho_{SI}(t)}{dt} = \int_0^t dt_1 \left(\frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t)\}\right] \right. \\ \left. -\frac{1}{2\hbar^2} D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t)]\right] \right) \tag{3.25}$$

3.2.1 Justifying the semi-Markov Approximation

Physical Justification

Recall section 1.3 and equations 1.14 and 1.16, in particular. The dissipation kernel $\Sigma(t)$ goes as $\omega_p^2 e^{-\omega_p t}$. As we increase ω_p, this function is going to get steeper at $t = 0$. So, in the equation 3.23, the first term will have a contribution only from $t = t_1$ as ω_p grows larger. Hence, replacing $\rho_{SI}(t_1) \to \rho_{SI}(t)$ is not really an approximation unless ρ_{SI} itself evolve with ω_p. This is not the case since the density matrix decays with a time-scale $1/\gamma$. We can say this because we have seen that the moments decay with a time-scale of $1/\gamma$ (see any $g(t)$ that we obtained in the section 2.2). Hence, until we ensure $\gamma << \omega_p$, the first step of the approximation is justified.

We need to do a similar analysis for $D_1(t) \sim \omega_p e^{-\omega_p t} + |\nu_n| e^{-|\nu_n| t}$. For $n = 0$, we just have to worry about the first exponential which has ω_p. For $n \neq 0$, the slowest frequency scale among ν_n is ν_1. So, if the slowest of ν_1 and ω_p decays faster compared to γ, the second step is also good and hence, $\gamma << \min\{\omega_p, \nu_1\}$ is required for the second step.

Let us now discuss why we did not put $x_I(t_1)$ to $x_I(t)$. Note that x_I evolves with a timescale of ω_0^{-1}, which is faster than γ^{-1}. In this approximation, we do the change only to the slowest evolving term.

This now justifies why we always focused on the limit $\gamma << \omega_0 << \omega_p$ while doing the Langevin analysis. It satisfies conditions for both the Born as well as the semi-Markov approximation.

Mathematical Justification

[4] We will try to justify the transition from equation 3.23 to equation 3.24a and further to equation 3.24b. Let us see a typical term in equation 3.23. It is of the form $x_I(t)I(t)$ with:

$$I(t) = \int_0^t dt_1 K_0(t, t_1)\rho_{SI}(t_1)$$

where $K_0(t, t_1)$ can be $\Sigma(t - t_1)\, x_I(t_1)$ (call it K_0^{Σ}) or $D_1(t - t_1)\, x_I(t_1)$ (call it K_0^{D}). Let us define a new quantity $K_1(t, t_1)$ such that

$$K_1(t, t_1) = \int_0^{t_1} dt_2 K_0(t, t_2) \implies K_0(t, t_1) = \frac{\partial}{\partial t_1} K_1(t, t_1); \quad K_1(t, 0) = 0 \tag{3.26}$$

Re-writing $I(t)$ in terms of $K_1(t, t_1)$ and then doing integration by parts, we get:

$$I(t) = \int_0^t dt_1 \left(\frac{\partial}{\partial t_1} K_1(t, t_1)\right) \rho_{SI}(t_1) = K_1(t, t)\rho_{SI}(t) - \int_0^t dt_1 K_1(t, t_1) \frac{d\rho_{SI}(t_1)}{dt_1} \tag{3.27}$$

We will repeat this process. After one more iteration, we will get:

$$K_2(t, t_1) = \int_0^{t_1} dt_2 K_1(t, t_2) \implies K_1(t, t_1) = \frac{d}{dt_1} K_2(t, t_1); \quad K_2(t, 0) = 0 \tag{3.28}$$

$$I(t) = K_1(t, t)\rho_{SI}(t) - K_2(t, t)\frac{d\rho_{SI}(t)}{dt} + \int_0^t dt_1 K_2(t, t_1) \frac{d^2\rho_{SI}(t_1)}{dt_1^2} \tag{3.29}$$

Upon multiple iterations, we get:

$$I(t) = K_1(t, t)\rho_{SI}(t) - K_2(t, t)\frac{d\rho_{SI}(t)}{dt} + K_3(t, t)\frac{d^2\rho_{SI}(t)}{dt^2} + \cdots \tag{3.30}$$

with

$$\begin{aligned} K_1(t, t) &= \int_0^t dt_1 K_0(t, t_1) \\ K_2(t, t) &= \int_0^t dt_1 \int_0^{t_1} dt_2 K_0(t, t_2) \\ K_3(t, t) &= \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 K_0(t, t_3) \\ \vdots &= \vdots \end{aligned} \tag{3.31}$$

Let us consider a specific case of a Drude bath. We have $K_0^{\Sigma}(t,t_1) \propto \Sigma(t-t_1) \sim \omega_p^2 e^{-\omega_p t}$ and $K_0^{D}(t,t_1) \propto D_1(t-t_1) \sim \omega_p e^{-\omega_p t} + |\nu_n| e^{-|\nu_n| t}$. Following the definition of K_1, we observe $K_1^{\Sigma} \sim \omega_p e^{-\omega_p t} \sim \frac{1}{\omega_p} K_0^{\Sigma}(t,t_1)$. Similarly, $K_1^{D}(t,t_1) \sim e^{-\omega_p t} + e^{-|\nu_n| t}$

So, higher orders of K gets divided by the bath frequency. As we justified in the previous section all moments and hence ρ_{SI} approximately relaxes as $e^{-\gamma t}$. So, $\frac{d^n \rho_{SI}(t)}{dt^n}$ brings a factor of γ^n. This tells us that the equation 3.30 is nothing but a series in γ/bath frequency.

For the first term of equation 3.23, the relevant bath frequency is ω_p and hence if $\gamma << \omega_p$, we can neglect the higher-order terms in equation 3.23:

$$I(t) = \int_0^t dt_1 K_0^{\Sigma}(t,t_1)\,\rho_{SI}(t_1) \approx \rho_{SI}(t) K_1^{\Sigma}(t,t) = \rho_{SI}(t) \int_0^t dt_1 \Sigma(t-t_1) x_I(t_1) \tag{3.32}$$

which justifies going from equation 3.23 to equation 3.24a. To justify the transition from equation 3.24a to equation 3.24b, we can give a similar argument. The only difference would be that now the relevant frequencies are ω_p and all ν_n ($n \neq 0$). Since this lies in the denominator, we want the smallest of them to be much larger than γ. Hence, $\gamma << \min\{\omega_p, \nu_1\}$ justifies that step.

Dynamics of Moments

From the Born semi-Markov master equation 3.24b, we can obtain the equation of motion for expectation of any system operator A using equation 3.8:

$$\begin{aligned}\frac{d\langle A\rangle_t}{dt} = \frac{i}{\hbar}\langle [H_0, A]\rangle_t + \int_0^t dt_1 \Bigg(&\frac{i}{2\hbar}\Sigma(t-t_1)\mathrm{tr}_S\left(\{[A_I(t), x_I(t)], x_I(t_1)\}\rho_{SI}(t)\right) \\ &- \frac{1}{2\hbar^2} D_1(t-t_1)\mathrm{tr}_S\left([[A_I(t), x_I(t)], x_I(t_1)]\rho_{SI}(t)\right)\Bigg)\end{aligned} \tag{3.33}$$

We now want to write $x_I(t_1)$ in terms of $x_I(t)$ and $p_I(t)$. For that, we will use the following relations which can be obtained by inverting equation 3.12:

$$\begin{aligned} x_I(t_1) &\approx x_I(t)\cos(\omega_0(t-t_1)) - \frac{p_I(t)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0} \\ p_I(t_1) &\approx p_I(t)\cos(\omega_0(t-t_1)) + M\omega_0 x_I(t)\sin(\omega_0(t-t_1)) \end{aligned} \tag{3.34}$$

Using this equations into equation 3.33. First moments:

$$\begin{aligned}\frac{d\langle x\rangle_t}{dt} = \frac{\langle p\rangle_t}{M}, \quad \frac{d\langle p\rangle_t}{dt} &= -M\omega_n^2\langle x\rangle_t + \int_0^t dt_1 \Sigma(t-t_1)\mathrm{tr}\{x_I(t_1)\rho_{SI}(t)\} \\ &= -M\omega_n^2\langle x\rangle_t + \langle x\rangle_t \int_0^t dt_1 C(t-t_1) - \frac{\langle p\rangle_t}{M}\int_0^t dt_1 S(t-t_1)\end{aligned} \tag{3.35}$$

The first line follows in an exactly similar fashion, as shown in the appendix 3.A.2. In fact, the only difference is we will have $\rho_{SI}(t)$ instead of $\rho_{SI}(t_1)$ throughout that calculation. We have just used equation 3.34 in the second line.

Second moments (refer to appendix 3.A.2):

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t - \frac{2\langle p^2\rangle_t}{M}\int_0^t d\tau S(\tau) + \langle xp+px\rangle_t\int_0^t d\tau C(\tau) + h(t) \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t - \frac{\langle xp+px\rangle_t}{M}\int_0^t d\tau S(\tau) + 2\langle x^2\rangle_t\int_0^t d\tau C(\tau) + \frac{f(t)}{M}
\end{aligned} \tag{3.36}$$

Let us now try to simplify this further. For that, we will put the explicit form of $C(t)$ and $S(t)$ (see equation 3.16) and stare at the integrals in above equations. For a Drude bath:

$$\begin{aligned}
\int_0^t d\tau C(\tau) = \gamma_0\omega_p^2\int_0^t d\tau e^{-\omega_p\tau}\cos(\omega_0\tau) &= \frac{\gamma_0\omega_p^2\left(\omega_p + e^{-\omega_p t}\left(\omega_0\sin(\omega_0 t) - \omega_p\cos(\omega_0 t)\right)\right)}{\omega_0^2+\omega_p^2} \\
\text{(putting } \omega_0 = 0\text{):} &= \gamma_0\omega_p(1-e^{-\omega_p t}) = \gamma(0)-\gamma(t) \\
\int_0^t d\tau S(\tau) = \frac{\gamma_0\omega_p^2}{\omega_0}\int_0^t d\tau e^{-\omega_p\tau}\sin(\omega_0\tau) &= \frac{\gamma_0\omega_p^2\left(\omega_0 - e^{-\omega_p t}\left(\omega_0\cos(\omega_0 t) + \omega_p\sin(\omega_0 t)\right)\right)}{\omega_0(\omega_0^2+\omega_p^2)} \\
\text{(putting } \omega_0 = 0\text{):} &= \gamma_0\left[1 - e^{-\omega_p t}\left(1+\omega_p t\right)\right]
\end{aligned} \tag{3.37}$$

For an Ohmic bath (put $\omega_p = \infty$ in the above equations and use $\lim_{\omega_p\to\infty}\omega_p e^{-\omega_p t} = \delta(t)$):

$$\begin{aligned}
&\int_0^t d\tau C(\tau) = \gamma_0\omega_p(1-e^{-\omega_p t}) = \gamma(0)-\gamma(t) \\
&\int_0^t d\tau S(\tau) = \gamma_0
\end{aligned} \tag{3.38}$$

So, in the system of equations 3.36, the coefficients are time-dependent for the case of a Drude bath. It will be a bit tedious to simplify them with these coefficients. So, we will make a mathematical approximation to make our lives simpler:

Assumption: In the limit $\omega_p >> \omega_0 >> \gamma$, we can safely use equations 3.38 instead of equations 3.37 for a Drude bath.

Motivation: In the section 2.2, we show that the form of $g(t)$ was exactly same for an Ohmic bath and for a Drude bath in the limit $\omega_p >> \omega_0 >> \gamma$. For example, compare equations 2.12 and 2.13. We will put a question mark over this assumption if our analysis gives some very absurd results.

In equation 3.36, we will do a further an approximation of replacing $\gamma(t)\langle A\rangle_t$ by $\gamma(t)\langle A\rangle_0$ in the limit of large ω_p. The motivation is that $\gamma(t)$ behaves almost like a delta function in this limit. Again, we will come back to this if our analysis gives us absurd results.

