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Thermal conduction in a chain of oscillators

Dissertação de Mestrado

Thesis presented to the Programa de Pós–graduação em Física da PUC-Rio in partial fulfillment of the requirements for the degree of Mestre em Física .

Advisor: Profa. Celia Beatriz Anteneodo de Porto

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dedication.

Acknowledgments

I would like to first thank my advisor ...

Then I wish to thank ...

Abstract

We simulate fourier's law of heat conduction by means of a model consisting of a chain os oscillators and then show that with a few small changes this model can describe the so called thermal diodes.

Keywords

Resumo

Abreu Almeida, Alexandre Augusto; Anteneodo, Celia. **Condução térmica em uma cadeia de osciladores**. Rio de Janeiro, 2020. 38p. Dissertação de Mestrado – Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro.

Nós simulamos a lei de fourier da condução de calor por meio de um modelo consistindo em uma cadeia de osciladores e mostramos que com algumas pequenas mudanças esse modelo pode descrever os chamados diodos térmicos.

Palavras-chave

Table of contents

List of figures

List of tables

My beautifull epigraph

Alguém, *Algum livro.*

List of Abreviations

ADI – Análise Digital de Imagens

BIF – *Banded Iron Formation*

... – ...

1
Introduction

1. Thermodynamics, Transport Phenomena and Non Equilibrium Thermo-dynamics (Quantum Thermodynamics?) [Truesdell, Mazur]

   Importance and Applications, Transport Phenomena x Non Equilibrium Thermodynamics, Achievements [?]

2. Statistical Physics [?]

3. Interests in non equilibrium physics [McQuarrie, Prigogine] [Fermi-Pasta-Ulam-Tsingou?]

1.1
Heat transport

1. Fourier Law

2. Solids [Ashcroft & Mermin]

3. Problems with linear harmonic chain [Aschroft & Mermin, Rieder]

One of the most common ways of thinking about solids is as being composed of many particles bounded together by first neighbors interactions.

This picture is commonly used in undergraduate Solid State Physics books as a toy model consisting of a one dimensional chain of classical particles interacting with their neighbors by quadratic potentials (an harmonic chain) mainly to introduce in its quantum analogue the concept of phonons [1] and how they affect some of the equilibrium and transport properties of metals and insulators [2].

Quoting from the book by Ashcroft & Mermin:

"The harmonic approximation is the starting point for all theories of lattice dynamics[...]"

1.2
Objective

1. What has been done [Lebowitz, Lepri, Casati, Baowen Li, Celia]

2. What we wish to do

What we wish to do is to try and simulate the Fourier equation in one dimension from first principles, using a microscopic model.

From there, we will then try to simulate a thermal diode.

The simplest model for heat transfer one might think about as a first idea is a linear chain of harmonic oscillators, like the common toy model for lattice vibrations seen in undergraduate physics courses in solid state theory [oxfordsolid], but with two heat baths on each side. However, it is known that this model does reproduce the linear temperature profile in accordance with Fourier's law, giving a flat profile instead [rieder].

Many models have been proposed to try to reproduce this linear profile, most of them consisting of adding anharmonic terms either in the potential of interaction between particles or in an external potential, although there are some that change the dynamics completely.

We shall try to use anharmonic terms to simulate such heat transfer using two stochastic models for the heat baths.

Since the model uses a linear harmonic chain, we will first review numerical methods for solving a simple harmonic oscillator, which will give us insights on their behavior for the couples oscillators. Then, we will review the methods used for simulating heat baths, which in our case will be Langevin heat baths (although in the literature, we can also see cases of Nose-Hoover Thermostats being used for heat baths, see [BaowenLi1] and [Lepri].

After that, we discuss the results for the simulation of harmonic and anharmonic chains.

2
Modelling Heat Flow

2.1
1D Heat Transport

Before diving in the microscopic models, let us first describe the basic heat flow problem from a macroscopic point of view so that afterwards it can be compared to our toy model. Suppose we have a solid bar with length L, cross sectional area A and thermal conductivity κ in contact with two thermal baths, one on each side and with temperatures T_1, T_2 such that $T_1 > T_2$.
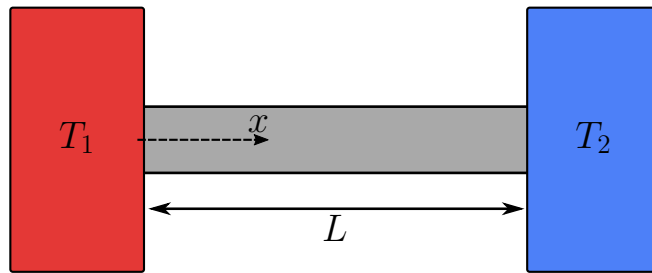
Figure 2.1: one dimensional heat transport

