



Alexandre Augusto Abreu Almeida

Study of a simple model for a thermal diode

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.

Acknowledgments

I would like to first thank my advisor ...

Then I wish to thank ...

Abstract

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We simulate a thermal diode by means of a chain of oscillators with nonlinear potentials and show the effects of a power law potential in such a model.

Keywords

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

Resumo

Abreu Almeida, Alexandre Augusto; Anteneodo, Celia. **Estudo de um modelo simples para um diodo térmico**. Rio de Janeiro, 2020. 53p. Dissertação de Mestrado – Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro.

Nós simulamos um diodo térmico a partir de uma cadeia de osciladores com potenciais não lineares e mostramos os efeitos de um potencial do tipo lei de potência neste modelo.

Palavras-chave

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

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My beautifull epigraph

Alguém, *Algum livro.*

List of Abbreviations

ADI – Análise Digital de Imagens

BIF – *Banded Iron Formation*

... – ...

1

Introduction

In 2006, four researchers from the University of California at Berkeley published what was perhaps the first experimental evidence of a thermal diode, a material whose thermal conductivity along a given axis changed depending on the direction of the heat flux along it [1].

They used an experimental apparatus consisting of two pads with platinum resistors that could operate as either a heater - through Joule effect - or as a sensor - through their resistivity variation with temperature.

Each pad was connected to each end of a nanotube which was coated inhomogeneously with Trimethyl-cyclopentadienyl platinum ($C_9H_{16}Pt$) and measured the conductivity along its axis with two different configurations, the first one with the heater on the side with more mass and then with the heater on the side with less mass, effectively changing the direction of heat flow. The experiment was repeated with different materials (carbon nanotubes - CNTs - and boron nitride nanotubes - BNNTs) which had high thermal conductivity, when compared to the hydrocarbon, dominated by phononic carriers.

What was surprising was that the magnitude of the heat flow changed, with the material's thermal conductivity changing as much as 7%. After that, different groups were able to devise new ways of obtaining such asymmetric conductivity obtaining higher and higher differences [2, 3].

Many theoretical ways of building such a device were proposed before this first experimental evidence with the first such case that we found dating as far back as 2002 by Terraneo, Peyrad and Casati [4], but to even begin to study how this phenomenon occurs a first discussion on the basics of heat conduction and of the theory of thermal conductivity in solids is needed.

1.1

Theory of heat conduction

Before diving into the microscopic understanding of the problem at hand, we need first to look at the basic macroscopic heat conduction problem to develop some intuition.

First consider a system describing a given volume $V \in \mathbb{R}^3$ with normal vector \vec{n} pointing outside, as in figure 1.1.

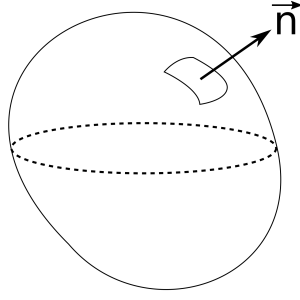


Figure 1.1: Control volume system

The first law of thermodynamics tells us that

$$\frac{dU}{dt} = \dot{Q} - \dot{W},$$

where \dot{Q} is the rate of heat that enters my system and U is our internal energy. Assuming no external work is applied, we get a kind of continuity equation using the specific internal energy u (which is an internal energy density) and rewriting the rate of heat as the surface integral of the heat flux through our system, giving us

$$\frac{d}{dt} \iiint_V u dV + \iint_{\partial V} \vec{q} \cdot \vec{n} dS = 0,$$

where the change in the heat signal is due to it being antiparallel to the surface normal vector.

Now assuming our system is sufficiently smooth so that we can put the derivative inside the integral and apply Gauss' theorem on the second term, together with rewriting everything using the specific heat capacity $u = C\rho T$ gives us

$$\iiint_V C\rho \frac{\partial T}{\partial t} + \vec{\nabla} \cdot \vec{q} dV = 0 \implies C\rho \frac{\partial T}{\partial t} + \vec{\nabla} \cdot \vec{q} = 0.$$

In the XIX century, the mathematician Jean-Baptiste Joseph Fourier coined the law that takes his name, Fourier's law of conduction, which says that the flow of heat that appears in a material due to a temperature gradient is linear with respect to such a gradient, so mathematically we have

$$\vec{q} = -\kappa \vec{\nabla} T$$

where \vec{q} is the flux of heat through a given system and κ is the system's thermal conductivity, that is always positive. Together with the first law of thermodynamics, we have a derivation of the famous heat equation

$$\alpha^2 \frac{\partial T}{\partial t} - \nabla^2 T = 0,$$

where $\alpha = C\rho/\kappa$, which describes the dynamics of the temperature of our system with time.

Let us look at a simple one dimensional case. 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 $T_1 > T_2$.

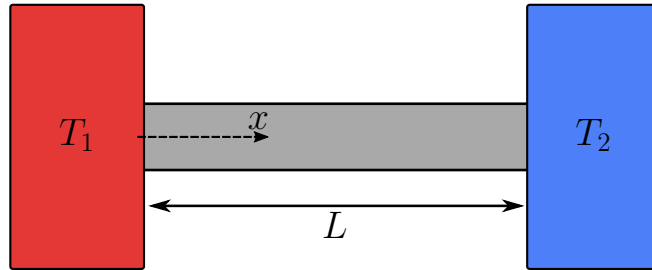


Figure 1.2: one dimensional heat transport

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, as in figure 1.1. This can also be rigorously proven from an analysis of the heat equation.