Using these approximations in equation 3.36:

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_0^2\langle xp+px\rangle_t - \frac{2\gamma_0\langle p^2\rangle_t}{M} - \gamma(t)\langle xp+px\rangle_0 + h(t) \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_0^2\langle x^2\rangle_t - \frac{\gamma_0\langle xp+px\rangle_t}{M} - 2\gamma(t)\langle x^2\rangle_0 + \frac{f(t)}{M}
\end{aligned} \tag{3.39}$$

3.2.2 Solving BSMME for a Bounded Particle

We now directly write equation 3.39 in the Laplace space:

$$\begin{aligned}
&z\langle\tilde{x}^2\rangle(z) - \langle x^2\rangle_0 = \frac{\langle xp\tilde{+}px\rangle(z)}{M} \\
&z\langle\tilde{p}^2\rangle(z) - \langle p^2\rangle_0 = -M\omega_0^2\langle xp\tilde{+}px\rangle(z) - \frac{2\gamma_0\langle\tilde{p}^2\rangle(z)}{M} - \tilde{\gamma}(z)\langle xp+px\rangle_0 + \tilde{h}(z) \\
&z\langle xp\tilde{+}px\rangle(z) - \langle xp+px\rangle_0 = \frac{2\langle\tilde{p}^2\rangle(z)}{M} - 2M\omega_0^2\langle\tilde{x}^2\rangle(z) - \frac{\gamma_0\langle xp\tilde{+}px\rangle(z)}{M} - 2\tilde{\gamma}(z)\langle x^2\rangle_0 + \frac{\tilde{f}(z)}{M}
\end{aligned} \tag{3.40}$$

It gives:

$$\begin{aligned}
\langle\tilde{x}^2\rangle(z) = &\frac{2M\tilde{h}(z) + (Mz+2\gamma_0)\tilde{f}(z) + M[2M^2\omega_0^2 + (Mz+2\gamma_0)(Mz+\gamma_0-2\tilde{\gamma}(z))]\langle x^2\rangle_0}{(Mz+\gamma_0)(4M^2\omega_0^2 + Mz(Mz+2\gamma_0))} \\
&+ \frac{M(2\langle p^2\rangle_0 + [Mz+2\gamma_0-2\tilde{\gamma}(z)]\langle xp+px\rangle_0)}{(Mz+\gamma_0)(4M^2\omega_0^2+Mz(Mz+2\gamma_0))}
\end{aligned} \tag{3.41}$$

with

$$\tilde{h}(z) = \frac{\tilde{D}_1(z-i\omega_0)+\tilde{D}_1(z+i\omega_0)}{2z}, \quad \tilde{f}(z) = \frac{\tilde{D}_1(z-i\omega_0)-\tilde{D}_1(z+i\omega_0)}{2iz\omega_0},$$
$$\tilde{D}_1(z) = \frac{2\hbar\gamma_0\omega_p^2}{\pi}\frac{z\ln(z/\omega_p)}{z^2-\omega_p^2}; \text{ for zero temperature}, \quad \tilde{D}_1(z) = \frac{2k_BT\gamma_0\omega_p}{z+\omega_p}; \text{ for } k_BT >> \hbar\omega_p$$

Once again, we can separate the homogeneous and inhomogeneous parts as we did earlier. We did the inverse Laplace transform for the inhomogeneous part numerically and plotted them in figures 3.1.1 and 3.1.2. Let us analyse the asymptotic limits of the inhomogeneous part:

1. $k_BT >> \hbar\omega_p$ and $z \to 0$:

$$\langle\tilde{x}^2\rangle(z) \to \frac{k_BT\omega_p(M\omega_p+\gamma_0)}{M^2\omega_0^2(\omega_0^2+\omega_p^2)z} \implies \langle x^2\rangle_{t\to\infty} = \frac{k_BT\omega_p(M\omega_p+\gamma_0)}{M^2\omega_0^2(\omega_0^2+\omega_p^2)} \to \frac{k_BT}{M\omega_0^2}.$$

where we have used $\omega_p >> \omega_0 >> \gamma$ in the last line.

2. $k_BT >> \hbar\omega_p$ and $z \to \infty$:

$$\langle\tilde{x}^2\rangle(z) \to k'\frac{6k_BT}{M^2z^5} \implies \langle x^2\rangle_t = k'\frac{k_BT}{4M^2}t^4 \text{ as } t \to 0$$

3. $k_BT = 0$ and $z \to 0$:

$$\langle\tilde{x}^2\rangle(z) \to \frac{\hbar\omega_p^2\left[M\pi\omega_0 + 2\gamma_0\ln\left(\frac{\omega_0}{\omega_p}\right)\right]}{2\pi M^2\omega_0^2(\omega_0^2+\omega_p^2)z} \implies \langle x^2\rangle_{t\to\infty} = \frac{\hbar\omega_p^2\left[M\pi\omega_0 + 2\gamma_0\ln\left(\frac{\omega_0}{\omega_p}\right)\right]}{2\pi M^2\omega_0^2(\omega_0^2+\omega_p^2)} \to \frac{\hbar}{2M\omega_0}$$

where we have used $\omega_p >> \omega_0 >> \gamma$ in the last line.

4. $k_BT = 0$ and $z \to \infty$:

$$\langle\tilde{x}^2\rangle(z) \to \frac{2\hbar\omega_p^2\gamma_0}{\pi M^2z^5}\left[3\ln(z/\omega_p) - 1\right] \implies \langle x^2\rangle_{t\to 0} = \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7 - 4\gamma_E - 4\ln(\omega_p t)\right]$$

All these asymptotic results match exactly with what we obtained using the exact Langevin approach in the section 2.3.2. In fact, figure 3.1.1 and 3.1.2 suggests that Born semi-Markov approximation is exact for **all temperatures** and all times for inhomogeneous parts in the weak coupling regime. This is a very surprising result since the Born semi-Markov approximation is not supposed to work for zero temperature. Remember in section 3.2.1, we justified that we need $\gamma << \min\{\omega_p, \nu_1\}$. For zero temperature case, $\nu_1 = 0$ and the inequality is totally ruined. We will learn the reason behind this in the section 5.2.1. In one line, we can say that as far as the second moments are concerned, ν_1 time-scale is nearly irrelevant for making a semi-Markov approximation.

> For a bounded particle, the Born semi-Markov approximation is exact in the limit $\gamma << \omega_0 << \omega_p$, i.e. it predicts correct results for all time and for **all temperatures**.

This also justifies that our assumption of using equation 3.38 instead of equation 3.37 and replacing $\gamma(t)\langle A\rangle_t$ by $\gamma(t)\langle A\rangle_0$ was harmless.

3.2.3 A Word of Caution about the Ohmic Bath

You might ask that if the goal was to simplify the system of equations 3.36 easy, then why didn't we use the Ohmic bath only? Why did we bother to do all those approximations for the Drude approach?

The answer is that the Ohmic bath is pathological. Look at the asymptotic form of $\langle x^2 \rangle_{t\to\infty}$ for zero temperatures (bulletin 3): The subleading term is $-\gamma_0 \ln(\omega_p)/\omega_0^2$. For the Drude case, as the inequality $\gamma << \omega_0 << \omega_p$ grows stricter, this term becomes insignificant. However, for the Ohmic case, this term is diverging logarithmically and is no longer subleading. Also, This divergence happens to $-\infty$ (also reported in [4]). This is very unphysical as $\langle x^2 \rangle$ is a positive operator. Obviously, this is a limitation of the Born semi-Markov approximation. The exact results don't give such divergence to $-\infty$ even for an Ohmic bath (it has a term $-\ln(\omega_p)/\omega_p^2$, see equation 2.32). This also means that the subleading terms predicted by the Born semi-Markov approximation are incorrect. Hence, the approximation is valid only when the weak coupling inequality is very strict.

Divergence to ∞ is nothing new for Ohmic baths. Even from exact results, we will see that $\langle p^2 \rangle_{t\to\infty}$ diverges to ∞ for any kind of trap ([5]). This divergence stems from the zero-point energy of the high-energy modes of an Ohmic bath. To escape such pathological problems, we use a Drude bath with a large cutoff which can act as a Markovian bath but is free of pathologies.

3.2.4 Solving BSMME for a Free Particle

We just need to replace ω_0 by 0 (now, $M\omega_n^2 = k'$) in equation 3.41:

$$\langle \tilde{x}^2 \rangle(z) = \frac{2M\tilde{h}(z) + (Mz + 2\gamma_0)\tilde{f}(z)}{Mz(Mz+\gamma_0)(Mz+2\gamma_0)} + \frac{2\langle p^2\rangle_0 + [Mz + 2\gamma_0 - 2\tilde{\gamma}(z)]\langle xp+px\rangle_0 + [(Mz+2\gamma_0)(Mz+\gamma_0 - 2\tilde{\gamma}(z))]\langle x^2\rangle_0}{z(Mz+\gamma_0)(Mz+2\gamma_0)} \tag{3.42}$$

with

$$\tilde{h}(z) = \frac{\tilde{D}_1(z)}{z}, \quad \tilde{f}(z) = -\frac{1}{z}\frac{d\tilde{D}_1(z)}{dz}, \quad \tilde{D}_1(z) = \frac{2\hbar\gamma_0\omega_p^2}{\pi}\frac{z\ln(z/\omega_p)}{z^2-\omega_p^2}; \text{ for zero temperature}$$

$$\tilde{D}_1(z) = \frac{2k_BT\gamma_0\omega_p}{z+\omega_p}; \text{ for } k_BT >> \hbar\omega_p$$

We did the inverse Laplace transforms of the inhomogeneous part numerically and plotted in the figure 3.1.3 for zero temperature and $T = 10000$ (where $k_BT >> \hbar\omega_p$ is valid). Let us find the asymptotic results of the inhomogeneous part:

1. $k_BT >> \hbar\omega_p$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2(\gamma_0 + M\omega_p)k_BT}{M\omega_p\gamma_0 z^2} - \frac{k_BT(3M^2\omega_p^2 + 4M\omega_p\gamma_0 + 4\gamma_0^2)}{M\omega_p^2\gamma_0^2 z} \implies$$
$$\langle x^2 \rangle_{t\to\infty} = \frac{2(\gamma_0 + M\omega_p)k_BT}{M\omega_p\gamma_0}t - \frac{k_BT(3M^2\omega_p^2 + 4M\omega_p\gamma_0 + 4\gamma_0^2)}{M\omega_p^2\gamma_0^2} \to \frac{2k_BT}{\gamma_0}t - \frac{3k_BT}{4M\gamma^2}$$

   where we have used the inequality $\omega_p >> \omega_0 >> \gamma$ in the last line.

2. $k_BT >> \hbar\omega_p$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to k' \frac{6k_BT}{M^2 z^5} \implies \langle x^2 \rangle_{t\to 0} = k' \frac{k_BT}{4M^2}t^4$$

3. $k_BT = 0$ and $z \to 0$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2\hbar}{M\pi z^2}\left[1 + \ln(z/\omega_p)\right] \implies \langle x^2 \rangle_{t\to\infty} = \frac{2\hbar t}{M\pi}\left[2 - \gamma_E - \ln(\omega_p t)\right]$$

4. $k_BT = 0$ and $z \to \infty$:

$$\langle \tilde{x}^2 \rangle(z) \to \frac{2\hbar\omega_p^2\gamma_0}{\pi M^2 z^5}\left[3\ln(z/\omega_p) - 1\right] \implies \langle x^2 \rangle_{t\to 0} = \frac{\hbar\omega_p^2\gamma_0 t^4}{16\pi M^2}\left[7 - 4\gamma_E - 4\ln(\omega_p t)\right]$$

For the limit $k_BT >> \hbar\omega_p$, the leading term and even the subleading term are the same as the exact Langevin results (equation 2.24). In fact, the figure 3.1.3 suggests that this is true for all times. Now, this is very surprising as the BME gave horribly wrong results, but doing a semi-Markov approximation on top of it made it give correct answers. We will discuss more about it in the next chapter.

For the zero temperature case, it agrees with the Langevin results for small times (see equation 2.35). But, for large times, it goes horribly wrong. It predicts $-t$ indicating the violation of positive semi-definiteness.

For a free particle, the BME predicts correct behaviour only for very small times in the limit $\gamma << \omega_p$ (irrespective of the temperature).
The BSMME (which is one approximation on top of BME) is exact in the limit $\hbar\gamma << \hbar\omega_p << k_BT$, i.e. it predicts correct results for **all times** (not just small times).
However, for the zero temperature case, BSMME predicts the correct answer only for very small times. For long times, it violates the positivity deviating from both the exact results as well as the BME results.

3.3 Born Markov Master Equation (BMME)

Markov Approximation: On top of the semi-Markov approximation we did, we also put the upper limit of integrals to infinity, i.e. in equation 3.24b, make the upper limit of integral $t \to \infty$. This gives us the **Born-Markov master equation**:

$$\boxed{\begin{aligned} \frac{d\rho_{SI}(t)}{dt} = \int_0^\infty dt_1 \Bigg(& \frac{i}{2\hbar}\Sigma(t-t_1)\left[x_I(t), \{x_I(t_1), \rho_{SI}(t)\}\right] \\ & -\frac{1}{2\hbar^2} D_1(t-t_1)\left[x_I(t), [x_I(t_1), \rho_{SI}(t)]\right]\Bigg) \end{aligned} \qquad (3.43)}$$

This is what we see in the literature as a Markovian approximation[3].

Justification: Since the kernels $\Sigma(t-t_1)$ is dirac-delta type in the limit $\gamma << \omega_0 << \omega_p$, the only significant contribution in the integral is from $t = t_1$ and the additional integral from t to ∞ will not have any significant contribution.

Let us try to solve our problem using this approach and try to seek the reason why we proposed the semi-Markov approximation. Dynamics of second moments will still be governed by equation 3.36 with a slight change:

$$\begin{aligned} \frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\ \frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t - \frac{2\langle p^2\rangle_t}{M}\int_0^\infty d\tau S(\tau) + \langle xp+px\rangle_t \int_0^\infty d\tau C(\tau) + h(t) \\ \frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t - \frac{\langle xp+px\rangle_t}{M}\int_0^\infty d\tau S(\tau) + 2\langle x^2\rangle_t \int_0^\infty d\tau C(\tau) + \frac{f(t)}{M} \end{aligned} \qquad (3.44)$$

Now, the simplification of the integrals will also be simpler (put $t \to \infty$ in equation 3.37):

$$\begin{aligned} \int_0^\infty d\tau C(\tau) &= \gamma_0\omega_p^2 \int_0^\infty d\tau e^{-\omega_p \tau}\cos(\omega_0\tau) = \frac{\gamma_0\omega_p^3}{\omega_0^2+\omega_p^2} \\ &\text{(putting } \omega_0 = 0\text{): } = \gamma_0\omega_p = \gamma(0) \\ \int_0^\infty d\tau S(\tau) &= \frac{\gamma_0\omega_p^2}{\omega_0^2}\int_0^\infty d\tau e^{-\omega_p\tau}\sin(\omega_0\tau) = \frac{\gamma_0\omega_p^2}{(\omega_0^2+\omega_p^2)} \\ &\text{(putting } \omega_0 = 0\text{): } = \gamma_0 \end{aligned} \qquad (3.45)$$

[3] It is usually done to bring it closer to the Lindblad form of the master equation. If you don't perform $t \to \infty$, the master equation will not follow something called the property of "dynamical semigroup", which is a must for the Lindblad master equation.

We got the time-independent coefficients straightaway for a Drude bath. But, compare equation 3.45 to equation 3.38, which we used in the case of the semi-Markov approximation. We see that equation 3.45 don't have $-\gamma(t)$ term in $\int d\tau C(\tau)$. So, now which one is correct? - We will show that the semi-Markov scheme we proposed here is more appropriate than the traditional Markov approximation.