We further assume that $L^2 \gg A$, the lateral surface of the bar is isolated from the environment and κ does not vary with temperature. In this case Fourier's law takes the form

$$\dot{Q} = -\kappa \frac{dT}{dx}.$$

It is expected that, as time goes to infinity, our system approaches a steady state where the heat flux $\dot{Q}$ is constant, and as such we can use the boundary conditions $T(x = 0) = T_1$ and $T(x = L) = T_2$ to integrate our function and get

$$T = -\frac{(T_1 - T_2)}{L} \cdot x + T_1,$$

showing that the temperature profile along the bar in the steady state is linear.
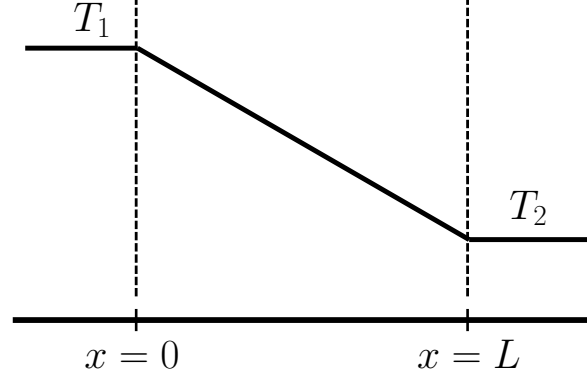
Figure 2.2: linear temperature profile.

It is also possible to use the heat equation to look at the dynamics of the system and see the evolution of the system as $t \to \infty$. In fact, if we divide the bar in small slabs of size Δx (partition the interval $[0, L]$ in intervals $[x, x+\Delta x]$) and then use the first law of thermodynamics to approximate for a given slab

$$(\dot{Q}(t, x) - \dot{Q}(t, x + \Delta x))A\Delta t = (u(t + \Delta t, x) - u(t, x))A\Delta x,$$

where u is the specific internal energy of the bar (considered homogeneous), then

$$-\frac{\partial \dot{Q}}{\partial x} = \frac{\partial u}{\partial t}$$

in the limit $\Delta x \to 0, \Delta t \to 0$. Now using the concept of specific heat capacity we could write $u = C\rho T$, and so

$$-\frac{\partial \dot{Q}}{\partial x} = C\rho\frac{\partial T}{\partial t},$$

which together with Fourier's law gives us the heat equation

$$\frac{\partial^2 T}{\partial x^2} = \alpha^2 \frac{\partial T}{\partial t},$$

where the definition $\alpha^2 = C\rho/\kappa$ was used. Considering that the bar have an initial temperature profile $f(x)$, its solution is given by

$$T(x, t) = -\frac{(T_1 - T_2)}{L} \cdot x + T_1 + \sum_{n=1}^{\infty} c_n e^{-(n\pi\alpha/L)^2 t} \sin\left(\frac{n\pi x}{L}\right),$$

where

$$c_n = \frac{2}{L} \int_0^L \left[f(x) - \frac{(T_2 - T_1)}{L} \cdot x - T_1 \right] \sin\left(\frac{n\pi x}{L}\right) dx,$$

from which it can be seen that the transient part goes to zero exponentially

with characteristic time $\tau \propto L^2/\alpha^2$.

2.2
Toy Model

A naive first idea for modeling this situation with the use of classical mechanics would be to replace the bar by a chain of particles with first-neighbors interaction through an harmonic potential.
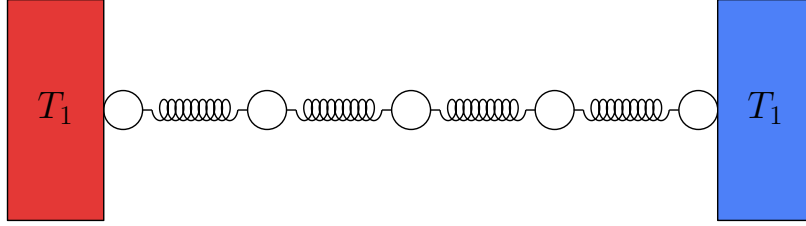
Figure 2.3: pictorial representation of the mathematical model

Along this text, many changes to this simple toy model will be discussed, but it is already worth noting that the failure of this model to reproduce the temperature profile given by Fourier's law has been known for some time ([3]) and nonlinear terms are needed to achieve this. The main toy model used in this work will be the so called Frenkel-Kontorova Model which add an external oscillating potential on the particles.

There many ways to simulate a constant temperature thermal baths in the literature and the one considered here will be using the dynamics of the Langevin equation.