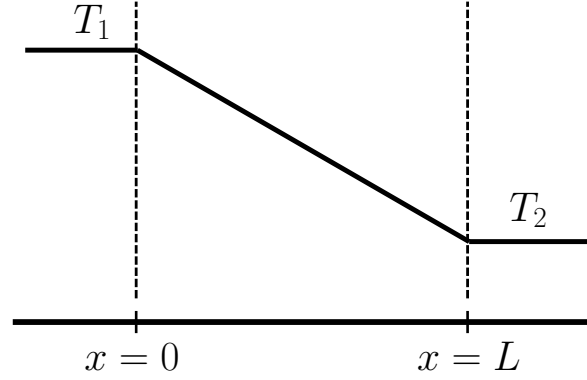


Figure 1.3: linear temperature profile.

If we replace this result back to Fourier's law we get

$$\frac{\dot{Q}}{\Delta T} = -\frac{\kappa}{L},$$

where $\Delta T = T_2 - T_1$, showing us that the heat flow is inversely proportional to the length of our bar.

The theoretical proposals for thermal diodes came as a development of many works that tried to understand what properties are needed by microscopic models to reproduce both these macroscopic heat conduction properties.

1.2

Thermal conductivity of solids

Most solids are composed by a regular lattice of atoms or ions that vibrates near their equilibrium positions. They can have first neighbors interactions or long range interactions, with the simplest description seen in introductory solid state physics books being a chain of atoms interacting harmonically with their first neighbors, such as depicted in figure 1.4.



Figure 1.4: Lattice of atoms

The vibrations of this lattice have varying degrees of importance for describing the thermal conductance of solids.

Solids are classified in accordance to its electrical conductance as conductors and insulators if their electrical conductivity is high or low, respectively. Conducting solids however are usually also good thermal conductors, for their

free electrons act as the main thermal energy carrier in the material. In this case, although the lattice vibrations have to be taken in account explain some phenomena, they are generally higher order corrections.

Insulators, however, although they do not have such good thermal conductance for they lack electrons in free conducting bands of energy, they do conduct heat with their main carrier being these lattice vibrations. These vibrations carry energy on their normal modes, which can interact between themselves and with other systems such as X-ray electrons, as well as propagate along the crystal as wave packets.

Quantum mechanically these excitations can be described as quasiparticles called phonons, permitting us to describe the heat transport of insulators by means of a kinetic theory of phonons. In this case, the phononic version of the Boltzmann equation is called Peierls-Boltzmann equation, in honor to sir Rudolf Ernst Peierls who first discovered it.

He is also credited with another important discovery for this work, which is the importance of anharmonic interaction terms to the conduction of heat. In fact, perfectly harmonic crystals would have infinite thermal conductivity.

The argument, which can be found in his book *Quantum theory of solids*, first published in 1955, and in [5], goes as follows: In a perfectly harmonic crystal the distribution of phonons is always composed of stationary states and as such if we prepared them in a way that they were transporting heat, they would stay that way forever, meaning that the crystal would have infinite thermal conductivity.

The Hamiltonians of a solid lattice then need to contain higher order potential energy terms

$$U_{anh} = \sum_{i,j,k} \frac{1}{3!} \frac{\partial^3 U}{\partial u_i \partial u_j \partial u_k} \bigg|_{\mathbf{u}=0} \cdot u_i u_j u_k + \sum_{i,j,k,l} \frac{1}{4!} \frac{\partial^4 U}{\partial u_i \partial u_j \partial u_k \partial u_l} \bigg|_{\mathbf{u}=0} \cdot u_i u_j u_k u_l,$$

to be able to describe the dynamics of heat flowing through a solid. These corrections give rise to umklapp processes, which are phonon-phonon interactions that do not conserve the total crystal momentum, giving rise to some thermal resistance in the material.

Problems with the harmonic model have also been shown from the point of view of classical statistical mechanics by Rieder, Lebowitz and Elliot Lieb in [6], where they solved exactly the problem of a harmonic chain of particles in contact with two heat baths at different temperatures using a generalized Liouville equation.

They showed that the chain shows a heat current proportional only to the temperature difference between both heat baths $J \propto (T_2 - T_1)$, instead of the

temperature gradient we saw in section 1.1, and that the kinetic temperature, defined as $\langle p_n \rangle$ where p_n is the momentum from the n -th particle, is uniform along the chain with value $0.5 \cdot (T_2 - T_1)$, instead of the linear temperature profile we would expect from Fourier's law.

After their work, many others followed suit to understand if anharmonicity was enough to reproduce the results from heat conduction or if other properties are needed, such as non conservation of momentum.

We can cite many models that were able to reproduce these results, such as the ding-a-ling model, the ding-dong model, the Frenkel-Kontorova model and the ϕ^4 model. Others, like the Fermi-Pasta-Ulam-Tsingou only approximately shows the wanted properties.

All these works culminated in the proposal of thermal rectification using an asymmetric chain of particles.

