Pontifícia Universidade Católica
do Rio de Janeiro

Alexandre Augusto Abreu Almeida

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

Rio de Janeiro
April 2020

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dedication.

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I would like to first thank my advisor ...

Then I wish to thank ...

Abstract

Abreu Almeida, Alexandre Augusto; Anteneodo, Celia (Advisor). **Thermal conduction in a chain of oscillators**. Rio de Janeiro, 2020. 31p. Dissertação de mestrado – Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro.

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

Thermal Conduction; Fourier's Law; Oscillator; Chain of Oscillators;

Resumo

Abreu Almeida, Alexandre Augusto; Anteneodo, Celia. **Condução térmica em uma cadeia de osciladores**. Rio de Janeiro, 2020. 31p. 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

Condução Térmica; Lei de Fourier; Oscilador; Cadeia de Osciladores;

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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 Thermodynamics (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 $T_1 > T_2$.

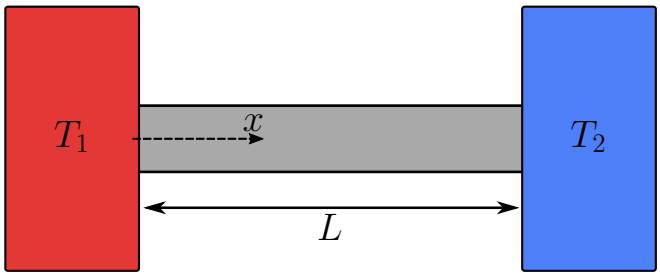

Figure 2.1: one dimensional heat transport

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.

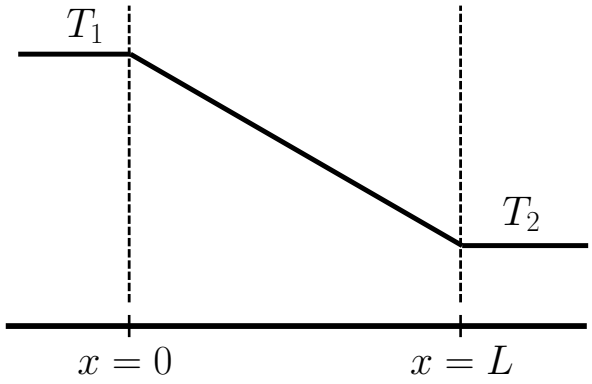

Figure 2.2: linear temperature profile.

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.

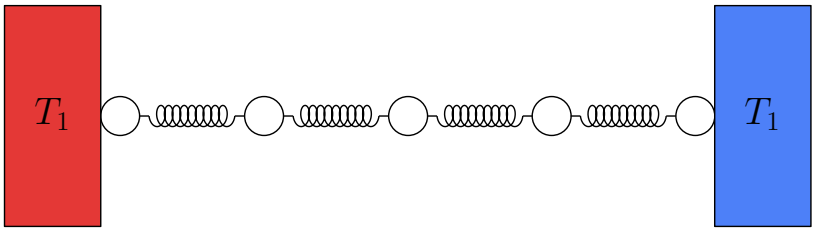

Figure 2.3: pictorial representation of the mathematical model

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

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

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 [7]. 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 [8].

Such an equation can be written as

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

where the $-\gamma\dot{r}$ term represents a drag force due to the media and η is a Wiener random process. The stochastic force represented by η can be seen as averaging all the fast degrees of motion from the system.

The solution of a particle that only follows this simple equation is already well established in the literature and it shall be shown here following [9] (use Green's function).

Let the Langevin equation in one dimension be rewritten as the system of equations

$$\begin{aligned} \frac{dv}{dt} &= -\gamma v + \eta\,(t)\,; \\ \frac{dx}{dt} &= v; \end{aligned} \tag{2-2}$$

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

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

v is the particle velocity and x is the particle position. Since η is a stochastic process, it follows that x and v are actually random variables in this description.

It can be shown that the following equations are valid for the mean and variance of the position and velocity:

$$\begin{aligned}
&\langle x(t)\rangle = x_0 + \frac{v_0}{\gamma}\left(1-e^{-\gamma t}\right);\\
&\sigma_x^2 = \frac{\Gamma}{\gamma^2}\left(t - \frac{2}{\gamma}(1-e^{-\gamma t}) + \frac{1}{2\gamma}\left(1-e^{-2\gamma t}\right)\right);\\
&\langle v(t)\rangle = v_0 e^{-\gamma t};\\
&\sigma_v^2 = \frac{\Gamma}{2\gamma}\left(1-e^{-2\gamma t}\right)
\end{aligned} \tag{2-3}$$

The parameters that describe this equation can also be related to the macroscopic thermodynamic variables describing the system. In the limit when $t \to \infty$ it achieves equilibrium and from the previous equations the ensemble average will be

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

and from classical statistical mechanics the equipartition theorem gives

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

result that can be replaced in the previous equation to show that

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

The asymptotic behavior of the position's variance relates with the diffusion coefficient such that

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

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

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].