The equations of motion will then be

$$\frac{dv_1}{dt} = -\gamma v_1 + \eta_1(t) - k\left(x_1 - x_2\right),$$
$$\frac{dv_i}{dt} = -k\left(2x_i - x_{i-1} - x_{i+1}\right), \tag{2-1}$$
$$\frac{dv_N}{dt} = -\gamma v_N + \eta_N(t) - k\left(x_N - x_{N-1}\right),$$

Both the chain of particles and the heat baths shall be further discussed in the next sections.

2.3
Heat Baths

In an equilibrium situation there are many techniques which are used to try and maintain the system at constant temperature, such as re-scaling the particle velocities in each time step, changing the Hamiltonian of the thermal

bath particles [4] and using stochastic equations to describe the thermal noise [5].

When trying to model low dimensional heat transfer, there are two main types of heat baths used, the Nose-Hoover thermostat and Langevin heat baths [5].

2.3.1
Nose-Hoover Thermostat

The Nose-Hoover thermostat consists of adding one more degree of freedom s, along with its conjugated momentum p_s, which represents somewhat an external system [4]. Using the same notation as in [6], let H_0 be the classical many body Hamiltonian of the particle, the *Nose Hamiltonian* is then defined as

$$H_N = H_0(q, p/s) + gKT \ln s + \frac{p_s^2}{2Q},$$

where g is the system's degrees of freedom and Q is a parameter

2.3.2
Langevin Equation

In the XIX century the botanist Robert Brown studied what is now called the *Brownian motion* which is the seemingly random motion of pollen grains in a viscous media such as water or acetone [17]. Paul Langevin tried to explain the phenomena using Newton's second law in 1908 by adding a random force which nowadays we recognize as being a Wiener random process and thus devising the so called Langevin equation [14].

Such an equation can be written as

$$m\ddot{r} = -\gamma\dot{r} + \eta,$$

where the $-\gamma\dot{r}$ term represents a viscous force due to the media and η is a Wiener random process.

2.4
Particle chain

Introductory texts in solid state physics commonly use the picture of a solid as being composed of many classical particles interacting with their first neighbors through springs that follows Hooke's law as a first toy model to explain the effect of lattice vibrations in some phenomena such as the law of Dulong and Petit [2].

Such an idea is commonly developed on the basis of two main assumptions, namely the small oscillations assumption that the atoms that constitute the solid only show small displacements from their equilibrium position and the harmonic approximation assumption that these small oscillations can be well described by a Taylor expansion up to second order.

Although the first assumption is a good enough approximation, the second fails to explain both equilibrium properties such as thermal expansion and transport properties such as thermal conductivity.

In fact in a paper from 1966 Z. Rieder, J. L. Lebowitz and E. Lieb showed, using a generalized form of the Liouville Equation, that such an harmonic crystal in a stationary state between two heat baths of unequal temperatures actually shows a flat temperature profile along the chain with average bath temperature. They used the kinetic energy of the particles as a proxy for the temperature (the kinetic temperature) [3].

$$
\boxed{
\begin{aligned}
\frac{dv_1}{dt} &= -\gamma v_1 + \eta_1(t) - k\left(x_1 - x_2\right); \\
\frac{dv_i}{dt} &= -k\left(2x_i - x_{i-1} - x_{i+1}\right); \\
\frac{dv_N}{dt} &= -\gamma v_N + \eta_N(t) - k\left(x_N - x_{N-1}\right);
\end{aligned}
}
\tag{2-2}
$$

Where $i = 2, 3, ..., N-1$, and x_i is the displacement from equilibrium for each particle, which is given by:

$$
\frac{dx_1}{dt} = v_1, \; \frac{dx_i}{dt} = v_i, \; \frac{dx_N}{dt} = v_N;
$$

The variables η_1 and η_2 are uncorrelated Gaussian processes, γ is the drag coefficient for the Langevin baths and k can be seen as the spring constant (assuming unit mass for all particles), or as the rescaled spring constant with respect to the particle masses, but either way it's assumed to be the same for all interactions.

The Hamiltonian corresponding to the linear chain is given by:

$$
H = \sum_{i=2}^{N} \frac{p_i^2}{m_i} + \frac{k}{2}(x_i - x_{i-1})^2;
$$

Discussing Rieder and Lebowitz finding that the fourier profile is not achieved.

2.4.1
Fermi Pasta Ulam Tsingou

???????

2.4.2
The Frenkel-Kontorova Model

The Frenkel Kontorova model for a linear chain of particles can be seen as being described by a Hamiltonian of the form

$$\mathcal{H} = K + U_{int} + U_{sub}$$

– K is the kinetic energy

– U_{int} is the interaction potential between the particles

– U_{sub} is a "substrate" potential characterizing the interaction of the particles with its surrounding.