1.3

Thermal diode

In 2002, Terraneo, Peyrad and Casati [4] published a paper on low dimensional heat conduction using harmonic interactions between the particles and a Morse external potential $V(x) = D(\exp(-\alpha x) - 1)^2$, and showed that when D varies along the chain we could theoretically have a thermal rectifier.

The rationale presented was that changing this parameter, the phonon bands in different parts of the chain stop overlapping impeding the phonons to travel along.

Following this work, Baowen Li, Lei Wang and Casati showed in 2004 [7] such a heat current rectifying mechanism in a 1D nonlinear lattice with a Frenkel-Kontorova external potential $A \cos(2\pi x_i)$ and an harmonic interaction by choosing different parameters for the left and right segments of the lattice.

Like we stated previously, then came the experimental confirmation of a thermal diode in 2006 [1], albeit with a really small efficiency. Many other papers followed suit with new ways of achieving this asymmetrical thermal conductivity, striving to achieve higher and higher efficiencies, with a work in 2015 by Martínez-Pérez, Fornieri and Giazotto, from Italy, showing a heat current in one direction two orders of magnitude higher than the heat current in the opposite direction when combining normal metals with superconductors [3].

Such devices could be very interesting from an applied point of view due to their potential uses in nanoscale thermal transport, for example in solar cells for energy harvesting, although it could also be used for radiation detection or in the field of quantum information [3], and the control of phonons is already a

field of its own called phononics where they can be used as information carriers [29], in stark contrast with their view nowadays as wasted energy.

The study of thermal transport in low dimensions still have many lingering questions being explored [32], and in this work we shall look at the effects of power law potentials on thermal diodes.

2

Modelling Heat Flow

2.1

Toy Models

(best to put something more generic)

(Put some results on heat transport in this chapter)

(we don't need to say that are springs that follows Hooke's law. Try to be more general)

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 a harmonic potential.

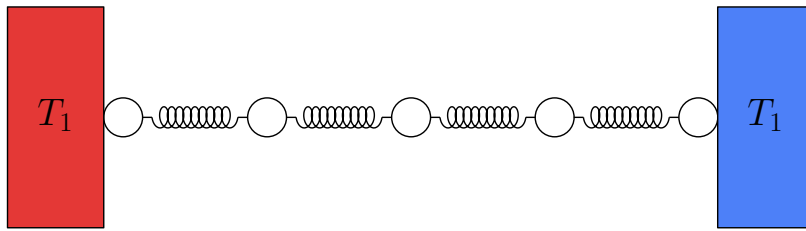


Figure 2.1: pictorial representation of the mathematical model

Many changes to this simple toy model will be discussed throughout the text, 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 ([6]) 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 adds 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.

(instead of $k(x_1-x_2)$, put a Force $F(x_{i-1}, x_i, x_{i+1})$, something more generic)

(We will discuss here that we use Langevin, but after we remember that there are other methods, and the result should not depend on the specific bath chosen)

The equations of motion will then be

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

(Here what is important is that the middle are not affected by the thermal baths terms directly)

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

2.2

Heat Baths

In an equilibrium situation, many techniques are used to try and maintain the system at a constant temperature, such as re-scaling the particle velocities in each time step, changing the Hamiltonian of the thermal bath particles [8], and using stochastic equations to describe the thermal noise [9].

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 [9].

2.2.1

Nose-Hoover thermostat

(Nose-Hoover is a deterministic equation, other implementation)

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 [8]. Using the same notation as in [10], 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

We use the stochastic approach with the Langevin equation.

2.2.2

Langevin thermostat

(try to avoid putting everything with upper case letters!!!!)

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 [11]. Paul Langevin tried to explain the phenomena using Newton's second law in 1908 by adding a random force that nowadays we recognize as being a Wiener random process and thus devising the Langevin equation [12].

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 [13] (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:

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

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

and from classical statistical mechanics the equipartition theorem gives

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

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

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

(maybe do this development by text)

(Green kubo is interesting, but no time)

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

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

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

2.3

Particle chain

(here we can rewrite F using Hooke's law)

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 [5].

Such an idea is commonly developed based on 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 a harmonic crystal in a stationary state between two heat baths of unequal temperatures 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) [6].

(Discuss the solution of the corresponding Fokker Planck equation in [9])

(Discuss Peierls, 1929?)

(How to introduce the first models that work?)

(Try to discuss harmonic, FPUT - both of which doesn't follow Fourier - quartic and frenkel kontorova)

(Maybe cite Carlos Olivarez, because his was a more general case of ours)

2.3.1

Anharmonic models

> Fermi Pasta Ulam Tsingou

(this is not a quartic pinning, its a quartic interaction between neighbors)

2.3.2

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 $i = 2, 3, \dots, N-1$:

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

Rewriting,

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

$$\mathcal{H} = \sum_{n=1}^N \frac{p_n^2}{2m_n} + \frac{k_n}{2} (x_n - x_{n-1} - a)^2 + V_{0,n} \left[1 - \cos\left(\frac{2\pi x_n}{a_s}\right) \right],$$

where x_n denotes the position of the n -th particle. However, we can remove the distance a between equilibrium positions from the hamiltonian by using the displacement from equilibrium $q_n = x_n - n \cdot a$ and assuming that the minima from the periodic potential coincides with the equilibrium positions (said another way, $a/a_s \in \mathbb{N}$), we rewrite our equation as

$$\mathcal{H} = \sum_{n=1}^N \frac{p_n^2}{2m_n} + \frac{k_n}{2} (q_n - q_{n-1})^2 + V_{0,n} \left[1 - \cos\left(\frac{2\pi q_n}{a_s}\right) \right],$$

2.4

Thermal Diode

Try to make something more general, so always try to describe in greater generality.