3.3.1 semi-Markov vs Markov Approximation

Let us compare equations governing dynamics of first moments from exact Langevin, BMME and BSMME approaches. For this illustration, we will stick to a very simple Ohmic bath.

Exact Langevin Approach

We need to recall the Langevin equation for a bounded particle (equation 2.8). If we take trace of that equation with respect to the initial system state, we get:

$$\begin{aligned}
\langle \dot{x} \rangle_t = \frac{\langle p \rangle_t}{M}, \quad \langle \dot{p} \rangle_t &= -M\omega_n^2 \langle x \rangle_t + \int_0^t dt_1 \langle x \rangle_{t_1} \Sigma(t - t_1) \\
&= -M\omega_n^2 \langle x \rangle_t - \int_0^t d\tau \langle x \rangle_{t-\tau} \dot{\gamma}(\tau) \\
&= -M\omega_n^2 \langle x \rangle_t - \left(\gamma(\tau) \langle x \rangle_{t-\tau} \big|_0^t + 2\gamma_0 \int_0^t d\tau \langle \dot{x} \rangle_{t-\tau} \delta(\tau) \right) \\
&= -M\omega_0^2 \langle x \rangle_t - 2\gamma_0 \delta(t) \langle x \rangle_0 - \frac{\gamma_0 \langle p \rangle_t}{M}
\end{aligned} \tag{3.46}$$

where we have used $\gamma(\tau) = 2\gamma_0 \delta(\tau)$ for the Ohmic bath.

BSMME Approach

Refer to equation 3.35 and use results for Ohmic bath (equation 3.38):

$$\frac{d\langle x \rangle_t}{dt} = \frac{\langle p \rangle_t}{M}, \quad \frac{d\langle p \rangle_t}{dt} = -M\omega_0^2 \langle x \rangle_t - 2\gamma_0 \delta(t) \langle x \rangle_0 - \frac{\gamma_0 \langle p \rangle_t}{M} \tag{3.47}$$

This is exactly the same as what we obtained from the Langevin approach. This is expected since we are in the limit $\gamma << \omega_0 << \omega_p$, where BSMME is exact.

BMME Approach

We still need to use equation 3.35, but with the upper limit of integral being ∞:

$$\begin{aligned}\frac{d\langle x\rangle_t}{dt} = \frac{\langle p\rangle_t}{M}, \quad \frac{d\langle p\rangle_t}{dt} &= -M\omega_n^2\langle x\rangle_t + \langle x\rangle_t\int_0^\infty d\tau C(\tau) - \frac{\langle p\rangle_t}{M}\int_0^\infty d\tau S(\tau) \\ &= -M\omega_0^2\langle x\rangle_t - \frac{\gamma_0\langle p\rangle_t}{M}\end{aligned} \tag{3.48}$$

So, BMME misses the boundary terms proportional to $\gamma(t)$. This leads to incorrect predictions of the homogeneous parts in transients. As we have seen earlier, this problem is persistent even for higher moments. The Born semi-Markov theme formulated here fixes this problem for all the moments.

Problem: What is the problem with the Markov approximation, and what about the justification that we gave earlier in favour of the Markov approximation?

Resolution: We think that making the upper limit of integral in equation 3.24b is not appropriate. If we look at the master equation 3.24b, we find that the argument t is present in the integrand as well. In the Markov approximation, we partially replace t to ∞. If we also replace t inside the integrand with ∞, we will get an equation for the steady-state.

The problem with justification is that in the limit $\gamma << \omega_p$, the dissipation kernel behaves like a delta function, but it is not exactly a delta function. Actually, it is $\sim \frac{d}{dt}\delta(t)$. So, if we do integration by parts and write Σ kernel in terms of the damping kernel $\gamma(t)$ (which $\sim \delta(t)$ in the limit $\gamma << \omega_p$), we will get a crucial boundary term. The Markov approximation misses this term.

Appendix

3.A Detailed Calculations

3.A.1 Born Master Equation

In this appendix, we will justify equations 3.14 and 3.15 given equation 3.13. Let us re-write equation 3.13:

$$\frac{d\langle A\rangle_t}{dt} = \frac{i}{\hbar}\langle[H_0, A]\rangle_t + \int_0^t dt_1 \Bigg(\frac{i}{2\hbar}\Sigma(t-t_1)\mathrm{tr}_S\left(\{[A_I(t), x_I(t)], x_I(t_1)\}\rho_{SI}(t_1)\right) \\ - \frac{1}{2\hbar^2}D_1(t-t_1)\mathrm{tr}_S\left([[A_I(t), x_I(t)], x_I(t_1)]\rho_{SI}(t_1)\right)\Bigg) \tag{3.49}$$

Recall $H_0 = \frac{p^2}{2M} + \frac{1}{2}M\omega_n^2 x^2$. To proceed, We will need all the basic commutation relations:

$$[p,x] = -i\hbar, \quad \{x,p\} = 2xp - i\hbar, \quad [p^2, x] = -2i\hbar p, \quad [x^2, p] = 2i\hbar x, \quad [xp+px, x] = -2i\hbar x \\ [x^2, p^2] = 2i\hbar(xp+px), \quad [x^2, xp+px] = 4i\hbar x^2, \quad [p^2, xp+px] = -4i\hbar p^2 \tag{3.50}$$

Now, we just have to plug various operators in equation 3.49 and use equation 3.50. For first moments:

$$\frac{d\langle x\rangle_t}{dt} = \frac{i}{\hbar}\langle[H_0, x]\rangle_t = \frac{\langle p\rangle_t}{M} \\ \frac{d\langle p\rangle_t}{dt} = \frac{i}{\hbar}\langle[H_0, p]\rangle_t + \int_0^t dt_1 \Bigg(\frac{i}{2\hbar}\Sigma(t-t_1)\mathrm{tr}_S\left(\{[p_I(t), x_I(t)], x_I(t_1)\}\rho_{SI}(t_1)\right) \\ - \frac{1}{2\hbar^2}D_1(t-t_1)\mathrm{tr}_S\left([[p_I(t), x_I(t)], x_I(t_1)]\rho_{SI}(t_1)\right)\Bigg) \\ = -M\omega_n^2\langle x\rangle_t + \int_0^t dt_1 \Sigma(t-t_1)\langle x\rangle_{t_1} \tag{3.51}$$

The dissipative part does not contribute for $x(t)$ since $[x, x] = 0$. Using the same logic:

$$\frac{d\langle x^2\rangle_t}{dt} = \frac{i}{\hbar}\langle[H_0, x^2]\rangle_t = \frac{\langle xp + px\rangle_t}{M} \tag{3.52}$$

Among $\langle p^2\rangle_t$ and $\langle xp + px\rangle_t$, we will only do $\langle p^2\rangle_t$. The other is exactly similar.

$$\begin{aligned}
\frac{d\langle p^2\rangle_t}{dt} &= \frac{i}{\hbar}\langle[H_0, p^2]\rangle_t + \int_0^t dt_1\Bigg(\frac{i}{2\hbar}\Sigma(t-t_1)\mathrm{tr}_S\left(\{[p_I^2(t), x_I(t)], x_I(t_1)\}\rho_{SI}(t_1)\right) \\
&\qquad - \frac{1}{2\hbar^2}D_1(t-t_1)\mathrm{tr}_S\left([[p_I^2(t), x_I(t)], x_I(t_1)]\rho_{SI}(t_1)\right)\Bigg) \\
&= -M\omega_n^2\langle xp + px\rangle_t + \int_0^t dt_1\Bigg(\Sigma(t-t_1)\mathrm{tr}_S\left(\{p_I(t), x_I(t_1)\}\rho_{SI}(t_1)\right) \\
&\qquad + \frac{i}{\hbar}D_1(t-t_1)\mathrm{tr}_S\left([p_I(t), x_I(t_1)]\rho_{SI}(t_1)\right)\Bigg)
\end{aligned} \tag{3.53}$$

At this point, we need to write $x_I(t)$ in terms of operators at time t_1 using equation 3.12:

$$\begin{aligned}
x_I(t) &\approx x_I(t_1)\cos(\omega_0(t-t_1)) + \frac{p_I(t_1)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0} \\
p_I(t) &\approx p_I(t_1)\cos(\omega_0(t-t_1)) - M\omega_0 x_I(t_1)\sin(\omega_0(t-t_1))
\end{aligned} \tag{3.54}$$

Using them:

$$\begin{aligned}
\frac{d\langle p^2\rangle_t}{dt} &= \int_0^t dt_1\Sigma(t-t_1)\left(\cos(\omega_0(t-t_1))\langle xp + px\rangle_{t_1} - 2M\omega_0^2\frac{\sin(\omega_0(t-t_1))}{\omega_0}\langle x^2\rangle_{t_1}\right) \\
&\quad + \int_0^t dt_1\left[D_1(t-t_1)\cos(\omega_0(t-t_1))\right] - M\omega_n^2\langle xp + px\rangle_t \\
&= -M\omega_n^2\langle xp + px\rangle_t + \int_0^t dt_1\left[C(t-t_1)\langle xp + px\rangle_{t_1} - 2M\omega_0^2 S(t-t_1)\langle x^2\rangle_{t_1}\right] + h(t)
\end{aligned} \tag{3.55}$$

This is what we were looking for. Let us briefly discuss about deriving equation 5.20, which is an expression to find $\frac{d\langle p^3\rangle_t}{dt}$ using the BME. We will now need the following commutation relation:

$$[p^3, x] = -3i\hbar p^2, \quad [x^2, p^3] = 2i\hbar(xp^2 + pxp + p^2x) = 3i\hbar(p^2x + xp^2) \tag{3.56}$$

Doing a similar exercise starting from equation 3.49 as we did above, we obtain:

$$\begin{aligned}
\frac{d\langle p^3\rangle_t}{dt} &= -\frac{3M\omega_n^2}{2}\langle xp^2 + p^2x\rangle_t + \frac{3}{2}\int_0^t dt_1\Bigg(\Sigma(t-t_1)\mathrm{tr}_S\left(\{p_I^2(t), x_I(t_1)\}\rho_{SI}(t_1)\right) \\
&\qquad + \frac{i}{\hbar}D_1(t-t_1)\mathrm{tr}_S\left([p_I^2(t), x_I(t_1)]\rho_{SI}(t_1)\right)\Bigg)
\end{aligned} \tag{3.57}$$

We now need to use

$$
\begin{aligned}
p_I^2(t) \approx p_I^2(t_1)\cos^2(\omega_0(t-t_1)) + M^2\omega_0^2 x_I^2(t_1)\sin^2(\omega_0(t-t_1)) \\
- M\omega_0 \sin(\omega_0(t-t_1))\cos(\omega_0(t-t_1))[p_I x_I + x_I p_I](t_1)
\end{aligned}
\tag{3.58}
$$

Using this and simplifying all commutations, we finally get equation 5.20.

3.A.2 Born semi-Markov Master Equation

We will try to get equation 3.36 using equations 3.33 and 3.34. The derivations is along the exact similar lines as the previous appendix. Nothing changes for $\frac{d\langle x^2\rangle_t}{dt}$ and it has same expression. It will change for $\langle p^2\rangle_t$ and $\langle xp+px\rangle_t$. Here, we will just show it for $\langle p^2\rangle_t$, the other has a very similar derivation.

We will start from equation 3.53 with $\rho_{SI}(t_1)$ replaced by $\rho_{SI}(t)$:

$$
\begin{aligned}
\frac{d\langle p^2\rangle_t}{dt} = -M\omega_n^2\langle xp+px\rangle_t + \int_0^t dt_1 \Bigg(\Sigma(t-t_1)\mathrm{tr}_S\left(\{p_I(t), x_I(t_1)\}\rho_{SI}(t)\right) \\
+ \frac{i}{\hbar} D_1(t-t_1)\mathrm{tr}_S\left([p_I(t), x_I(t_1)]\rho_{SI}(t)\right) \Bigg)
\end{aligned}
\tag{3.59}
$$

Instead of using equation 3.12, we will here use equation 3.34 to write operators at time t_1 in terms of operators at time t. In particular:

$$
\begin{aligned}
x_I(t_1) &\approx x_I(t)\cos(\omega_0(t-t_1)) - \frac{p_I(t)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0} \\
p_I(t_1) &\approx p_I(t)\cos(\omega_0(t-t_1)) + M\omega_0 x_I(t)\sin(\omega_0(t-t_1))
\end{aligned}
\tag{3.60}
$$

Using this:

$$
\begin{aligned}
\frac{d\langle p^2\rangle_t}{dt} = \langle xp+px\rangle_t \int_0^t dt_1 \Sigma(t-t_1)\cos(\omega_0(t-t_1)) - \frac{2\langle p^2\rangle_t}{M}\int_0^t dt_1 \Sigma(t-t_1)\frac{\sin(\omega_0(t-t_1))}{\omega_0} \\
+ \int_0^t dt_1 \left[\cos(\omega_0(t-t_1))D_1(t-t_1)\right] - M\omega_n^2\langle xp+px\rangle_t
\end{aligned}
\tag{3.61}
$$

This is same as equation 3.36. Let us try to look at the expression of $\frac{d\langle p^3\rangle_t}{dt}$ using this scheme. If we do the entire exercise for p^3, we will get an equation similar to equation 3.57 with $\rho_{SI}(t)$ instead of $\rho_{SI}(t_1)$:

$$\frac{d\langle p^3\rangle_t}{dt} = -\frac{3M\omega_n^2}{2}\langle xp^2 + p^2x\rangle_t + \frac{3}{2}\int_0^t dt_1 \Bigg(\Sigma(t-t_1)\mathrm{tr}_S\left(\{p_I^2(t), x_I(t_1)\}\rho_{SI}(t)\right) + \frac{i}{\hbar}D_1(t-t_1)\mathrm{tr}_S\left([p_I^2(t), x_I(t_1)]\rho_{SI}(t)\right)\Bigg) \tag{3.62}$$

We just need to write operators at time t_1 in terms of operators at time t using same equations 3.12 and simplify to get:

$$\begin{aligned}\frac{d\langle p^3\rangle_t}{dt} &= -\frac{3M\omega_n^2}{2}\langle\{p^2, x\}\rangle_t + 3\langle p\rangle_t h(t) \\ &\quad + \frac{3\langle\{p^2, x\}\rangle_t}{2}\int_0^t dt_1 C(t-t_1) - \frac{3\langle p^3\rangle_t}{M}\int_0^t dt_1 S(t-t_1)\end{aligned} \tag{3.63}$$

Chapter 4

Comparisons between Both Approaches

In this chapter, we will try to compare the analysis that we did in the previous two chapters. The comparison of homogeneous parts is due, and we will do that in this chapter. The comparison of inhomogeneous parts and their conclusions are mostly presented in the previous chapter. However, we will do some more calculations to understand them and summarise them. So, let us first start by comparing homogeneous parts.