Opening each term, we have:

$$\mathcal{H} = \underbrace{\sum_{i=1}^{N} \frac{p_i^2}{2m_i}}_{K} + \underbrace{\sum_{i=1}^{N} \frac{k_i}{2}(x_i - x_{i-1} - a)^2}_{U_{int}} + \underbrace{\sum_{i=1}^{N} V_{0,i}\left[1 - \cos\left(\frac{2\pi x_i}{a_s}\right)\right]}_{U_{sub}}$$

Where x_i is the position of the i-th particle. Assuming the equilibrium position of i-th particle is given by $i \cdot a$, we can write $x_i = ia + q_i$, where q_i is the particle displacement from equilibrium. Also:

$$\frac{dx_i}{dt} = \frac{dq_i}{dt}$$

From which we can rewrite:

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} \frac{k_i}{2}(q_i - q_{i-1})^2 + \sum_{i=1}^{N} V_{0,i}\left[1 - \cos\left(\frac{2\pi ia}{a_s} + \frac{2\pi q_i}{a_s}\right)\right]$$

We can see that U_{sub} is periodic with period a_s, where the $x_i = na_s$ is the minimum of the potential (equilibrium position).

Assuming that $a/a_s = k \in \mathbb{N}$, we get:

$$\cos\left(\frac{2\pi ia}{a_s} + \frac{2\pi q_i}{a_s}\right) = \cos\left(2\pi ki + \frac{2\pi q_i}{a_s}\right) = \cos\left(2\pi k' + \frac{2\pi q_i}{a_s}\right)$$

Which is just

$$\cos\left(\frac{2\pi q_i}{a_s}\right)$$

Hence,

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} \frac{k_i}{2}(q_i - q_{i-1})^2 + \sum_{i=1}^{N} V_{0,i}\left[1 - \cos\left(\frac{2\pi q_i}{a_s}\right)\right]$$

The equations of motion are

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}, \quad \dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i},$$

Assuming the particles $i = 1, N$ represent the thermal baths, we have for $i = 2, 3, \ldots, N - 1$:

$$\frac{dq_i}{dt} = \frac{p_i}{m_i}$$

$$\frac{dp_i}{dt} = -k_i(q_i - q_{i-1}) + k_i(q_{i+1} - q_i) - \frac{2\pi V_{0,i}}{a_s} \sin\left(\frac{2\pi q_i}{a_s}\right)$$

Rewriting,

$$\frac{dq_i}{dt} = \frac{p_i}{m_i}$$

$$\frac{dp_i}{dt} = -k_i(q_i - q_{i-1}) - k_i(q_i - q_{i+1}) - \frac{2\pi V_{0,i}}{a_s} \sin\left(\frac{2\pi q_i}{a_s}\right)$$

3
Computational Methods

3.1
Deterministic

3.2
Stochastic

We will give a summary of Langevin simulation here.

The Langevin equation is:

$$\boxed{\frac{dv}{dt} = -\gamma v + \eta\left(t\right)}$$

$$\frac{dx}{dt} = v$$

Where $\eta\left(t\right)$ is a gaussian stochastic process defined by the autocorrelation function:

$$\langle \eta\left(t\right)\eta\left(t'\right)\rangle = \Gamma\delta\left(t - t'\right)$$

3.3
Solution

Theoretical Formulae:

$$\boxed{\langle v(t)\rangle = v_0 e^{-\gamma t}}$$

$$\boxed{\sigma_v^2 = \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right)}$$

$$\boxed{\langle x(t)\rangle = x_0 + \frac{v_0}{\gamma}\left(1 - e^{-\gamma t}\right)}$$

$$\boxed{\sigma_x^2 = \frac{\Gamma}{\gamma^2}\left(t - \frac{2}{\gamma}(1 - e^{-\gamma t}) + \frac{1}{2\gamma}\left(1 - e^{-2\gamma t}\right)\right)}$$

3.3.1
Macroscopic Variables

We can relate our parameters with thermodynamics variables.

The ensemble average in the equilibrium (the limit when $t \to \infty$) is:

$$\left\langle v^2 \right\rangle = \frac{\Gamma}{2\gamma}$$

From the kinetic theory, we also know that

$$\frac{1}{2}m \left\langle v^2 \right\rangle = \frac{1}{2}k_B T$$

Using the two equations together, we get:

$$\boxed{\Gamma = \frac{2\gamma k_B T}{m}}$$

Looking at the asymptotic behavior of the variance of the position of the particle, which gives us a relation with the diffusion coefficient.

$$2D = \frac{\Gamma}{\gamma^2}$$

$$D = \frac{k_B T}{m\gamma}$$

$$\boxed{\gamma = \frac{k_B T}{mD}}$$

However, for spherical particles of radius a, we could also use stokes-law for the drag coefficient.

$$\boxed{\gamma = \frac{6\pi\mu a}{m}}$$

3.3.2
Simulation

And can be solved by the Euler method, using the iterations:

$$\boxed{v_{n+1} = v_n - \tau\gamma v_n + \sqrt{\tau\Gamma}\xi_n}$$

$$\boxed{x_{n+1} = x_n + \tau v_n}$$

Where $\tau = \Delta t$ is the time step used in the method and ξ_n is a sequence of random variables sampled from a gaussian distribution $\mathcal{N}(0,1)$.