Always go from "General" \Rightarrow "Particular"

Show the results we have for Kontorova too, it is interesting.

But we can discuss it at the end of the thermal diode part.

REMEMBER TO DISCUSS THE FIXED BOUNDARY CONDITIONS.

Show Fourier's law.

For the ϕ^4 , the results are known. But for Frenkel Kontorova, we don't know.

2.4.1

Assymetry

2.4.2

Interphase Potential

3

Solution Methods

3.1

Analytical Methods

3.2

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 find 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 $t_1 = a, t_2, t_3, \dots, t_N = b$ all separated by a constant time step $\Delta t = \tau$, meaning that $t_{n+1} - t_n = \tau$ for all $n \in \{1, 2, 3, \dots, N\}$. 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 be 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 latter 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)

(The comparison of methods we have done, put here! Describe more with graphs, not only text)

3.2.1

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]

3.2.1.1

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, $\tau \rightarrow 0$, the approximate solution is known to converge (zero-stability) under certain weak assumptions on the ODEs [14] 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 [15].

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

$$\begin{aligned} \frac{dv}{dt} &= -\frac{k}{m}x \\ \frac{dx}{dt} &= v. \end{aligned}$$

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

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

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).

3.2.1.2 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 conserve energy, the energy changes very little with each step of the method. Because of this, the phase space looks very much like a closed ellipse.

The fourth 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 these oscillations are, the system's orbit describes an almost perfect ellipse in phase space.

3.2.1.3 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 [16]. 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 $i\mathcal{L}\mathcal{A} = \{\mathcal{A}, \mathcal{H}\}$, 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:

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

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

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

3.2.2 Stochastic

Computational models for solving stochastic differential equations.

[Discuss pseudo random number generators?]

3.2.2.1**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

Results

In chapter 2 we have discussed the main building blocks for a simple toy model that reproduce the same linear temperature profile as a diffusion problem following Fourier's law, and we have also discussed how the rectification of heat current can come from asymmetries in the particle chain. Now we shall put everything together and see how some of them affect the rectification of the heat current, focusing mainly on changing the parameters for the interphase potential.

The Hamiltonian of the chain of particles will be

$$\mathcal{H} = \sum_{n=1}^N \frac{p_n^2}{2m_n} + U_{int,n}(q_n, q_{n-1}) + U_{ext,n}(q_n),$$

and we then find the dynamics of the system by means of Hamilton's equations.

The chain is always assumed to be composed of two parts, a left one consisting of particles $n \leq N/2$ and a right one for particles $n > N/2$ and although the functional form of the potentials for each one will be the same, their parameters will be different.

For the first neighbor interaction potential inside each part, we used the harmonic potential $U_{int} = k_n (q_n - q_{n-1})^2 / 2$, where $k_n = k_L$ for particles on the left chain and $k_n = k_R$ for the ones on the right chain, while the interphase interaction between them was described by a power law potential

$$U_{int}(q_{N/2}, q_{N/2+1}) = \frac{k_\mu}{\mu} |q_{N/2} - q_{N/2+1}|^\mu.$$

For the external potential $U_{ext,n}(q_n)$ we first used the Frenkel-Kontorova potential

$$U_{ext,n} = V_n \left[1 - \cos \left(\frac{2\pi q_n}{a_s} \right) \right],$$

and afterwards the ϕ^4 potential

$$U_{ext,n} = \frac{V_n}{4} q_n^4$$

was used, which showed better convergence properties. In both cases we consider that $V_n = V_L$ for $n \leq N/2$ and $V_n = V_R$.

The thermal baths have temperatures T_L and T_R and are in contact with particles 1 and N , respectively. They are modeled as Langevin heat baths by the addition of a drag force $-\gamma p_n/m_n$ and white noises η_L and η_R , each one with variances $2\gamma k_B T_L/m_1$ and $2\gamma k_B T_R/m_N$, to the equations of motion for the momenta of these particles because such a heat bath cannot be written as a Hamiltonian.

The last important block to finish building our toy model are the boundary conditions, which in our case were fixed boundary conditions meaning that they can be thought of as virtual particles ("zeroth particle" and a "N+1-th particle") that are always at their equilibrium positions $q_0(t) = q_{N+1}(t) = 0$ and only interacts with the first and last particles, respectively.

4.1

Simulations

Due to the considerations laid out on chapter 3, all simulations were made using the fourth order stochastic Runge Kutta method, taking advantaged of the fact that our model for the Langevin heat bath consist only of additive noise terms.

One last consideration for the simulation is that instead of inputting all the parameters directly in the simulation, we defined some closely related ones that gives us deeper physical understanding of the system while decreasing the number of inputs. This was also done in order to more closely follow and compare our results with the work by Baowen Li, Lei Wang and Giulio Casati [7], although we make one small change.