4.1 Comparing the Homogeneous Parts

We will again observe $\langle x^2\rangle_t$ for comparisons. Let us recall the homogeneous part of $\langle x^2\rangle_t$ that we separated out from all three approaches. The homogeneous parts of $\langle x^2\rangle_t$ (recall equations 2.19, 3.20 and 3.41):

$$\begin{aligned}
&\text{Langevin}: \ \langle x^2\rangle_t = \dot{g}^2(t)\langle x^2\rangle_0 + \frac{g^2(t)}{M^2}\langle p^2\rangle_0 + \frac{\dot{g}(t)g(t)}{M}\langle xp+px\rangle_0 \\
&\text{BME}: \ \langle \tilde{x}^2\rangle(z) = \frac{2\langle p^2\rangle_0 + Mz\langle xp+px\rangle_0 + M[z(Mz-\tilde{S}(z)) + 2(M\omega_n^2 - \tilde{C}(z))]\langle x^2\rangle_0}{4M\omega_0^2\tilde{S}(z) + Mz^2(Mz-\tilde{S}(z)) + 4Mz(M\omega_n^2-\tilde{C}(z))} \\
&\text{BSMME}: \ \langle \tilde{x}^2\rangle(z) = \frac{2\langle p^2\rangle_0 + [Mz+2\gamma_0-2\tilde{\gamma}(z)]\langle xp+px\rangle_0}{(Mz+\gamma_0)(4M\omega_0^2+z(Mz+2\gamma_0))} \\
&\qquad\qquad + \frac{[2M^2\omega_0^2 + (Mz+2\gamma_0)(Mz+\gamma_0-2\tilde{\gamma}(z))]\langle x^2\rangle_0}{(Mz+\gamma_0)(4M\omega_0^2+z(Mz+2\gamma_0))}
\end{aligned} \tag{4.1}$$

We will take some arbitrary initial conditions. For the master equation case, we again will do the inverse Laplace transforms numerically. For the Langevin case, we just need corresponding

$g(t)$. We have plotted all of them in figure 4.1.1 for a bounded particle. Figures 4.1.2 and 4.1.3 shows corresponding figures for a free particle with different parameters. Let us summarise the conclusions:

- All three approaches agree for all times for the case of a bounded particle.
- For the case of a free particle, exact results and BME results disagree heavily. But, BSMME results, which we obtained by doing a semi-Markov approximation on top of BME, agree with the exact results. This behaviour is the same as what we saw even for the inhomogeneous part in the previous chapter.
- Let us say that t^* is the time at which Born results start deviating from exact results. We wanted to check if t^* increases upon making the inequality $\gamma << \omega_p$ stricter. So, we studied the free particle case for a different set of parameters in figures 4.1.2 and 4.1.3.
- It seems like t^* doesn't depend on the strictness of the inequality. For example, increasing k' while keeping other parameters constant doesn't change t^* (figures 4.1.2 and 4.1.3). If we change γ_0, then t^* will change since we are changing the relaxation rate. But, it has nothing to do with the strictness of inequality.

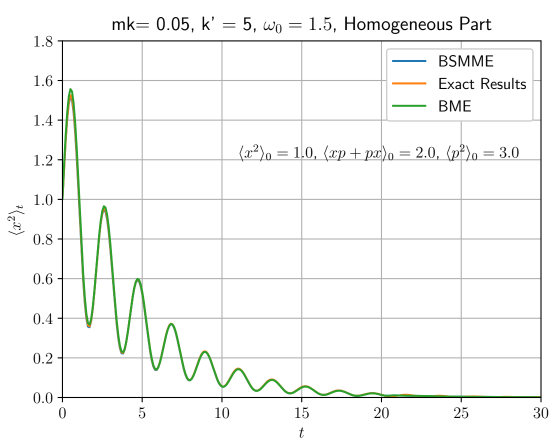


Figure 4.1.1: *Comparison of homogeneous part of $\langle x^2\rangle_t$ from different approaches for a bounded particle in the limit $\gamma << \omega_0 << \omega_p$.*

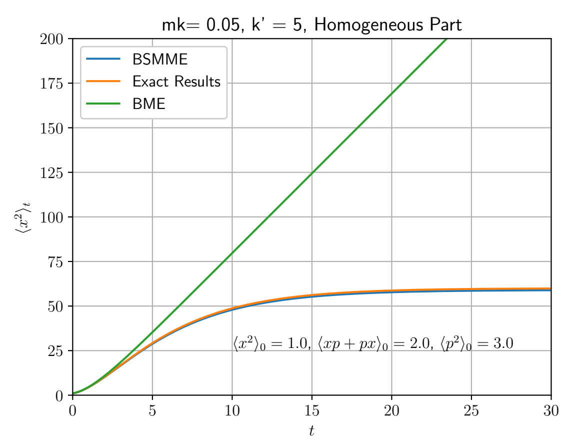


Figure 4.1.2: *Comparison of homogeneous part of $\langle x^2\rangle_t$ from different approaches for a free particle in the limit $\gamma << \omega_p$.*

There are two puzzles that we are carrying from the previous chapter:

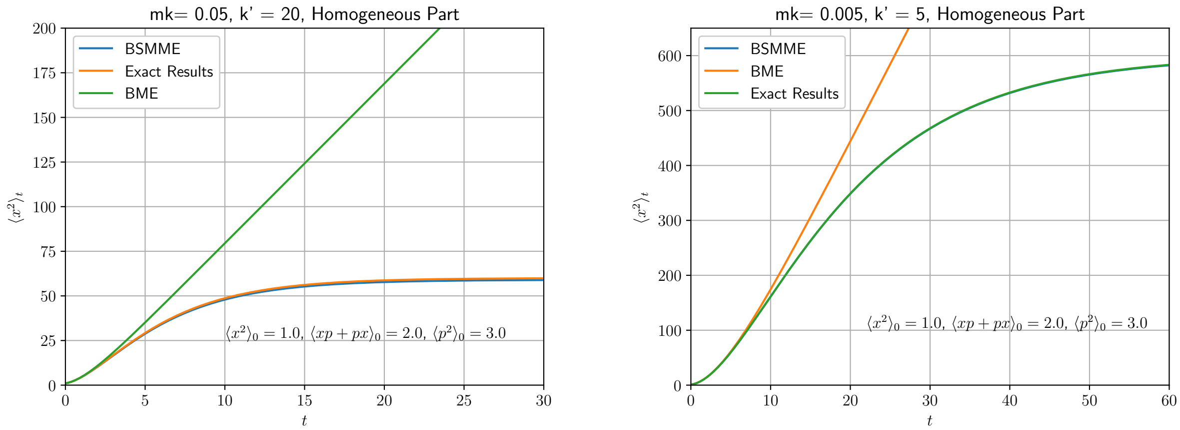


Figure 4.1.3: *Comparison of homogeneous part of* $\langle x^2 \rangle_t$ *from different approaches for a free particle with different parameters in the limit* $\gamma << \omega_0 << \omega_p$.

1. Why does BME work fine for a Bounded particle but doesn't work for a free particle?

2. Why does BSMME work for a free particle but BME doesn't, given that BSMME has one extra approximation on top of BME? This kind of "correction" is seen only in the $k_B T >> \hbar\omega_p$ limit. For the zero temperature case, all three approaches deviate. Why?

Answering the second question above will also explain our conclusions about homogeneous parts.

4.2 Free Particle Limit of a Bounded Particle

One answer to the first question above is that a free particle case violates the inequality $\gamma << \omega_0 << \omega_p$. And so, the hypothesis is that the BME works only if the inequality $\gamma << \omega_0 << \omega_p$ is satisfied. Let us test this hypothesis by studying a bounded particle in the limit $\omega_0 << \gamma << \omega_p$. We call it a "free particle limit" since the trap frequency ω_0 is the smallest energy scale. Putting $\omega_0 = 0$ will actually give us the free particle.

4.2.1 Langevin Equation Approach

Equation 2.37 will still be our starting point:

$$\langle x^2 \rangle_t = \frac{2\gamma\hbar\omega_p^2}{\pi M} \int_0^\infty d\omega \frac{\omega}{\omega^2 + \omega_p^2} \coth\left(\frac{\hbar\beta\omega}{2}\right) f(\omega, t) \tag{4.2}$$

We will now use the $g(t)$ corresponding to this limit. We found it in the equation 2.12:

$$g(t) = \frac{2\gamma \left(e^{-2\gamma t} - e^{-(\omega_0^2/2\gamma)t} \right)}{\omega_0^2 - (2\gamma)^2}$$

Using this $g(t)$ will yield some complicated $f(\omega, t)$. Using this $f(\omega, t)$, we can find exact numerical results. These results are plotted in figures 4.2.1 and 4.2.2. Let us try to see the long-time results analytically. We will write $f(\omega, t)$ in this limit:

$$f(\omega, t \to \infty) \approx \frac{4\gamma^2(\omega_0^4 - 8\gamma^2\omega_0^2 + 16\gamma^4)}{(\omega_0^2 - 4\gamma^2)^2(\omega^2 + 4\gamma^2)(\omega_0^4 + 4\gamma^2\omega^2)} \tag{4.3}$$

Putting this into the equation 4.2 and doing the integral:

1. $\langle x^2 \rangle \to \frac{k_B T}{M\omega_0^2}$ (same as weak coupling) for $k_B T >> \hbar\omega_p$.
2. $\langle x^2 \rangle \to \frac{\hbar}{M\pi\gamma} \ln\left(\frac{2\gamma}{\omega_0}\right)$ (not same as weak coupling) for $k_B T = 0$.

The figure 4.2.3 shows the numerical behaviour for small times. It is compared against the results obtained using the master equation approach.

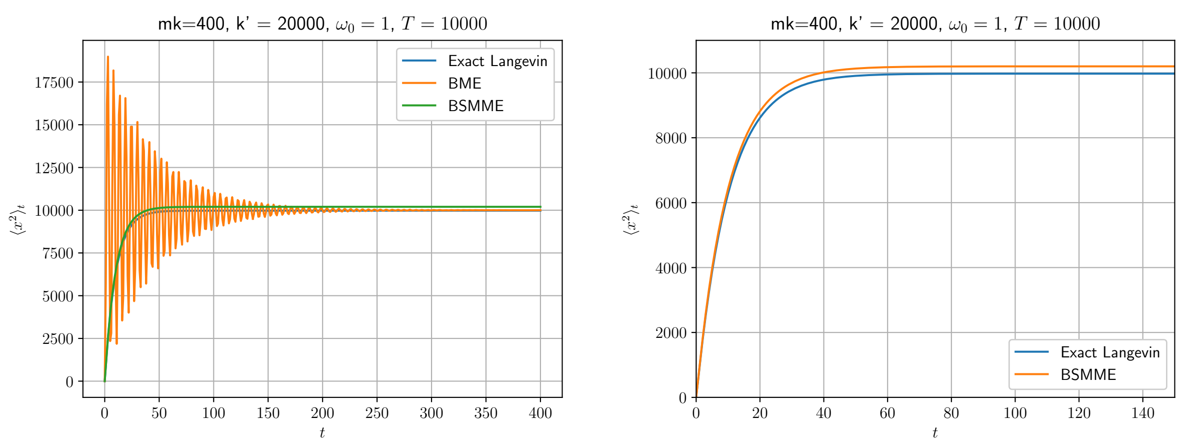


Figure 4.2.1: *Comparison of inhomogeneous part of $\langle x^2 \rangle_t$ from different approaches for a bounded particle in the limit $\hbar\omega_0 << \hbar\gamma << \hbar\omega_p << k_B T$.*

4.2.2 Master Equation Approach

In the master equation approach, the results remain the same. We still need to find the inverse Laplace transform of equations 3.18 and 3.41, but with parameters that satisfy the inequality $\omega_0 << \gamma << \omega_p$. These are plotted in figures 4.2.1, 4.2.2 and 4.2.3.

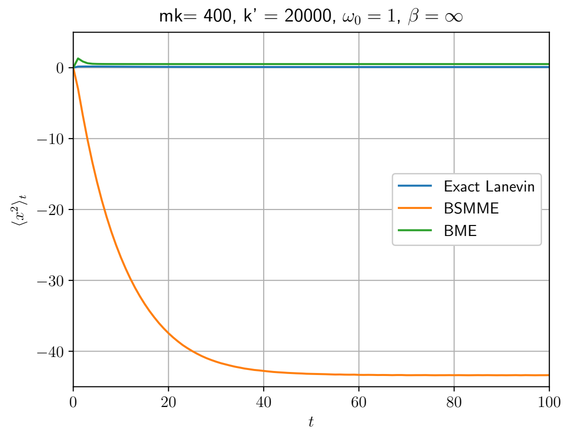


Figure 4.2.2: *Comparison of the inhomogeneous part of $\langle x^2 \rangle_t$ from different approaches for a bounded particle in the limit $k_BT << \hbar\omega_0 << \hbar\gamma << \hbar\omega_p$.*

Let us list down our observations from these comparisons:

1. For the limit $k_BT >> \hbar\omega_p$, BSMME and exact approaches match for all times (figure 4.2.1). They might seem a bit different at large times. But, as we increase ω_p, they will grow closer.