The used parameters and the results are given below.

 – Noise amplitude: $\Gamma = 0.1$

 – drag coefficient: $\gamma = 0.1$

 – initial velocity: $v_0 = 1.0$

 – initial position: $x_0 = 0.0$

 – time step: $\tau = 0.0001$

 – Number of particles in the ensemble: $N_p = 200$

3.3.2.1
Euler

3.3.2.2
Stochastic Runge Kutta

3.4
Solution 1 - Euler's Method

3.4.1
Theory

The Euler's method for the solution of differential equations and of the Langevin Bath is based on the simple and naive idea of partitioning the simulation time interval in small discrete steps $\Delta t = \tau$ and approaching the evolution of the system in each step by a taylor series truncated at the linear terms.

$$\mathbf{u}(t + \tau) \approx \mathbf{u}(t) + \tau \frac{d\mathbf{u}}{dt}$$

Where the derivative is given by the differential equation.

$$\frac{d\mathbf{u}}{dt} = f(\mathbf{u}, t)$$

The bold font is used to indicate vector quantities.

For the solution of a single Langevin bath, this method works reasonably well. However, when used to simulate the motion of an oscillator subject to an elastic potential of the form $kx^2/2$, the method gives an error for the amplitude of oscillation that grows exponentially with the number of time steps in the simulation ().

The reason for this is that Euler's method does not conserve energy, and instead increases it exponentially. This can be seen from a simple calculation for the equations of motion of a simple harmonic oscillator (system of equations 3.4.1). First, let us show that such a system should conserve energy.

$$\frac{dv}{dt} = -\frac{k}{m}x$$
$$\frac{dx}{dt} = v$$

Multiplying the first equation in the system 3.4.1 by mv and the second by kx and summing both of them, we see that the variation of the total energy with time is zero.

$$\frac{m}{2}\frac{dv^2}{dt} = \frac{dE_c}{dt} = -kxv, \quad \frac{k}{2}\frac{dx^2}{dt} = \frac{dE_p}{dt} = kxv$$

$$\frac{dE_c}{dt} + \frac{dE_p}{dt} = \frac{dE_T}{dt} = 0$$

Now, using the approximation of the Euler's method for the equations:

$$v_{n+1} = v_n - \frac{k}{m}x_n\tau$$

$$x_{n+1} = x_n + v_n\tau$$

Squaring both sides of the equations, multiplying them by $m/2$ and $k/2$, respectively, and then summing them we get:

$$E_{c,n+1} = E_{c,n} - kx_nv_n\tau + \frac{k}{m}\tau^2 E_{p,n}, \quad E_{p,n+1} = E_{p,n} + kx_nv_n\tau + \frac{k}{m}\tau^2 E_{c,n}$$

$$E_{T,n+1} = E_{T,n}\left(1 + \frac{k}{m}\tau^2\right)$$

Showing that the energy increases with a fixed ratio simply because of the approximations used.

Mathematically,

It's also possible to see this using new coordinates $x' = \sqrt{k/2}x$ and $v' = \sqrt{m/2}v$, the energy being just the distance from the point (x', v') to the origin in the phase space. With each new iteration, this point goes further and further away from the origin. (In the harmonic oscillation, the trajectory in this phase space would be a circle centered at the origin).

The problem would still continue even if we displaced the particle from the origin (just change the frame of reference by translation $x' = x - a$) and even if we added many elastic forces to the particle (since all forces are linear with respect to displacement $F_{el} = k(x - a)$, the resulting force will also be linear with respect to displacement $F_R = k'(x - a')$).

This means that, for our case, the euler's method will make the energy of the middle particle increase indefinitely. In the next part, we will see the

results from the simulations.

3.4.1.1
Results

Now lets compile the results of using the Euler's Method for both equation 2-2 and 3.4.1. The parameters used are given as bellow:

- $\gamma = 0.1$ the drag coefficient at the langevin baths
- $\tau = 0.001s$ timestep in seconds
- $tempo = 120.0s$ total simulation time in seconds
- $A_e = 0.1$ variance of the process for the bath at temperature T_1
- $A_d = 2.0$ variance of the process for the bath at temperature T_2
- $k = 0.1$ spring constant (same for all springs)
- $N_P = 100$ number of different simulations

The initial conditions are that all displacements and velocities are zero.