Thus to begin with we define the mean temperature between the baths as $T_m = (T_L + T_R)/2$ and their difference, as a percentage of this mean temperature, is given by $\Delta = (T_L - T_R)/T_m$, while the ratio between the properties of the left and the right chain is $\lambda = k_R/k_L = V_R/V_L$. We shall also consider all particles as having unit mass $m_n = 1$ and in the case of the Frenkel-Kontorova potential we assume $a_s = 1$, making its minima coincide with the equilibrium positions of each particle (assumed to be on the integer values of the real line).

All simulations are wrote in terms of velocities, which can be gotten from the momenta equations by using $v_n = p_n/m_n$, but since in our case we assume unit masses, the numerical value of the both will be the same and the equations will have the same functional forms.

4.1.1

The Frenkel-Kontorova model

As seen previously, the Frenkel-Kontorova model consists of adding a periodic external potential to our system, which together with our previous considerations gives us for the momenta of the particles in contact with the baths,

$$\begin{aligned}\frac{dp_1}{dt} &= -k_L(2q_1 - q_0 - q_2) - 2\pi V_L \sin(2\pi q_1) - \gamma p_1 + 2\gamma k_B T_L \epsilon_1(t), \\ \frac{dp_N}{dt} &= -k_R(2q_N - q_{N-1} - q_{N+1}) - 2\pi V_R \sin(2\pi q_N) - \gamma p_N + 2\gamma k_B T_R \epsilon_2(t),\end{aligned}$$

where $\epsilon_1(t)$ and $\epsilon_2(t)$ are white noises with zero mean and unit variances $\langle \epsilon_1(t) \epsilon_1(t') \rangle = \delta(t - t')$ and $\langle \epsilon_2(t) \epsilon_2(t') \rangle = \delta(t - t')$, while for the interphase particles between both sides of the chain we have

$$\begin{aligned}\frac{dp_{\frac{N}{2}}}{dt} &= -k_L(q_{\frac{N}{2}} - q_{\frac{N}{2}-1}) - k_\mu \frac{|q_{\frac{N}{2}} - q_{\frac{N}{2}+1}|^\mu}{q_{\frac{N}{2}} - q_{\frac{N}{2}+1}} - 2\pi V_L \sin(2\pi q_{\frac{N}{2}}), \\ \frac{dp_{\frac{N}{2}+1}}{dt} &= -k_R(q_{\frac{N}{2}+1} - q_{\frac{N}{2}+2}) - k_\mu \frac{|q_{\frac{N}{2}+1} - q_{\frac{N}{2}}|^\mu}{q_{\frac{N}{2}+1} - q_{\frac{N}{2}}} - 2\pi V_R \sin(2\pi q_{\frac{N}{2}+1}),\end{aligned}$$

and finally for the rest of the particles the momenta equations of motion are

$$\begin{aligned}\frac{dp_n}{dt} &= -k_L(2q_n - q_{n-1} - q_{n+1}) - 2\pi V_n \sin(2\pi q_n), \\ n &= 2, 3, \dots, \frac{N}{2} - 1, \frac{N}{2} + 2, \frac{N}{2} + 3, \dots, N - 1,\end{aligned}$$

where $V_n = V_L$ for the left chain particles and $V_n = V_R$ for the right chain particles.

The equations of motion for particle's displacements from equilibrium are

$$\frac{dq_n}{dt} = p_n, n = 1, 2, \dots, N,$$

and the initial conditions for the simulation were $q_n(0) = p_n(0) = 0$.

4.1.1.1

FK-Fourier varying VL

Simulation parameters:

- Number of samples: 100
- Number of particles: 20
- Time step: 0.001

- Total simulation time: 300000.0
- Transient time: 100000.0
- Mean temperature: 0.09
- Temp diff: 0.5
- chain ratio $\lambda = 1.0$,
- spring constant between segments $k_{int} = 1.0$,
- power law coefficient $\mu = 2.0$,
- amplitude of the potential on the left [varying],
- chain spring constant on the left $k_L = 1.0$,
- drag coefficient, $\gamma = 1.0$,