2. Since the BSMME at small times still goes as $k'\frac{k_BT}{4}t^4$, we can conclude that even Langevin results goes as $k'\frac{k_BT}{4}t^4$ for small times (see figure 4.2.3).

3. BME agrees to the other two only for very small (figure 4.2.3) and very large times. Intermediary transients from BME are significantly different (figure 4.2.1). In the limit $\omega_0 \to 0$, the oscillations from BME will not saturate to $\frac{K_BT}{M\omega_0^2}$ and hence for the free particle case, it can only correctly predict small-time results.

4. For zero temperature, three approaches just disagree for all times. For very small times (figure 4.2.3), BME and BSMME agree (expected), but it is different from the exact results (it is still of the form $[a + b\ln(t)]t^4$). Saturation results are different in all three approaches, and BSMME again seems to violate positive semi-definiteness.

- The BME is highly sensitive to the inequality $\gamma << \omega_0$, so much so that it fails for the free particle case (where $\omega_0 = 0$).

- The BSSME is not sensitive to the inequality $\gamma << \omega_0$ if the inequality $\hbar\omega_p << k_BT$ is ensured. Otherwise, it will agree to exact results only in the limit $\gamma << \omega_0$.

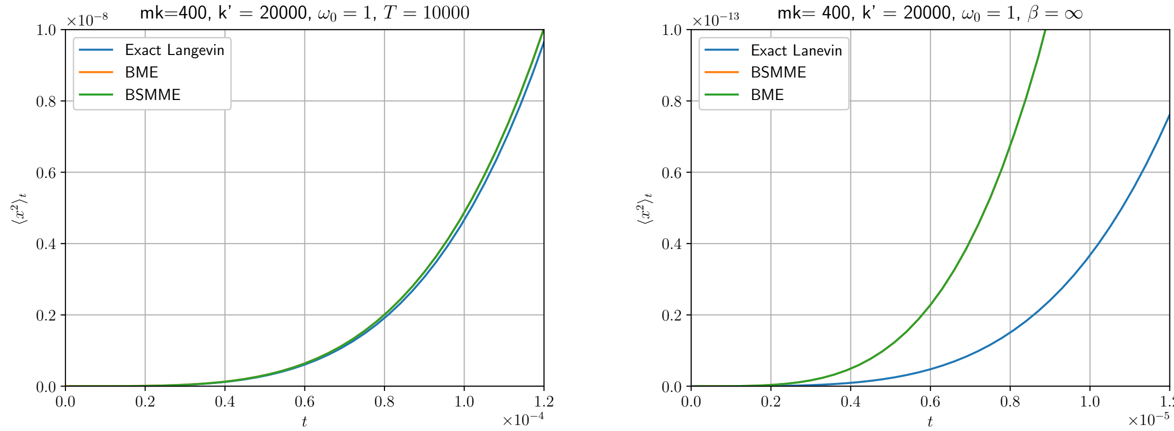


Figure 4.2.3: *Comparison of inhomogeneous part of $\langle x^2 \rangle_t$ from different approaches for a bounded particle as $t \to 0$ in the limit $k_BT << \hbar\omega_0 << \hbar\gamma << \hbar\omega_p$ and $\hbar\omega_0 << \hbar\gamma << \hbar\omega_p << k_BT$.*

Let us also compare the homogeneous parts in this limit. We still need to use equation 4.1 to find the homogeneous parts using various approaches. We use parameters and $g(t)$ corresponding to this limit. The results are shown in the figure 4.2.4. The comparison shows that all three approaches

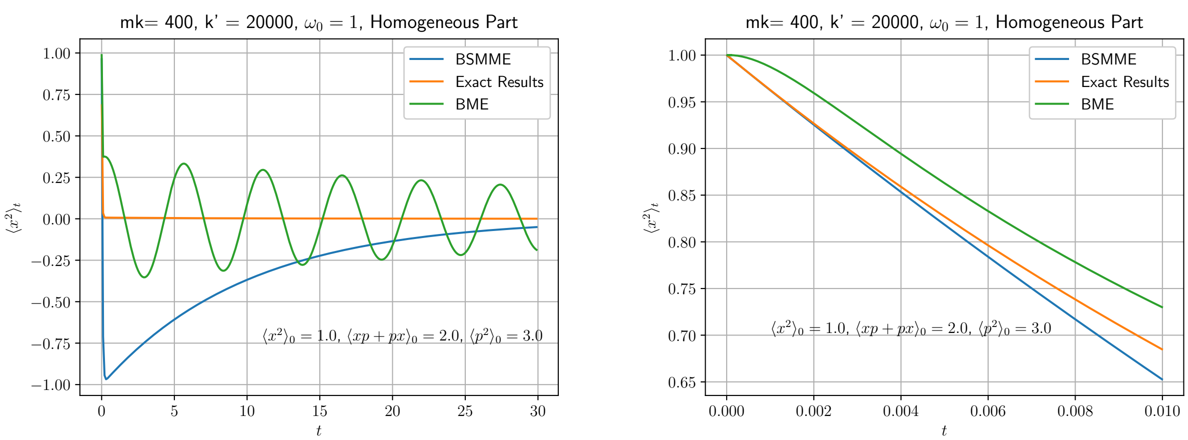


Figure 4.2.4: *Comparison of homogeneous part of $\langle x^2 \rangle_t$ from different approaches for a bounded particle in the limit $\hbar\omega_0 << \hbar\gamma << \hbar\omega_p$.*

disagree for transients. However, it will dampen out to zero for all approaches since it is a trap. So, at very large time, all of them will agree. But, this will not happen for a free particle. The other figure shows the behaviour at very small times. Here, BSMME agrees with Langevin for very small times. However, BME disagrees with both BSMME and exact Langevin at small times.

4.3 Comparing BME and BSMME using the Ohmic Bath

Let us do an interesting study. When justifying the Markov approximation, i.e. going from equation 3.23 to equation 3.24b, we argued that since the kernels peak around $t = t_1$ and hence replacing $\rho_{SI}(t_1)$ with $\rho_{SI}(t)$ is not really an approximation. Now, we know that for an Ohmic bath and the high-temperature limit, both the kernels $\Sigma(t)$ and $D_1(t)$ are fully Markovian (see section 1.3.3) and hence going from equation 3.23 to 3.24a should have no approximation involved. In this limit, we expect results from BME and BSMME to be exactly the same, right? - Let us check.

4.3.1 BME using the Ohmic bath

After doing the Born approximation, we obtained the following system of equations (equation 3.15):

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}\\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t + \underbrace{\int_0^t dt_1\left[C(t-t_1)\langle xp+px\rangle_{t_1} - 2M\omega_0^2 S(t-t_1)\langle x^2\rangle_{t_1}\right]}_{I(t)} + h(t)\\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t + \int_0^t dt_1\left[2C(t-t_1)\langle x^2\rangle_{t_1} + S(t-t_1)\frac{\langle xp+px\rangle_{t_1}}{M}\right] + \frac{f(t)}{M}
\end{aligned} \tag{4.4}$$

Let us now simplify this for an Ohmic bath. We will put $\Sigma(t) = -\frac{d\gamma(t)}{dt} = -2\gamma_0\frac{d\delta(t)}{dt}$ directly here. Let us focus only on terms that depend on $\Sigma(t)$. For instance, the term denoted by $I(t)$ above. We write $C(t)$ and $S(t)$ in terms of $\Sigma(t)$ and do a variable change $\tau = t - t_1$:

$$\begin{aligned}
I(t) &= \int_0^t d\tau\Sigma(\tau)\left[\cos(\omega_0\tau)\langle xp+px\rangle_{t-\tau} - 2M\omega_0\sin(\omega_0\tau)\langle x^2\rangle_{t-\tau}\right]\\
&= -\int_0^t d\tau\frac{d\gamma(\tau)}{d\tau}\left[\cos(\omega_0\tau)\langle xp+px\rangle_{t-\tau} - 2M\omega_0\sin(\omega_0\tau)\langle x^2\rangle_{t-\tau}\right]\\
&= -\left[\gamma(\tau)\left(\cos(\omega_0\tau)\langle xp+px\rangle_{t-\tau} - 2M\omega_0\sin(\omega_0\tau)\langle x^2\rangle_{t-\tau}\right)\right]_0^t\\
&\quad + \int_0^t d\tau\gamma(\tau)\Bigg[\omega_0\sin(\omega_0\tau)\left(2M\frac{d\langle x^2\rangle_{t-\tau}}{d(t-\tau)} - \langle xp+px\rangle_{t-\tau}\right)\\
&\qquad\qquad - \cos(\omega_0\tau)\left(\frac{d\langle xp+px\rangle_{t-\tau}}{d(t-\tau)} + 2M\omega_0^2\langle x^2\rangle_{t-\tau}\right)\Bigg]\\
&= k'\langle xp+px\rangle_t - 2\gamma_0\delta(t)\langle xp+px\rangle_0 - \gamma_0\left[2M\omega_0^2\langle x^2\rangle_t + \frac{d\langle xp+px\rangle_t}{dt}\right]
\end{aligned} \tag{4.5}$$

Substituting this $I(t)$ back in second eqation of 4.4, we get:

$$\frac{d\langle p^2\rangle_t}{dt} = -M\omega_0^2\langle xp+px\rangle_t - 2\gamma_0\delta(t)\langle xp+px\rangle_0 - \gamma_0\left[2M\omega_0^2\langle x^2\rangle_t + \frac{d\langle xp+px\rangle_t}{dt}\right] + h(t) \tag{4.6}$$

Similarly, we can simplify the third equation of 4.4:

$$\frac{d\langle xp+px\rangle_t}{dt} = \frac{2\langle p^2\rangle_t}{M} - 2M\omega_0^2\langle x^2\rangle_t - \frac{\gamma_0}{M}\langle xp+px\rangle_t - 4\gamma_0\delta(t)\langle x^2\rangle_0 + \frac{f(t)}{M} \tag{4.7}$$

Plugging equation 4.7 into equation 4.6, we get the final set of differential equations:

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M} \\
\frac{d\langle p^2\rangle_t}{dt} &= M\left(\frac{\gamma_0^2}{M^2} - \omega_0^2\right)\langle xp+px\rangle_t - \frac{2\gamma_0}{M}\langle p^2\rangle_t + h(t) \\
&\qquad - \gamma_0\frac{f(t)}{M} - 2\gamma_0\delta(t)\langle xp+px\rangle_0 + 4\gamma_0^2\delta(t)\langle x^2\rangle_0 \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_0^2\langle x^2\rangle_t - \frac{\gamma_0}{M}\langle xp+px\rangle_t - 4\gamma_0\delta(t)\langle x^2\rangle_0 + \frac{f(t)}{M}
\end{aligned} \tag{4.8}$$

4.3.2 BSMME using the Ohmic Bath

We had equations 3.36 after doing the Born semi-Markov approximation. Let us use equations 3.38 to simplify them:

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_0^2\langle xp+px\rangle_t - \frac{2\gamma_0\langle p^2\rangle_t}{M} - 2\gamma_0\delta(t)\langle xp+px\rangle_0 + h(t) \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_0^2\langle x^2\rangle_t - \gamma_0\frac{\langle xp+px\rangle_t}{M} - 4\gamma_0\delta(t)\langle x^2\rangle_0 + \frac{f(t)}{M}
\end{aligned} \tag{4.9}$$

Recall that $f(t) \sim \int_0^t dt_1 \sin(\omega_0 t_1) D_1(t_1)$. For high temperature and the Ohmic bath, $D_1(t) \sim \delta(t)$ and hence $f(t) = 0$ in this limit.

When substitute it in equations 4.8 and 4.9 and then compare them, they do not match! For a bounded particle, we may even assume that $\omega_0 >> \frac{\gamma_0}{M}$ (weak coupling) and put $\frac{\gamma_0^2}{M^2} - \omega_0^2 \sim -\omega_0^2$. After doing this, two set of differential equations still differ by a boundary term.

In the case of a free particle, the difference is much more stark as we can't employ $\omega_0 >> \frac{\gamma_0}{M}$. This extra term brings a very non-trivial difference in results predicted by BME and BSMME. This analysis suggests further that the results predicted by BME and BSMME can be significantly different for the case of a free particle.

Employing Markovian kernels (Ohmic bath and high temperatures) to the BME is not equivalent to the BSMME.

Chapter 5

Born-Markov Approximations in the Langevin Approach

In this chapter, we will formulate a prescription to perform the Born and semi-Markov approximation in the Langevin formalism. This will help us understand the nature of these approximations better. In particular, we will get the answer to why the Born semi-Markov approximation worked at zero temperatures.

For complicated systems, it is very hard to study the dynamics of the exact different-time correlation functions of the system. We often use the Markovian master equation to study them using something called as the "quantum regression theorem". Now, the quantum regression theorem has its own set of difficulties in its application. For example, we can't apply it to non-Markovian master equations. A formulation of Born and Markov approximation in the Langevin formalism can help study these correlations easily.