For each group of equations, we will take a look at the averages for the squared velocity of each particle $\langle v^2 \rangle$, looking at the time average and the ensemble average. The reason for this is that, from the equipartition theorem, we have:

$$T_i = \frac{m}{2} \left\langle v^2 \right\rangle$$

If the system is ergodic, it doesn't matter if we look at this average as being a time average or an ensemble average, it should be the same. For the cases of time average, we use the first out of the 100 simulations.

The results for the group of equations 2-2 is given below. In them we can see that, on average, all the simulations are such that the middle particle energy grows indefinitily (looking at the ensemble average). We can also see that the time average of the middle particle for the simulation we look at is always bigger than the time average of the baths (which must be due to the increasing energy with each iteration).

Now we take a look at the results for the group of equations 3.4.1 below. In this case, we will change the spring constant to $k = 0.01$ so that the result will be easier to see. This time, we can see that it's as if the middle particle doesn't move at all, although the heat baths don't change much (aside from their velocity oscilating very fast).

First, let us see the simple one dimensional harmonic oscillator consisting of a particle subject to an elastic force which obeys Hooke's law. This problem is described by the linear second order ODE

$$\ddot{x}(t) = -\omega^2 x(t),$$

where $\omega^2 = k/m$ (k being the elastic constant and m the particle mass) and its general solution for any initial value conditions $x(0)$ and $\dot{x}(0)$ is given by [Symon Mechanics]

$$x(t) = x(0) \cos \omega t + \frac{\dot{x}(0)}{\omega} \sin \omega t.$$

It is important to notice that our ODE can be written as a system of first order ODEs if we define a new variable $v(t) = \dot{x}(t)$ [Smale ODE], the velocity, which gives us

$$\dot{x}(t) = v(t)$$

$$\dot{v}(t) = -\omega^2 x(t),$$

because we will use this version of the equation for all the numerical solutions.

There are two other important things to remember about the dynamics. The first one is that this system conserves energy, which can be seen from the following derivation

$$mv \frac{dv}{dt} = \frac{m}{2} \frac{dv^2}{dt} = \frac{dE_k}{dt} = -kxv$$

$$kx \frac{dx}{dt} = \frac{k}{2} \frac{dx^2}{dt} = \frac{dE_p}{dt} = kxv$$

$$\frac{dE_k}{dt} + \frac{dE_p}{dt} = \frac{dE_T}{dt} = 0,$$

which means that the orbit of our system in the phase space is described by an ellipse [TaylorMechanics]

$$\frac{x^2}{2/k} + \frac{v^2}{2/m} = E_t.$$

An example is given in [fig:1], where we have taken $k = 0.5$, $m = 2$ and $E_t = 1$, where we disregard the units, since they don't matter to this analysis.

To simplify our second commentary, let us assume that $\dot{x}(0) = 0$. Then, since the velocity of the particle oscillates, the kinetic energy also oscillates

$$E_k = \frac{1}{2}mv(t)^2 = \frac{1}{2}m\omega^2 x^2(0)sin^2(\omega t).$$

From a purely dynamical point of view, this oscillations might be interesting, but they don't give us a clear picture on how big the total kinetic energy of our particle is (just think about comparing the kinetic energy of two out of phase oscillators), since at times its higher or lower. If we want to better compare two particles to see how much more energetic one is than the other, we need to take the average kinetic energy along the oscillation period (giving us a constant picture of the kinetic energy with time), which is [Moyses 2]

$$\overline{E_k} = \frac{1}{2\pi}\int_0^{2\pi} E_k(t)dt = \frac{1}{4}m\omega^2 x^2(0).$$

Also, using $E_p = (1/2)kx^2(t)$, we can find the total energy

$$E_T = \frac{1}{2}m\omega^2 x^2(0),$$

showing that it indeed is a constant of the motion.

3.5
Computational Methods

To solve our problem by computational methods, we first partition the time interval $[a, b]$, for which we want the solution, in N points $t_1 = a, t_2, t_3, \ldots, t_N = b$ separated by a constant time step $\Delta t = \tau$, which means we can obtain each by

$$t_{n+1} = t_n + \tau,$$

and we then approximate the graph of the function by a sequence of points $(t_n, \mathbf{x}_n)$ [Smale ODE]. All the methods we use here follow the general equation [Chapra Numerico]

$$x_{n+1} = x_n + \phi\tau$$

for each of the components of the vectors $\mathbf{x_{n+1}}$ and $\mathbf{x_n}$, where ϕ can be seen as an increment which might depend on all components in a multitude of ways.