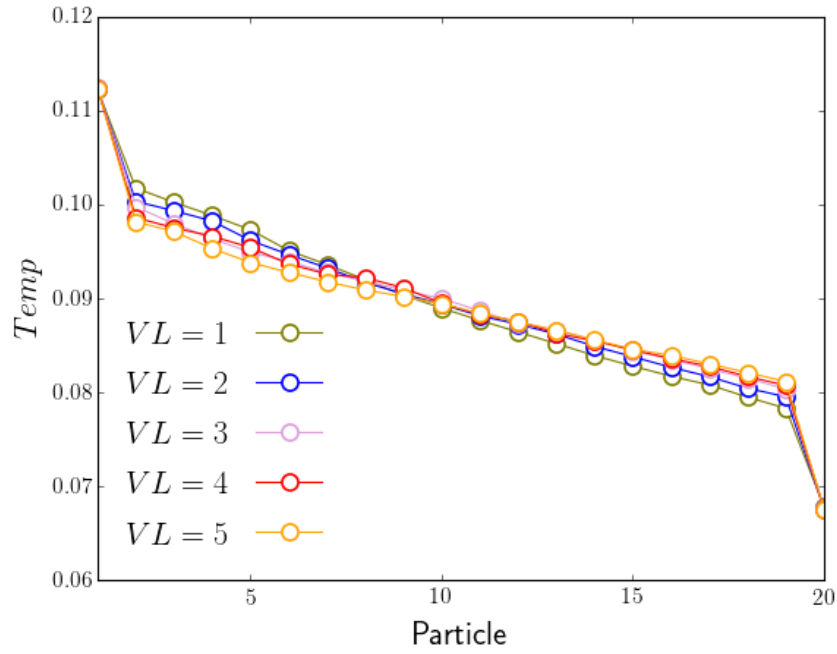
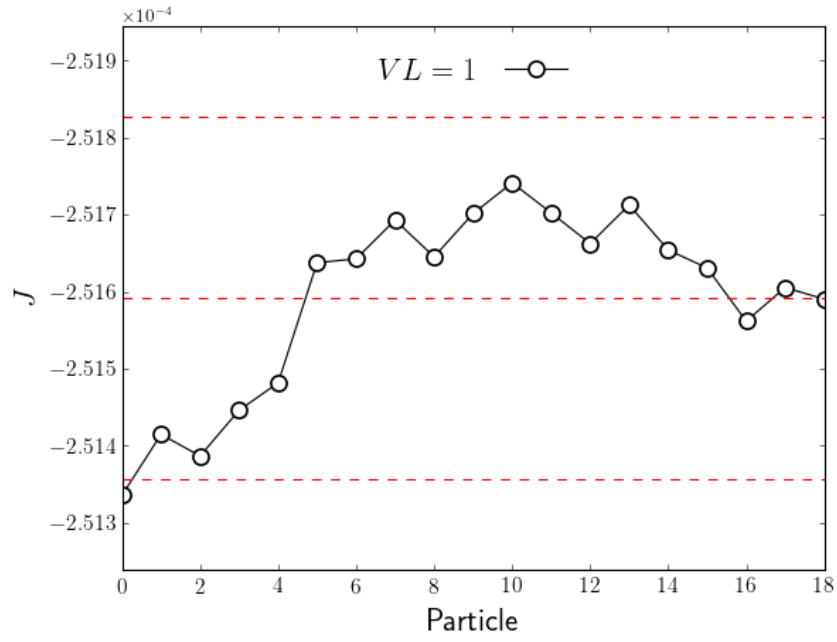
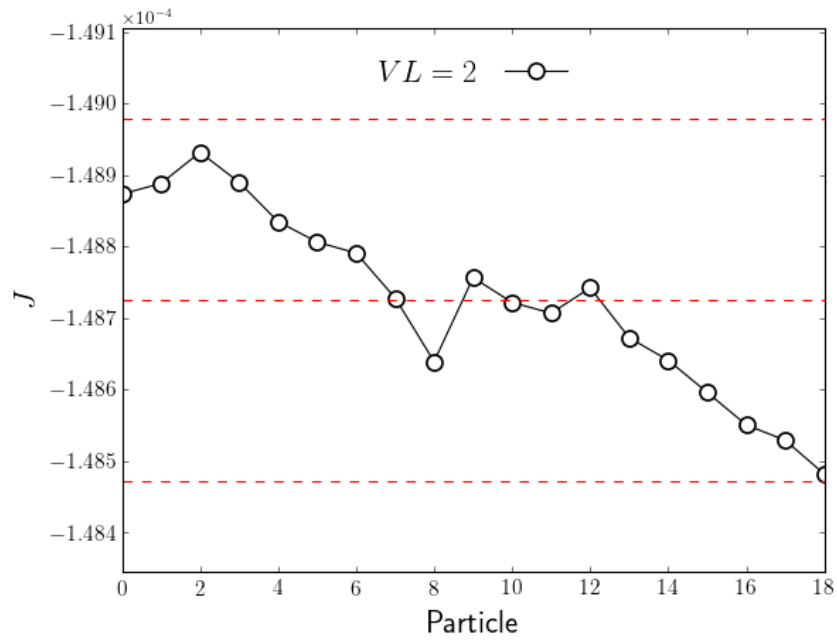