We start by recalling the Langevin equation 2.5 for the case of a bounded particle (use equation 2.7):

$$M\ddot{x}(t) + M\omega_n^2 x(t) = \int_0^t dt_1 x(t_1)\Sigma(t-t_1) + \eta(t) = B(t) \tag{5.1}$$

where

$$\Sigma(t) = \sum_s \frac{C_s^2}{\Omega_s}\sin(\Omega_s t), \quad \eta(t) = \sum_s C_s\sqrt{\frac{\hbar}{2\Omega_s}}(e^{i\Omega_s t}b_s^\dagger + e^{-i\Omega_s t}b_s) \tag{5.2}$$

We can multiply $\rho_S(0)$ above and then take the trace over the system to obtain:

$$M\langle\dot{x}\rangle_t = \langle p\rangle_t, \quad \langle\dot{p}\rangle_t + M\omega_n^2\langle x\rangle_t - \int_0^t dt_1\Sigma(t-t_1)\langle x\rangle_{t_1} = 0 \tag{5.3}$$

Remember that we just wrote Heisenberg's equation of motion to obtain the Langevin equation. In the same spirit, let us write the Heisenberg's equation for second moments (recall Hamiltonian 1.2):

$$
\begin{aligned}
\dot{x}^2(t) &= \frac{i}{\hbar}[H(t), x^2(t)] = \frac{i}{\hbar}[H_S(t), x^2(t)] = \frac{x(t)p(t)+p(t)x(t)}{M}, \\
\dot{p}^2(t) &= \frac{i}{\hbar}[H(t), p^2(t)] = \frac{i}{2\hbar}[M\omega_n^2 x^2(t), p^2(t)] - \frac{i}{\hbar}[x(t)B(t), p^2(t)] \\
&\qquad\qquad = -M\omega_n^2(x(t)p(t)+p(t)x(t)) + (p(t)B(t)+B(t)p(t)) \\
\frac{d[xp+px](t)}{dt} &= \frac{i}{\hbar}[H(t), (xp+px)(t)] = \frac{i}{\hbar}[H_S(t), (xp+px)(t)] - \frac{i}{\hbar}[x(t)B(t), (xp+px)(t)] \\
&\qquad\qquad = \frac{2p^2(t)}{M} - 2M\omega_n^2 x^2(t) + (x(t)B(t)+B(t)x(t))
\end{aligned}
\tag{5.4}
$$

Here, $B(t)$ is defined in equation 5.1. We have also used the fact that $[x(t), B(t)] = 0 = [p(t), B(t)]$. This is very easy to prove using the following argument: At $t = 0$, $[x(0), X_s(0)] = 0$ (they lie in different Hilbert spaces). Now evolve this commutator using the full propagator $U = e^{-iHt}$ to immediately see $[x(t), X_s(t)] = 0 \implies [x(t), B(t)] = 0$, where we have used the fact that $B(t) = \sum_s C_s X_s(t)$ (equation 2.7). But, if we explicitly write $X_s(t)$ using equation 2.4, it becomes a non-trivial statement:

$$
\boxed{[x(t), X_s(t)] = 0 \implies \int_0^t dt_1 [x(t), x(t_1)] \sin[\Omega_s(t-t_1)] = 0, \ \forall s \tag{5.5}}
$$

This is a non-trivial identity that can be used in the future.

5.1 Born Approximation

Let us now formulate the Born approximation. Equations 5.4 are the exact differential equations from the Langevin approach. We will apply the Born approximation to it. We will start by solving for $x(t)$ order by order in k' from the exact QLE (equation 5.1):

$$
M\ddot{x}(t) + M\omega_0^2 x(t) + k'x(t) = \int_0^t dt_1 x(t_1)\Sigma(t-t_1) + \eta(t) = B(t) \tag{5.6}
$$

Please note from the definition of $\eta(t)$ and $\Sigma(t)$ (equation 1.10) that we can write $B(t) = B^{(1)}(t) + B^{(2)}(t)$ with

$$
B^{(1)}(t) = \eta(t) \sim \mathcal{O}(k'), \quad B^{(2)}(t) = \int_0^t dt_1 x(t_1)\Sigma(t-t_1) \sim \mathcal{O}(k'^2) \tag{5.7}
$$

Keeping this in mind, the Langevin equation to different orders:

$$\begin{aligned}
&M\ddot{x}^{(0)}(t) + M\omega_0^2 x^{(0)}(t) = 0 \;\cdots\; \text{upto } \mathcal{O}(k') = 0. \\
&M\ddot{x}^{(1)}(t) + M\omega_0^2 x^{(1)}(t) = \eta(t) - k'x^{(0)}(t) \;\cdots\; \text{upto } \mathcal{O}(k') = 1. \\
&M\ddot{x}^{(2)}(t) + M\omega_0^2 x^{(2)}(t) = \int_0^t dt_1 x^{(0)}(t_1)\Sigma(t-t_1) - k'x^{(1)}(t) \;\cdots\; \text{upto } \mathcal{O}(k') = 2.
\end{aligned} \tag{5.8}$$

Solving them is easy. The first equation is the standard equation of motion for an oscillator, and hence the solutions are

$$x^{(0)}(t) = x(0)\cos(\omega_0 t) + \frac{p(0)}{M}\frac{\sin(\omega_0 t)}{\omega_0}, \quad p^{(0)}(t) = p(0)\cos(\omega_0 t) - M\omega_0 x(0)\sin(\omega_0 t) \tag{5.9}$$

The second and third equations are inhomogeneous differential equations. Now, we know the fact that

$$\mathcal{L}_t(x(t)) = f(t) \implies x(t) = \int_0^\infty dt_1 g^+(t-t_1)f(t_1) \text{ such that } \mathcal{L}_t(g^+(t)) = \delta(t) \tag{5.10}$$

For our case:

$$\mathcal{L}_t = M\left[\frac{d^2}{dt^2} + \omega_0^2\right] \implies g^+(t) = \frac{\sin(\omega_0 t)}{M\omega_0}\theta(t) \tag{5.11}$$

So, the solutions to next order differential equation are:

$$\begin{aligned}
x^{(1)}(t) &= \frac{1}{M\omega_0}\int_0^t dt_1 \sin(\omega_0(t-t_1))[\eta(t_1) - k'x^{(0)}(t_1)] \\
p^{(1)}(t) &= \int_0^t dt_1 \cos(\omega_0(t-t_1))[\eta(t_1) - k'x^{(0)}(t_1)] \\
x^{(2)}(t) &= \frac{1}{M\omega_0}\int_0^t dt_1 \sin(\omega_0(t-t_1))\left[\int_0^{t_1} dt_2 \left(\Sigma(t_1-t_2)x^0(t_2)\right) - k'x^{(1)}(t_1)\right] \\
p^{(2)}(t) &= \int_0^t dt_1 \cos(\omega_0(t-t_1))\left[\int_0^{t_1} dt_2 \left(\Sigma(t_1-t_2)x^0(t_2)\right) - k'x^{(1)}(t_1)\right]
\end{aligned} \tag{5.12}$$

We will now use these expressions of $x(t)$ and $p(t)$ to truncate equations 5.4 to the second order in the system-bath coupling. We will also make sure that we don't kill any system-system correlations. Remember that we only killed the system-bath correlations even in the master equation formalism.

So, let us try the first moments (equation 5.1): it has $B(t)$, which is just bath term and has no system bath correlations and so we will keep it as it is. First moments:

$$\langle \dot{x} \rangle_t = \frac{\langle p \rangle_t}{M}, \quad \langle \dot{p} \rangle_t = -M\omega_n^2 \langle x \rangle_t + \int_0^t dt_1 \langle x \rangle_{t_1} \Sigma(t-t_1) \tag{5.13}$$

We can check that this matches with the BME result that we obtained in the equation 3.14. Let us now turn to the second moments.

Note that $B^{(2)}(t)$ is not strictly up to the second order. It has $x(t)$, which has terms of all the orders. Ideally, we should write $x^{(0)}(t)$ instead of $x(t)$. But, as we shall see that doing this will end up killing higher-order system-system correlations.

For the second moments we will do the following truncation:

$$\begin{aligned}
x(t)B(t) &\approx [x^{(0)}(t) + x^{(1)}(t)]B^{(1)}(t) + x^{(0)}B^{(2)}(t) \\
p(t)B(t) &\approx [p^{(0)}(t) + p^{(1)}(t)]B^{(1)}(t) + p^{(0)}B^{(2)}(t)
\end{aligned} \tag{5.14}$$

Note that if we had truncated $x(t)$ inside $B(t)$, it would have also killed the higher-order $x - x$ and $x - p$ correlations in the above equations.

Since we finally want to work with moments, let us take the expectation of $x(t)B(t) + B(t)x(t)$ and $p(t)B(t) + B(t)p(t)$ and truncate it as prescribed above (see appendix 5.A.1):

$$\begin{aligned}
\langle xB + Bx\rangle_t \approx& \frac{1}{M}\int_0^t dt_1 \frac{\sin(\omega_0(t-t_1))}{\omega_0} D_1(t-t_1) \\
&+ \int_0^t dt_1 \Sigma(t-t_1)\left[2\langle x^2\rangle_{t_1}\cos(\omega_0(t-t_1)) + \frac{\langle xp+px\rangle_{t_1}}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0}\right], \\
\langle pB + Bp\rangle_t \approx& \int_0^t dt_1 \cos(\omega_0(t-t_1)) D_1(t-t_1) \\
&+ \int_0^t dt_1 \Sigma(t-t_1)\left[\langle xp+px\rangle_{t_1}\cos(\omega_0(t-t_1)) - 2M\omega_0^2\langle x^2\rangle_{t_1}\frac{\sin(\omega_0(t-t_1))}{\omega_0}\right].
\end{aligned} \tag{5.15}$$

Using this, finally equation 5.4 becomes:

$$\begin{aligned}
\frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\
\frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t + \int_0^t dt_1\left[C(t-t_1)\langle xp+px\rangle_{t_1} - 2M\omega_0^2 S(t-t_1)\langle x^2\rangle_{t_1}\right] + h(t), \\
\frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t + \int_0^t dt_1\left[2C(t-t_1)\langle x^2\rangle_{t_1} + S(t-t_1)\frac{\langle xp+px\rangle_{t_1}}{M}\right] + \frac{f(t)}{M}
\end{aligned} \tag{5.16}$$

with

$$\begin{aligned}
&C(t) = \Sigma(t)\cos(\omega_0 t), \quad S(t) = \Sigma(t)\frac{\sin(\omega_0 t)}{\omega_0} \\
&h(t) = \int_0^t d\tau \cos(\omega_0\tau) D_1(\tau), \quad f(t) = \int_0^t d\tau \frac{\sin(\omega_0\tau)}{\omega_0} D_1(\tau)
\end{aligned}$$

This is exactly the same as the equation 3.15 which we obtained from the Born ME approach.

5.2 semi-Markov Approximation

This approximation is exactly the same as what we did in the master equation approach. The only difference would be that in the master equation approach, we did it on the master equation. Here, we will do it on the differential equation governing the dynamics of various moments.

Let $\langle A\rangle_t$ is the expectation value of any system operator. Then, it can be written as $\langle A\rangle_t = \text{tr}(A_I(t_1)\rho_{SI}(t_1))$ in the interaction picture.

semi-Markov approximation: $\text{tr}(A_I(t_1)\rho_{SI}(t_1)) \to \text{tr}(A_I(t_1)\rho_{SI}(t))$ for any system operator A.

Intuitively, we might think that this has to work since it is exactly same as what we do in the master equation approach. But, let us show it explicitly for the first and second moments. We will need the following transformation (equation 3.34):

$$\begin{aligned} x_I(t_1) &= x_I(t)\cos(\omega_0(t-t_1)) - \frac{p_I(t)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0}, \\ p_I(t_1) &= p_I(t)\cos(\omega_0(t-t_1)) + M\omega_0 x_I(t)\sin(\omega_0(t-t_1)) \end{aligned} \tag{5.17}$$

First Moments: Do $\text{tr}(A_I(t_1)\rho_{SI}(t_1)) \to \text{tr}(A_I(t_1)\rho_{SI}(t))$ on the RHS of equation 5.13 (which we obtained after doing the Born approximation) and then use equation 5.17 to finally get (refer to appendix 5.A.2):

$$\langle \dot{x}\rangle_t = \frac{\langle p\rangle_t}{M}, \quad \langle \dot{p}\rangle_t = -M\omega_n^2\langle x\rangle_t + \langle x\rangle_t\int_0^t dt_1 C(t-t_1) - \frac{\langle p\rangle_t}{M}\int_0^t dt_1 S(t-t_1) \tag{5.18}$$

Second Moments: Do $\text{tr}(A_I(t_1)\rho_{SI}(t_1)) \to \text{tr}(A_I(t_1)\rho_{SI}(t))$ on the RHS of equation 5.16 and then use equation 5.17 to finally get (refer to appendix 5.A.2):

$$\begin{aligned} \frac{d\langle x^2\rangle_t}{dt} &= \frac{\langle xp+px\rangle_t}{M}, \\ \frac{d\langle p^2\rangle_t}{dt} &= -M\omega_n^2\langle xp+px\rangle_t + \langle xp+px\rangle_t\int_0^t d\tau C(\tau) - \frac{2\langle p^2\rangle_t}{M}\int_0^t d\tau S(\tau) + h(t) \\ \frac{d\langle xp+px\rangle_t}{dt} &= \frac{2\langle p^2\rangle_t}{M} - 2M\omega_n^2\langle x^2\rangle_t + 2\langle x^2\rangle_t\int_0^t d\tau C(\tau) - \frac{\langle xp+px\rangle_t}{M}\int_0^t d\tau S(\tau) + \frac{f(t)}{M} \end{aligned} \tag{5.19}$$

Both first and second moments are exactly similar to what we obtained from the BSMME (see equations 3.35 and 3.36).

5.2.1 Why BSMME Worked for Zero Temperatures?

To understand it, we will need to seek a justification of changing $\rho_{SI}(t_1) \to \rho_{SI}(t)$. The argument is along the same lines as we did in the master equation case in the section 3.2.1. If we closely look at equations on which we performed the semi-Markov approximation, i.e. equation 5.16, we find that typical terms on which we did the semi-Markov approximation are of the form:

$$\int_0^t dt_1 C(t-t_1)\langle A\rangle_{t_1} \text{ and } \int_0^t dt_1 S(t-t_1)\langle A\rangle_{t_1}$$

Both $C(t)$ and $S(t)$ has only the dissipation kernel $\Sigma(t)$, which has a frequency scale of ω_p associated with it. So, justifying the approximation in a way similar to section 3.2.1 will require us to ensure $\gamma << \omega_p$. We will not be required to ensure the other condition $\gamma << \nu_1$, which we needed while doing this approximation on the master equation. ν_1 was the temperature-dependent timescale that we required in the comparison. This explains why BSMME could explain the correct dynamics of the second moments even for zero temperature for the case of a bounded particle.