(Discuss the solution of the corresponding Fokker Planck equation in [5])

(Discuss Peierls, 1929?)

(How to introduce the first models that work?)

2.4.1 Anharmonic models

> 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

$$\dot{p_i} = -\frac{\partial \mathcal{H}}{\partial q_i},\ \dot{q_i} = \frac{\partial \mathcal{H}}{\partial p_i},$$

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

$$\begin{aligned}
\frac{dq_i}{dt} &= \frac{p_i}{m_i} \\
\frac{dp_i}{dt} &= -k_i(q_i - q_{i-1}) + k_i(q_{i+1} - q_i) - \frac{2\pi V_{0,i}}{a_s}\sin\left(\frac{2\pi q_i}{a_s}\right)
\end{aligned}$$

Rewriting,

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

2.5 Model used

3
Computational Methods

Depending on which of the toy models brought forward in chapter 2 for the bath and chain of particles one uses it may be really hard or even impossible to fin an analytical solution. Thus it is common to use computational methods to simulate such a system and watch its dynamical behavior in some time interval $[a, b]$.

To be able to use a computer for such a task one first needs to make a partition of the time interval. Consider then such a partition having N points $t_1 = a, t_2, t_3, \ldots, t_N = b$ all separated by a constant time step $\Delta t = \tau$, meaning that $t_{n+1} - t_n = \tau$ for all $n \in \{1, 2, 3, \ldots, N\}$. They can be written in terms of t_1 as

$$t_{n+1} = t_1 + n \cdot \tau.$$

In the case of deterministic baths the equations to be solved consist of a system of ordinary differential equations whose graph will me approximated on the partition points.

However when one is looking at the stochastic baths all the variables of interest have to be seen as random variables which means that instead of finding an approximation to a given graph what is needed is to make sure that the statistical properties of the equations are satisfied.

Since many methods for the solution of stochastic differential equations are adaptations of the deterministic ones, it is interesting to discuss the later first.

(Given that most of the chain do not interact directly with the random variables, maybe one can also draw approximate conclusions to the problem at hand)

3.1
Deterministic

In the case of a system of ordinary differential equations, the position of each particle may be seen as a function of time $x = x(t)$ to be approximated.

[Show the result of simulating a simple harmonic motion with each method]

3.1.1 Euler's Method

The Euler's Method consists of approaching 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 derivative is then given by the ordinary differential equation itself

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

(the bold font is here used to indicate vector quantities).

When the time step goes to zero, $\tau \to 0$, the approximate solution is known to converge (zero-stability) under certain weak assumptions on the ODEs [10] and thus it is to be expected that for small enough τ and a fixed time interval such a 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 [11].

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. Let the equations of motion be

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

Using the approximation for Euler's method one would then write

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

and squaring both sides of the equations, multiplying them by $m/2$ and $k/2$, respectively, and then summing them the end result is

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

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

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

Mathematically this problem is due to the region of "absolute stability" of the method.[?????]

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).

3.1.2 Runge Kutta

Another commonly used algorithm is the Runge Kutta family of methods, mostly the classical 2nd order and 4th order methods. In this method, the increment is approximated by a series.

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

For the second order, ...

In this case, although the method does not exactly conserves energy, the energy changes very little with each step of the metho. Because of this, the phase space looks very much like a closed ellipse.

The fourht order Runge Kutta ....

In this case, the energy actually oscillates with a very small amplitude. In fact, the oscillations can only be seen by looking at simulation results with a really small scale. Due to how small this oscillations are, the system's orbit describes an almost perfect ellipse in phase space.

3.1.2.1 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 [25]. 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 the 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, liquid simulation]) 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 the approximated evolution operator, one gets the system of equations:

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

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

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

3.2 Stochastic

Computational models for solving stochastic differential equations.

[Discuss pseudo random number generators?]

3.3 Euler's Method

The Langevin Equation 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 $\mathcal{N}(0, 1)$.

4
Thermal Diode

When simulating an asymmetrical particle chain with the many models discussed here one is faced with a thermal diode.

5
Conclusions

The conclusions are what we conclude.

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