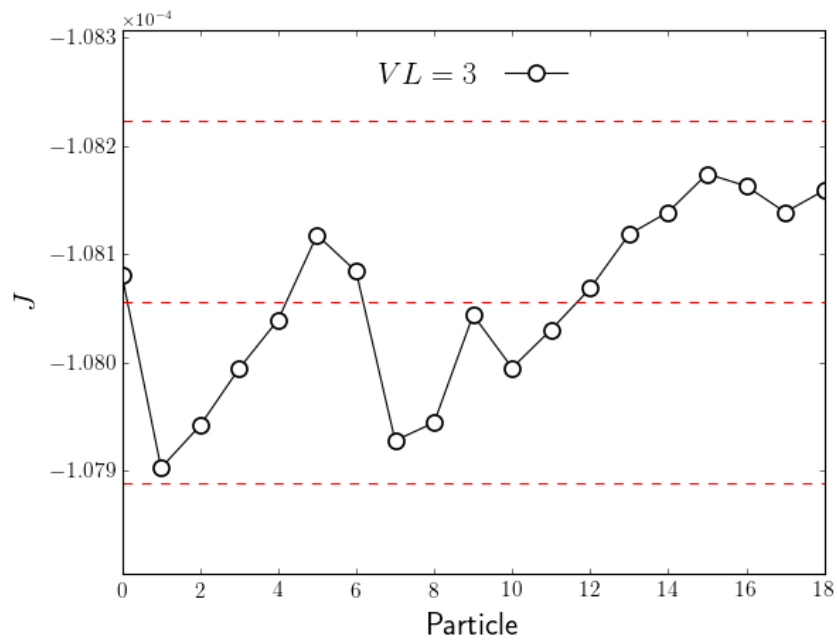
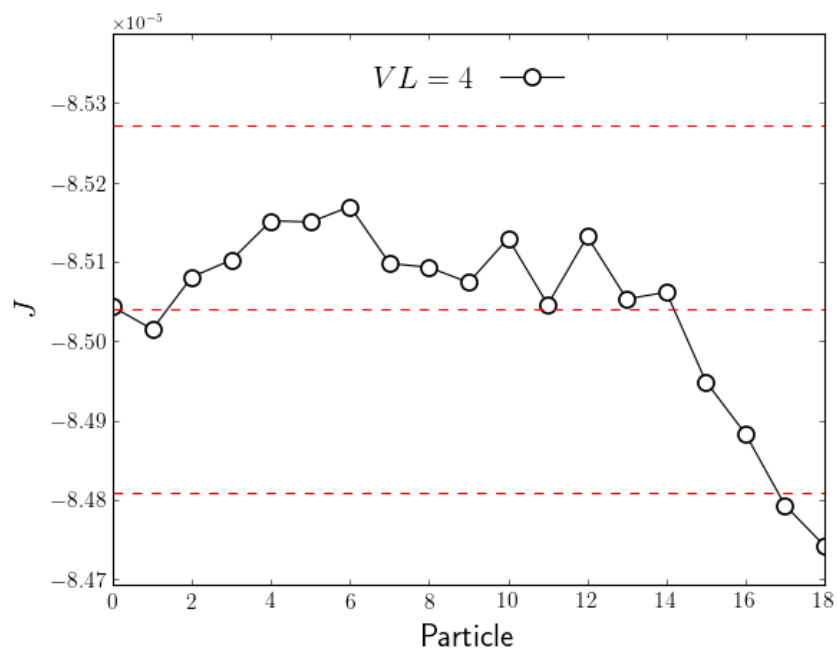
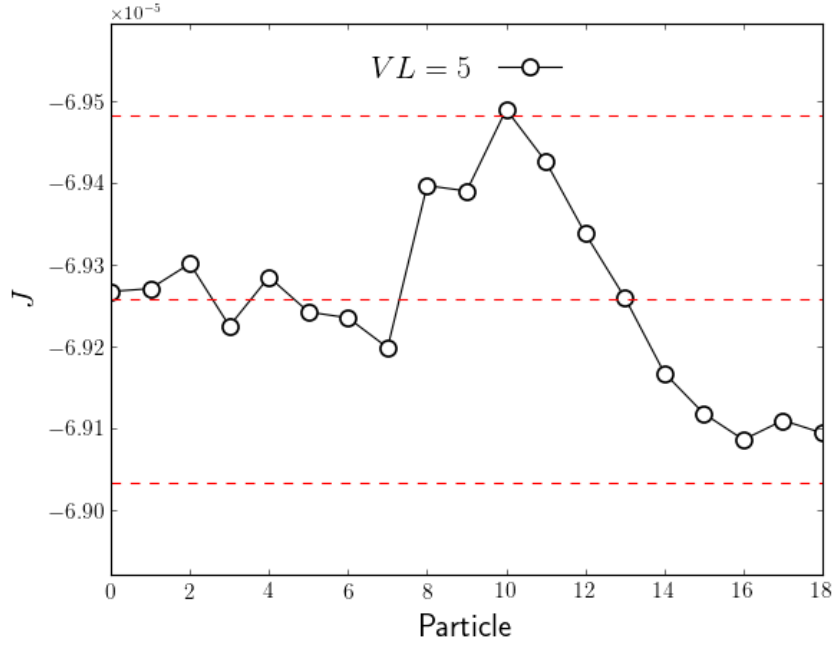