Temperature-dependent timescale is not relevant for the first two moments. However, we will be required to satisfy that inequality ($\gamma << \nu_1$) for higher moments. For example, we will check $\langle p^3\rangle_t$.

From BME: Use the equation 3.13 to obtain (see appendix 3.A.1):

$$\begin{aligned}\frac{d\langle p^3\rangle_t}{dt} = &-\frac{3M\omega_n^2}{2}\langle\{x,p^2\}\rangle_t \\ &+3\int_0^t dt_1 D_1(t-t_1)\left[\cos^2(\omega_0(t-t_1))\langle p\rangle_{t_1} - \frac{M\omega_0\sin(2\omega_0(t-t_1))}{2}\langle x\rangle_{t_1}\right] \\ &+\frac{3}{2}\int_0^t dt_1\Sigma(t-t_1)\Bigg[\cos^2(\omega_0(t-t_1))\langle\{x,p^2\}\rangle_{t_1} + 2\left(M\omega_0\sin(\omega_0(t-t_1))\right)^2\langle x^3\rangle_{t_1} \\ &\qquad - \frac{M\omega_0\sin(2\omega_0(t-t_1))}{2}\langle x^2p+2xpx+px^2\rangle_{t_1}\Bigg]\end{aligned} \tag{5.20}$$

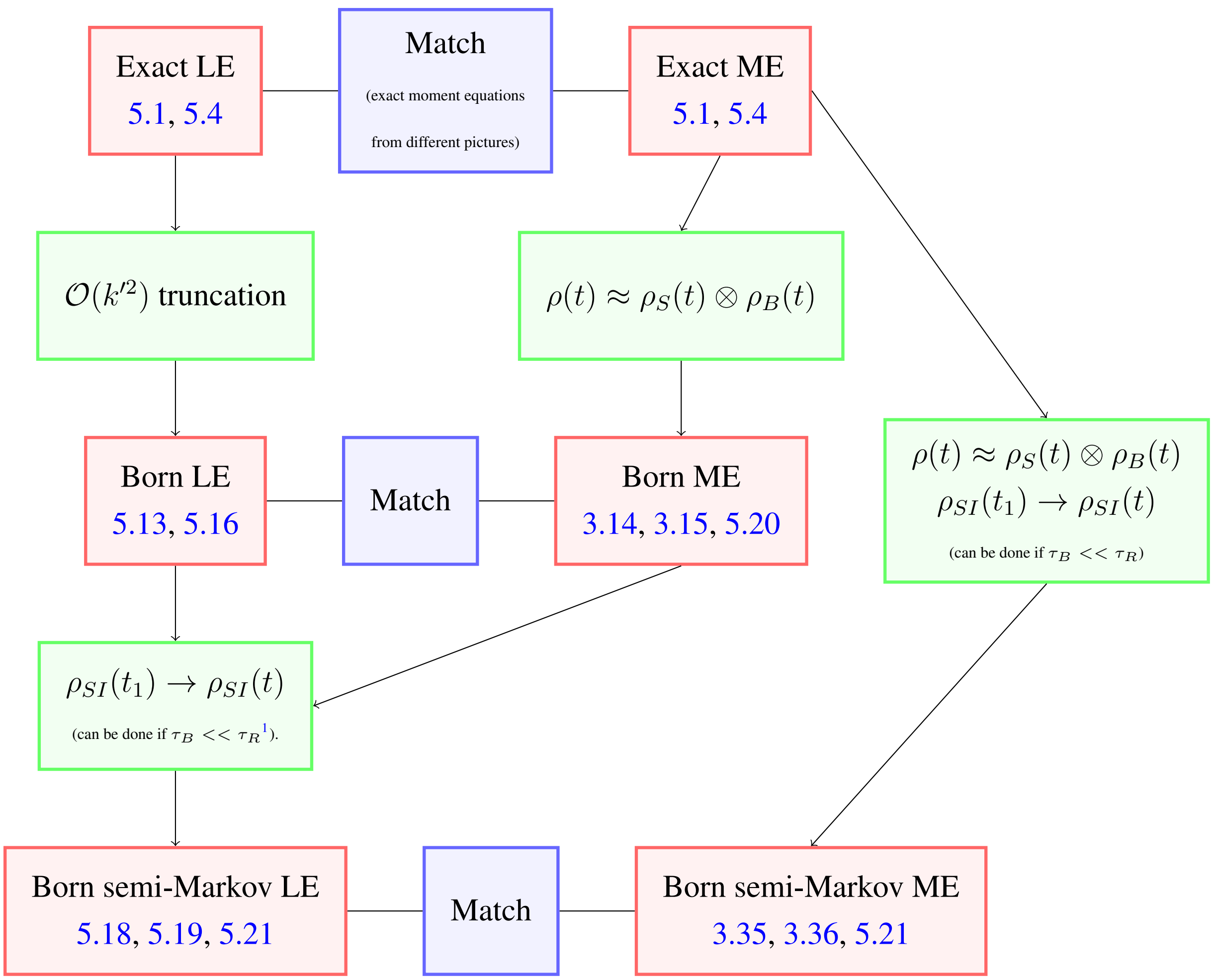
Now, there are also terms which have moments convoluted with the noise kernel, $D_1(t)$. So, while doing $\mathrm{tr}(A_I(t_1)\rho_{SI}(t_1)) \to \mathrm{tr}(A_I(t_1)\rho_{SI}(t))$ here, we will also be needed to ensure $\gamma << \nu_1$ alongside $\gamma << \omega_p$. Doing the approximation and simplifying, we get (the procedure is same as given in appendix 5.A.2):

$$\begin{aligned}\frac{d\langle p^3\rangle_t}{dt} = &-\frac{3M\omega_n^2}{2}\langle\{p^2,x\}\rangle_t + 3\langle p\rangle_t h(t) \\ &+\frac{3\langle\{p^2,x\}\rangle_t}{2}\int_0^t dt_1 C(t-t_1) - \frac{3\langle p^3\rangle_t}{M}\int_0^t dt_1 S(t-t_1)\end{aligned} \tag{5.21}$$

We can obtain this moment from BSMME, i.e. using the equation 3.33 (refer to appendix 3.A.2). That (equation 3.63) is exactly the same as equation 5.21. This gives us confidence that our formulation of Born and semi-Markov approximation is also valid for higher moments‘.

5.3 Summary Table

Let us summarise our understanding of this chapter. Let the bath correlation timescale $\tau_B = \max\{\frac{1}{\omega_p}, \frac{1}{\nu_1}\}$ and the system relaxation timescale $\tau_R = \frac{1}{\gamma}$. For equations that governs the dynamics of moments:



[1]up to second order, thermal time scale in τ_B is irrelevant

Appendix

5.A Detailed Calculations

5.A.1 Truncating the Moment Equations

We want to arrive at the equation 5.15 from the equation 5.14 using equations 5.7, 5.9 and 5.12. Let us rewrite these equations here:

$$B^{(1)}(t) = \eta(t), \quad B^{(2)}(t) = \int_0^t dt_1 x(t_1)\Sigma(t-t_1) \tag{5.22}$$

$$x^{(0)}(t) = x(0)\cos(\omega_0 t) + \frac{p(0)}{M}\frac{\sin(\omega_0 t)}{\omega_0}, \quad x^{(1)}(t) = \frac{1}{M\omega_0}\int_0^t dt_1 \sin(\omega_0(t-t_1))[\eta(t_1) - k' x^{(0)}(t_1)] \tag{5.23}$$

We want to simplify $\langle xB + Bx\rangle_t$ using $x(t)B(t) \approx [x^{(0)}(t) + x^{(1)}(t)]B^{(1)}(t) + x^{(0)}B^{(2)}(t)$. Let us do it term by term:

$$\begin{aligned}
\langle x^{(0)}B^{(1)} + B^{(1)}x^{(0)}\rangle_t &= 2\langle x^{(0)}\rangle_t\langle\eta\rangle_t = 0 \\
\langle x^{(1)}B^{(1)} + B^{(1)}x^{(1)}\rangle_t &= \frac{1}{M\omega_0}\int_0^t dt_1 \sin(\omega_0(t-t_1))[\langle\{\eta(t_1),\eta(t)\}\rangle - 2k'\langle x^{(0)}\rangle_{t_1}\langle\eta\rangle_t] \\
&= \frac{1}{M\omega_0}\int_0^t dt_1 \sin(\omega_0(t-t_1))D_1(t-t_1) \\
\langle x^{(0)}B^{(2)} + B^{(2)}x^{(0)}\rangle_t &= \int_0^t dt_1\Sigma(t-t_1)\langle x(t_1)x^{(0)}(t) + x^{(0)}(t)x(t_1)\rangle \\
&= \int_0^t dt_1\Sigma(t-t_1)\left[2\langle x^2\rangle_{t_1}\cos(\omega_0(t-t_1)) + \frac{\langle xp+px\rangle_{t_1}\sin(\omega_0(t-t_1))}{M\omega_0}\right]
\end{aligned} \tag{5.24}$$

where in the last line, I have used $x^{(0)}(t) = x(t_1)\cos(\omega_0(t-t_1)) + \frac{p(t_1)}{M}\frac{\sin(\omega_0(t-t_1))}{\omega_0}$, which follows directly from equation 5.9. We have also used the fact that $\langle\eta\rangle_t = 0$. Adding three contributions, we get equation 5.15. Truncation of $\langle pB + Bp\rangle_t$ is exactly similar and hence we will not show it here.

5.A.2 Born semi-Markov: Langevin Approach

We will get equations 5.18 and 5.19. Let us start with first moments. Changing $\rho_{SI}(t_1)$ to $\rho_{SI}(t)$ in equation 5.13 and then using equation 5.17:

$$
\begin{aligned}
\langle \dot{p} \rangle_t &= -M\omega_n^2 \langle x \rangle_t + \int_0^t dt_1 \mathrm{tr}_S \left(x_I(t_1) \rho_{SI}(t) \right) \Sigma(t-t_1) \\
\langle \dot{p} \rangle_t &= -M\omega_n^2 \langle x \rangle_t + \langle x \rangle_t \int_0^t dt_1 \Sigma(t-t_1) \cos(\omega_0(t-t_1)) - \frac{\langle p \rangle_t}{M} \int_0^t dt_1 \Sigma(t-t_1) \frac{\sin(\omega_0(t-t_1))}{\omega_0} \\
&= -M\omega_n^2 \langle x \rangle_t + \langle x \rangle_t \int_0^t dt_1 C(t-t_1) - \frac{\langle p \rangle_t}{M} \int_0^t dt_1 S(t-t_1)
\end{aligned}
\tag{5.25}
$$

$\langle \dot{x} \rangle_t$ has no t_1 and hence we are done with first moments. Similarly, the expression for $\langle \dot{x}^2 \rangle$ too won't change. For the rest of second moments, we will need the following equations which can be easily obtained from equation 5.17:

$$
\begin{aligned}
x_I^2(t_1) &= x_I^2(t) \cos^2(\omega_0(t-t_1)) + p_I^2(t) \frac{\sin^2(\omega_0(t-t_1))}{(M\omega_0)^2} - [xp+px]_I(t) \frac{\sin(2\omega_0(t-t_1))}{2M\omega_0} \\
p_I^2(t_1) &= p_I^2(t) \cos^2(\omega_0(t-t_1)) + x_I^2(t) (M\omega_0 \sin(\omega_0(t-t_1)))^2 + [xp+px]_I(t) \frac{M\omega_0 \sin(2\omega_0(t-t_1))}{2} \\
[xp+px]_I(t_1) &= [xp+px]_I(t) \cos(2\omega_0(t-t_1)) + M\omega_0 x_I^2(t) \sin(2\omega_0(t-t_1)) - p_I^2(t) \frac{\sin(2\omega_0(t-t_1))}{M\omega_0}
\end{aligned}
\tag{5.26}
$$

We will demonstrate the calculation only for $\langle p^2 \rangle_t$. Corresponding calculation for $\langle xp + px \rangle_t$ is very similar. Changing $\rho_{SI}(t_1)$ to $\rho_{SI}(t)$ in equation 5.16, we get:

$$
\begin{aligned}
\frac{d\langle p^2 \rangle_t}{dt} &= -M\omega_n^2 \langle xp+px \rangle_t + h(t) \\
&\quad + \int_0^t dt_1 \left[\underbrace{C(t-t_1) \mathrm{tr} \left([xp+px]_I(t_1) \rho_{SI}(t) \right) - 2M\omega_0^2 S(t-t_1) \mathrm{tr} \left(x_I^2(t_1) \rho_{SI}(t) \right)} \right]
\end{aligned}
\tag{5.27}
$$

For the ease of calculations, let us develop the following short-hand notations:

$$
\cos(\omega_0(t-t_1)) \equiv c, \quad \sin(\omega_0(t-t_1)) \equiv s, \quad \Sigma(t-t_1) \equiv \Sigma \tag{5.28}
$$

where A is any operator. Let us just focus on the underbraced part in the equation 5.27 (use equation 5.26):

$$
\begin{aligned}
LHS &= \text{tr}\left([xp+px]_I(t_1)\rho_{SI}(t)\right)\Sigma c - 2M\omega_0 \text{tr}\left(x_I^2(t_1)\rho_{SI}(t)\right)\Sigma s \\
&= \Sigma c\left(\langle xp+px\rangle_t(c^2-s^2) + 2M\omega_0 sc\langle x^2\rangle_t - \langle p^2\rangle_t \frac{2sc}{M\omega_0}\right) \\
&\qquad - 2M\omega_0\Sigma s\left(\langle x^2\rangle_t c^2 + \langle p^2\rangle_t \frac{s^2}{(M\omega_0)^2} - \langle xp+px\rangle_t \frac{sc}{M\omega_0}\right) \\
&= \langle xp+px\rangle_t\left(\Sigma c(c^2-s^2) + 2\Sigma s^2 c\right) + \langle x^2\rangle_t\left(2M\omega_0\Sigma sc^2 - 2M\omega_0\Sigma sc^2\right) \\
&\qquad - \langle p^2\rangle_t\left(\frac{2\Sigma sc^2}{M\omega_0} + \frac{2\Sigma s^3}{M\omega_0}\right) \\
&= \langle xp+px\rangle_t(\Sigma c) - \frac{2\langle p^2\rangle_t}{M}\left(\frac{\Sigma s}{\omega_0}\right) \\
&\equiv \langle xp+px\rangle_t C(t-t_1) - \frac{2\langle p^2\rangle_t}{M} S(t-t_1)
\end{aligned}
\tag{5.29}
$$

Putting this back into equation 5.27:

$$
\frac{d\langle p^2\rangle_t}{dt} = -M\omega_n^2\langle xp+px\rangle_t + \langle xp+px\rangle_t\int_0^t d\tau C(\tau) - \frac{2\langle p^2\rangle_t}{M}\int_0^t d\tau S(\tau) + h(t) \tag{5.30}
$$

which is exactly the same as equation 5.19.