In each of the simulations the parameters used were (the physical units are not important for the comparison of the computational methods):

– initial position $x(0) = 2$

– initial velocity $\dot{x}(0) = 0$

– mass $m = 1$

    – spring constant $k = 2$

    – time step $\tau = 0.01$

    – time interval size 30

With this, the exact solution is then $x(t) = 2cos(\sqrt{2}t)$.

For the comparison of the algorithms, we will be more interested in their energy conserving properties and thus shall look at the energy of the system along the time and its portrait in phase space.

3.5.1
Euler Method

The Euler Method is the simplest possible method, based on the approach of the evolution of the system by a taylor series truncated at the linear terms at each step

$$\mathbf{u}(t_n + \tau) \approx \mathbf{u}(t_n) + \tau \left(\frac{d\mathbf{u}}{dt} \right)_{t=t_n}$$

The resulting solution can be seen in figure [fig:2] together with the exact curve, letting us see how to Euler's method artificially makes the amplitude of the oscillations grow.

This method is convergent, meaning that for a fixed range of time, as $\tau \to 0$ we have that the approximation x_n converges to the true solution $x(t_n)$ [Quarteroni].

    > Absolute stability

However,

For small enough τ, this method works reasonably well since it is convergent (as $\tau \to 0$, the approximate solution converges to the true solution $x_n \to x(t_n)$ for a fixed time interval[Quarteroni]) it has the problem that, for a given time steps, the error grow without bounds as the time interval increases, so that the energy is not conserved, growing in an exponential rate [Giordano]. In fact, we have

$$v_{n+1} = v_n - \frac{k}{m}x_n\tau$$
$$x_{n+1} = x_n + v_n\tau$$

which we then square and multiply the first by $m/2$ and the second by $k/2$, getting

$$E_{c,n+1} = E_{c,n} - kx_nv_n\tau + \frac{k}{m}\tau^2 E_{p,n}$$

$$E_{p,n+1} = E_{p,n} + kx_n v_n \tau + \frac{k}{m}\tau^2 E_{c,n}$$

$$E_{t,n+1} = E_{t,n} + \frac{k}{m}\tau^2 E_{t,n}$$

showing that $E_{t,n}$ follows a geometric progression with rate $(1 + \frac{k}{m}\tau^2)$. Since this will be true even if we make any translation in the position, the Euler method also does not conserve energy for a linear harmonic chain.

In fact, a subtle increase can be observed in the amplitude of the oscillations in figure [fig:1], and the energy of our simulation is given in figure [fig:2], showing its growth by almost 35%.

We can also take a look at the phase space of the solution in figure [fig:3], which will be a spiral.

3.5.1.1
Runge Kutta

The second algorithm which we will use is the Runge Kutta family of methods, in specific the classical 2nd order and 4th order methods. In this method, we approximate the increment by a series.

$$\phi = \sum_{i=0}^{m}(a_i k_i)$$

For the second order, we have....

The resulting graph can be seen in figure [fig:4].

In this case, although the method does not exactly conserves energy, the energy changes very little with each step of the method, as seen in figure [fig:5]. Because of this, the phase space looks very much like a closed ellipse, as shown in figure [fig:6].

The fourht order Runge Kutta ....

The result is given in figure [fig:7].

In this case, the energy actually oscillates with a very small amplitude. In fact, we can only see the oscillations if we use a really small scale in our graph, as can be seen comparing figures [fig:8] and [fig:9]. Due to how small this oscillations are, the system's orbit describes an almost perfect ellipse in phase space, as seen in figure [fig:10].

3.5.1.2
Verlet

The Verlet algorithm is based on an approximation to the equation for the evolution of any quantity in the classical phase space

$$\frac{d\mathcal{A}}{dt} = \frac{\partial\mathcal{A}}{\partial t} + \{\mathcal{A}, \mathcal{H}\}$$

where $\{\mathcal{A}, \mathcal{H}\}$ is the Poisson Bracket, defined by the summation

$$\{\mathcal{A}, \mathcal{H}\} = \sum_{i=1}^{d \cdot N_p} \left[\frac{\partial\mathcal{H}}{\partial p_i}\frac{\partial\mathcal{A}}{\partial q_i} - \frac{\partial\mathcal{H}}{\partial q_i}\frac{\partial\mathcal{A}}{\partial p_i} \right] = \sum_{i=1}^{d \cdot N_p} \left[\dot{q}_i\frac{\partial\mathcal{A}}{\partial q_i} + \dot{p}_i\frac{\partial\mathcal{A}}{\partial p_i} \right]$$

which runs through the d degrees of freedom of each of the N_p particles ([salinas]). For the case of the density of states, Liouville's theorem states that $\frac{d\rho}{dt} = 0$.