Conclusions and Future Plans

In this thesis, we studied a quantum Brownian particle attached to a Rubin bath using various formalisms of open quantum systems, namely the quantum Langevin approach, the Born master equation and the Born-Markov master equation. We compared three approaches and understood the regimes of validity of both master equations. The regimes that we define are in terms of various frequency scales involved in the problem. Let us list them down:

1. $\gamma = \frac{\sqrt{mk}}{2M}$. m is the mass of bath oscillators, and k is the inter-bath coupling. M is the mass of the system oscillator (see figure 1.1). The system reaches equilibrium with a timescale $1/\gamma$.

2. ω_0: The trap frequency, i.e. the external potential on the system is $\frac{1}{2}M\omega_0^2x^2$.

3. $\omega_p = \frac{k'}{\sqrt{mk}}$: Drude cutoff in the Drude spectral density (equation 1.5). It determines the timescale with which bath correlation functions decay.

4. k_BT: The temperature of the bath. It also determines a time scale with which bath correlation functions decay.

A list of important conclusions:

- A Langevin equation is typically written in terms of a dissipation kernel. One needs to be careful about an algebraic subtlety involved while writing the same equation in terms of a damping kernel, as discussed in the section 2.1.1.

- If there is no external potential, then we observe four distinct behaviours in $\langle x^2\rangle_t$ of the system in the following order (increasing in time): 1. An initial t^4 growth, 2. A polynomial growth $\sim t^2$ (ballistic), 3. A subdiffusive logarithmic growth $\sim \ln(t)$, and finally 4. A diffusive growth $\sim t$. The times at which such crossover occurs seem to depend on various frequency scales involved in the system. However, further investigation needs to be done in order to establish a concrete mathematical statement.

- Behaviour of $\langle x^2 \rangle_t$ at any finite temperature matches to the zero temperature behaviour up to some crossover time t^*.
- In the formalism of open quantum systems, one should define the weak coupling limit by studying the spectral density and not by merely looking at the interaction Hamiltonian.
- In the literature, the Markovian approximation is done in two steps: 1. Replacing $\rho_{SI}(t_1)$ to $\rho_{SI}(t)$ in the Born master equation 3.23, and 2. Making the upper limit of the integral $t \to \infty$ in the same equation. We find that doing only the first step suffices the Markovian approximation. In fact, doing the second step leads to the incorrect prediction of transients even in the limits where the Markovian approximation is supposed to work. Hence, we have only done the first step in our study and called it a "semi-Markov approximation" to distinguish it from the traditional Markovian approximation.
- Using an Ohmic bath as a Markovian bath can be pathological, i.e. it can lead to ultraviolet divergences. Our study suggests that a Drude bath with a large cutoff can be safely used as a Markovian bath.

We will now summarise our conclusions from the comparisons.

- The dynamics of the first moments is totally unaffected by the Born approximation. Discussions in the upcoming bulletin points will be about the second moments, particularly $\langle x^2 \rangle_t$.
- Both the BME and BSMME works exactly **for all temperature and all times** for a bounded particle in the weak coupling limit $\gamma << \omega_0 << \omega_p$. As discussed in the section 5.2.1, the BSMME can work for zero temperature given we satisfy the inequality $\gamma << \omega_0 << \omega_p$.
- Irrespective of the temperature, the BME works only for very small times for a free particle even in the weak coupling limit $\gamma << \omega_p$. On the contrary, the BSMME—which is obtained by doing an extra approximation on the BME—works for all times for a free particle if we satisfy $\hbar\gamma << \hbar\omega_p << K_B T$. However, if the temperature decreases, the BSMME works only for very small times.
- To understand the free particle results, we study the bounded particle in the limit $\omega_0 << \gamma << \omega_p$. This suggests that the inequality $\gamma << \omega_0 << \omega_p$ is a must for the BME to work. However, BSMME can work even if we satisfy the inequality $k_B T >> \hbar\omega_p$ even if violate the inequality $\gamma << \omega_0$.

- Employing Markovian kernels (Ohmic bath and high temperatures) to the BME is not equivalent to the BSMME.
- It is possible to formulate the Born and Markov approximations in the Langevin equation formalism as shown in the chapter 5. This helped us identify that the BSMME can work for second moments even for the zero-temperature limit if we ensure an inequality $\gamma << \omega_0 << \omega_p$.

We will summarise all our comparisons in the form of a table.

Bounded Particle: $\gamma << \omega_0 << \omega_p$						
Time	BME			BSMME		
	Inhomogeneous Part		Homogeneous Part	Inhomogeneous Part		Homogeneous Part
	$T \to 0$	$T \to \infty$		$T \to 0$	$T \to \infty$	
$t \to 0$	✓	✓	✓	✓	✓	✓
Finite t	✓	✓	✓	✓	✓	✓
$t \to \infty$	✓	✓	✓	✓	✓	✓
Bounded Particle: $\omega_0 << \gamma << \omega_p$						
Time	BME			BSMME		
	Inhomogeneous Part		Homogeneous Part	Inhomogeneous Part		Homogeneous Part
	$T \to 0$	$T \to \infty$		$T \to 0$	$T \to \infty$	
$t \to 0$	×	✓	×	✖	✓	✓
Finite t	×	×	×	✖	✓	✖
$t \to \infty$	×	✓	✓	✖	✓	✓
Free Particle: $\gamma << \omega_p$						
Time	BME			BSMME		
	Inhomogeneous Part		Homogeneous Part	Inhomogeneous Part		Homogeneous Part
	$T \to 0$	$T \to \infty$		$T \to 0$	$T \to \infty$	
$t \to 0$	✓	✓	✓	✓	✓	✓
Finite t	×	×	×	✖	✓	✓
$t \to \infty$	×	×	×	✖	✓	✓

Table 5.1.1: *Summary of our results. The comparison is based on the behaviour of second moments. In particular,* $\langle x^2 \rangle_t$.

These are the conventions to understand the table:

1. A tick '✓' means that the result agrees with the exact Langevin approach.

2. A tick ‘✕’ means that the result does not agree with the exact Langevin approach.

3. A tick ‘✖’ will only be in the BSMME section. It means that the BSMME result disagrees with both exact Langevin and BME. If both BME and BSMME have a ‘✕’ , then both are the same but disagree with the exact approach.

Future Directions

In this project, there are a couple of results that we have not adequately understood. For example, why does doing a semi-Markov on top of the Born approximation make the BME to work for the high-temperature limit? We need to do further work to understand these puzzles. We also want to study different systems in a similar fashion to see the generalisability of our results. Currently, we are working on verifying our results on a different system. I will briefly describe the system in this section.

We take an empty open-ended tight-binding chain of N_S sites of Bosons/Fermions as a system. a_i is the annihilation operator of i^{th} site. We connect the m^{th} site of this chain to the first site of a semi-infinite tight-binding chain equilibrated temperature β and chemical potential μ. b_i is the annihilation operators of i^{th} bath site. The Hamiltonian setup is

$$H_S = g\sum_{i=1}^{N_S-1}\left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right), \quad H_B = t_B\sum_{i=1}^{\infty}\left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i\right), \quad \hat{H}_I = \epsilon\gamma_1\left(a_m^\dagger b_1 + b_1^\dagger a_m\right) \tag{5.31}$$

We try to study the dynamics of injection of particles, i.e. $N(t) = \sum_i \langle a_i^\dagger a_i\rangle_t$ with time. We also study the spread of the density profile (plots of $n_i = \langle a_i^\dagger a_i\rangle_t$ with site index i) with time t. We are doing this study using the following different approaches:

1. Exact Numerics.

2. Steady-state Langevin equation approach.

3. The Born Master Equation.

4. The Born semi-Markov Master Equation.

5. The Lindblad Master Equation.

Finally, we will compare the results obtained from all these approaches. Hopefully, this will enrich our understanding of the regimes of validity of master equations further.

Bibliography

[1] Vinay Ambegaokar. Quantum brownian motion and its classical limit. *Berichte der Bunsen-gesellschaft für physikalische Chemie*, 95(3):400–404, 1991.

[2] Janet Anders, Connor Sait, and Simon AR Horsley. Quantum brownian motion for magnets. *New Journal of Physics*, 2022.

[3] Giuseppe Argentieri, Fabio Benatti, Roberto Floreanini, and Marco Pezzutto. Violations of the second law of thermodynamics by a non-completely positive dynamics. *EPL (Europhysics Letters)*, 107(5):50007, 2014.

[4] Daniel Boyanovsky and David Jasnow. Heisenberg-langevin versus quantum master equation. *Physical Review A*, 96(6):062108, 2017.

[5] Heinz-Peter Breuer, Francesco Petruccione, et al. *The theory of open quantum systems*. Oxford University Press on Demand, 2002.

[6] Howard J Carmichael. *Statistical methods in quantum optics 2: Non-classical fields*. Springer Science & Business Media, 2009.

[7] Avijit Das, Abhishek Dhar, Ion Santra, Urbashi Satpathi, and Supurna Sinha. Quantum brownian motion: Drude and ohmic baths as continuum limits of the rubin model. *Physical Review E*, 102(6):062130, 2020.

[8] Suman G Das and Abhishek Dhar. Landauer formula for phonon heat conduction: relation between energy transmittance and transmission coefficient. *The European Physical Journal B*, 85(11):1–8, 2012.

[9] CH Fleming, Albert Roura, and BL Hu. Exact analytical solutions to the master equation of quantum brownian motion for a general environment. *Annals of Physics*, 326(5):1207–1258, 2011.

[10] Chris H Fleming and Nick I Cummings. Accuracy of perturbative master equations. *Physical Review E*, 83(3):031117, 2011.

[11] GW Ford and RF O'connell. Exact solution of the hu-paz-zhang master equation. *Physical Review D*, 64(10):105020, 2001.

[12] Vincent Hakim and Vinay Ambegaokar. Quantum theory of a free particle interacting with a linearly dissipative environment. *Physical Review A*, 32(1):423, 1985.

[13] Bei Lok Hu, Juan Pablo Paz, and Yuhong Zhang. Quantum brownian motion in a general environment: Exact master equation with nonlocal dissipation and colored noise. *Physical Review D*, 45(8):2843, 1992.

[14] Naim Kalantar, Bijay Kumar Agarwalla, and Dvira Segal. On the definitions and simulations of vibrational heat transport in nanojunctions. *The Journal of Chemical Physics*, 153(17): 174101, 2020.

[15] Amikam Levy and Ronnie Kosloff. The local approach to quantum transport may violate the second law of thermodynamics. *EPL (Europhysics Letters)*, 107(2):20004, 2014.

[16] Sabrina Maniscalco, Jyrki Piilo, F Intravaia, F Petruccione, and A Messina. Lindblad-and non-lindblad-type dynamics of a quantum brownian particle. *Physical Review A*, 70(3): 032113, 2004.

[17] Pietro Massignan, Aniello Lampo, Jan Wehr, and Maciej Lewenstein. Quantum brownian motion with inhomogeneous damping and diffusion. *Physical Review A*, 91(3):033627, 2015.

[18] Frederik Nathan and Mark S Rudner. Universal lindblad equation for open quantum systems. *Physical Review B*, 102(11):115109, 2020.

[19] Archak Purkayastha, Abhishek Dhar, and Manas Kulkarni. Out-of-equilibrium open quantum systems: A comparison of approximate quantum master equation approaches with exact results. *Physical Review A*, 93(6):062114, 2016.

[20] Angel Rivas, A Douglas K Plato, Susana F Huelga, and Martin B Plenio. Markovian master equations: a critical study. *New Journal of Physics*, 12(11):113032, 2010.

[21] Ingrid Rotter and JP Bird. A review of progress in the physics of open quantum systems: theory and experiment. *Reports on Progress in Physics*, 78(11):114001, 2015.

[22] Juzar Thingna, Jian-Sheng Wang, and Peter Hänggi. Generalized gibbs state with modified redfield solution: Exact agreement up to second order. *The Journal of chemical physics*, 136 (19):194110, 2012.

[23] Devashish Tupkary, Abhishek Dhar, Manas Kulkarni, and Archak Purkayastha. Fundamental limitations in lindblad descriptions of systems weakly coupled to baths. *Physical Review A*, 105(3):032208, 2022.

[24] Sai Vinjanampathy and Janet Anders. Quantum thermodynamics. *Contemporary Physics*, 57 (4):545–579, 2016.

[25] Hannu Wichterich, Markus J Henrich, Heinz-Peter Breuer, Jochen Gemmer, and Mathias Michel. Modeling heat transport through completely positive maps. *Physical Review E*, 76 (3):031115, 2007.