It is possible to define a Liouville operator $\mathcal{L}$ by means of $i\mathcal{L}A = \{A, \mathcal{H}\}$, which helps find the solution using the exponential of our operator. If the partial derivative with respect to time is zero, then

$$\mathcal{A}(\mathbf{q}(t), \mathbf{p}(t)) = e^{i\mathcal{L}t}\mathcal{A}(\mathbf{q}(0), \mathbf{p}(0))$$

The idea of the Verlet Algorithm ([allentildesley]) is to define two "Liouville like" operators, $i\mathcal{L}_1$ and $i\mathcal{L}_2$ corresponding to evolutions only on position and momentum, respectively, such that $i\mathcal{L} = i\mathcal{L}_1 + i\mathcal{L}_2$, and then approximate the exponential for the time evolution as being

$$e^{i\mathcal{L}\delta t} \approx e^{i\mathcal{L}_2\delta t/2}e^{i\mathcal{L}_1\delta t}e^{i\mathcal{L}_2\delta t/2}.$$

Using $\mathcal{A}$ as being the vector in the phase space and applying our approximated evolution operator, we get the system of equations:

$$\mathbf{p}(t + \delta t/2) = \mathbf{p}(t) + \frac{\delta t}{2}\frac{d\mathbf{p}(t)}{dt}$$

$$\mathbf{q}(t) = \mathbf{q}(t) + \delta t\frac{1}{m}\mathbf{p}(t)$$

$$\mathbf{p}(t + \delta t) = \mathbf{p}(t + \delta t/2) + \frac{\delta t}{2}\frac{d\mathbf{p}(t + \delta t)}{dt}$$

We will give a summary of Langevin simulation here.

The Langevin equation is:

$$\boxed{\frac{dv}{dt} = -\gamma v + \eta(t)}$$

$$\frac{dx}{dt} = v$$

Where $\eta(t)$ is a gaussian stochastic process defined by the autocorrelation

function:

$$\langle \eta(t) \eta(t') \rangle = \Gamma \delta(t - t')$$

3.5.2
Solution

Theoretical Formulae:

$$\boxed{\langle v(t) \rangle = v_0 e^{-\gamma t}}$$

$$\boxed{\sigma_v^2 = \frac{\Gamma}{2\gamma} \left(1 - e^{-2\gamma t}\right)}$$

$$\boxed{\langle x(t) \rangle = x_0 + \frac{v_0}{\gamma} \left(1 - e^{-\gamma t}\right)}$$

$$\boxed{\sigma_x^2 = \frac{\Gamma}{\gamma^2} \left(t - \frac{2}{\gamma}(1 - e^{-\gamma t}) + \frac{1}{2\gamma}\left(1 - e^{-2\gamma t}\right)\right)}$$

3.5.3
Macroscopic Variables

We can relate our parameters with thermodynamics variables.

The ensemble average in the equilibrium (the limit when $t \to \infty$) is:

$$\left\langle v^2 \right\rangle = \frac{\Gamma}{2\gamma}$$

From the kinetic theory, we also know that

$$\frac{1}{2} m \left\langle v^2 \right\rangle = \frac{1}{2} k_B T$$

Using the two equations together, we get:

$$\boxed{\Gamma = \frac{2\gamma k_B T}{m}}$$

Looking at the asymptotic behavior of the variance of the position of the particle, which gives us a relation with the diffusion coefficient.

$$2D = \frac{\Gamma}{\gamma^2}$$

$$D = \frac{k_B T}{m\gamma}$$

$$\gamma = \frac{k_B T}{mD}$$

However, for spherical particles of radius a, we could also use stokes-law for the drag coefficient.

$$\gamma = \frac{6\pi\mu a}{m}$$

3.6
Simulation

And can be solved by the Euler method, using the iterations:

$$v_{n+1} = v_n - \tau\gamma v_n + \sqrt{\tau\Gamma}\xi_n$$

$$x_{n+1} = x_n + \tau v_n$$

Where $\tau = \Delta t$ is the time step used in the method and ξ_n is a sequence of random variables sampled from a gaussian distribution $\mathcal{N}(0, 1)$.

The used parameters and the results are given below.

– Noise amplitude: $\Gamma = 0.1$

– drag coefficient: $\gamma = 0.1$

– initial velocity: $v_0 = 1.0$

– initial position: $x_0 = 0.0$

– time step: $\tau = 0.0001$

– Number of particles in the ensemble: $N_p = 200$

3.6.1
Euler

3.6.1.1
Stochastic Runge Kutta

4
Thermal Diode

5
Conclusions

The conclusions are what we conclude.

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Pseudo-Random Number Generator

Discussing RNGs.