Figure 4.1: Temperature along the chain varying amplitude

Figure 4.2: Heat current along the chain $VL=1$ Figure 4.3: Heat current along the chain $VL=2$

Figure 4.4: Heat current along the chain $VL=3$ Figure 4.5: Heat current along the chain $VL=4$

Figure 4.6: Heat current along the chain $VL=5$

4.1.1.2

FK-Fourier varying kL

Simulation parameters:

- Number of samples: 100
- Number of particles: 20
- Time step: 0.001
- Total simulation time: 300000.0
- Transient time: 100000.0
- Mean temperature: 0.09
- Temp diff: 0.5
- chain ratio $\lambda = 1.0$,
- spring constant between segments [varying],
- power law coefficient $\mu = 2.0$,
- amplitude of the potential on the left $V_L = 5$,
- chain spring constant on the left [varying],
- drag coefficient, $\gamma = 1.0$,

The constant between segments varied to always match the chain spring constant.

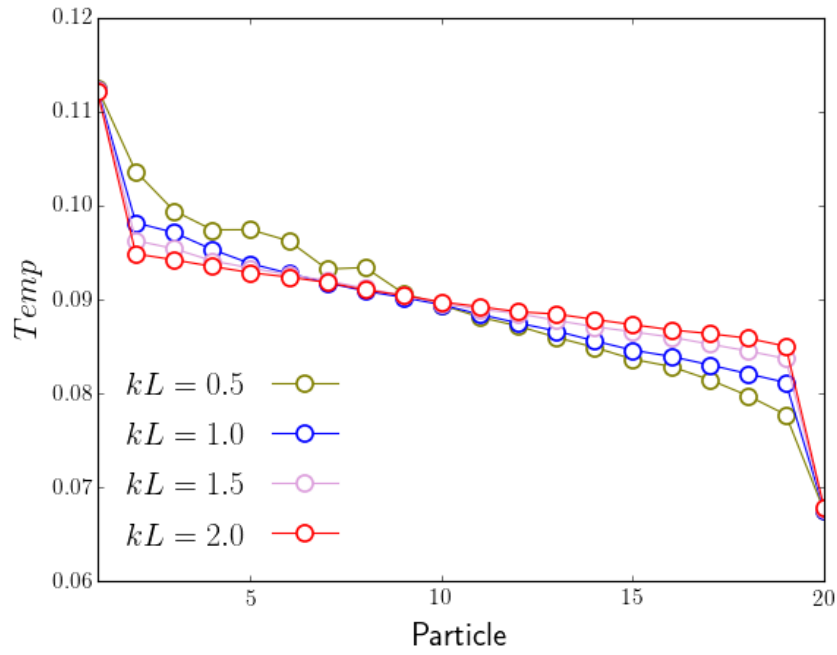


Figure 4.7: Temperature along the chain varying kL

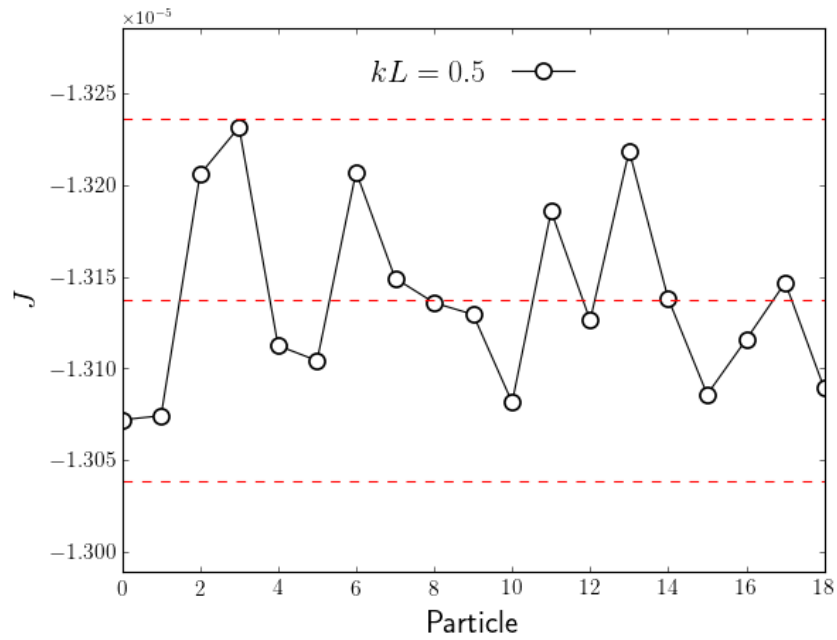
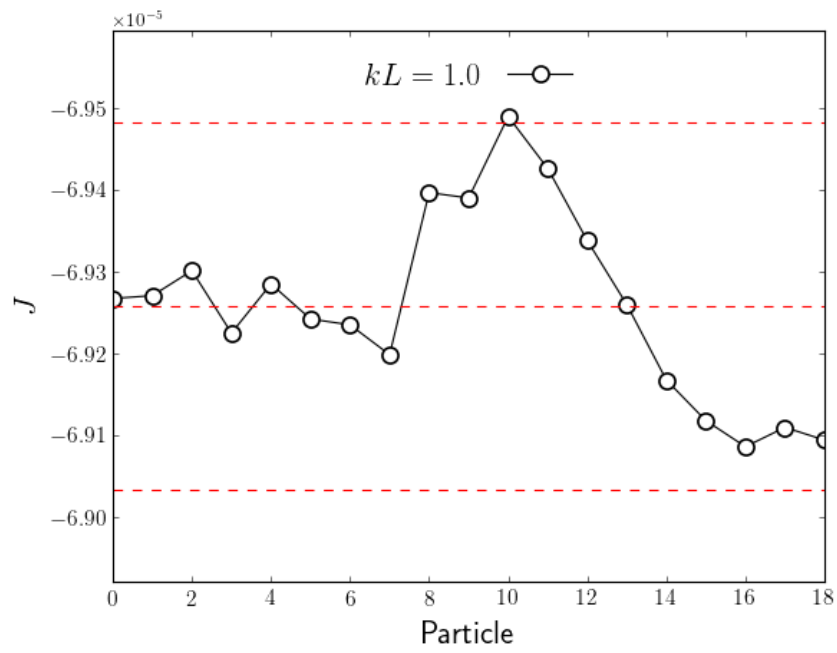
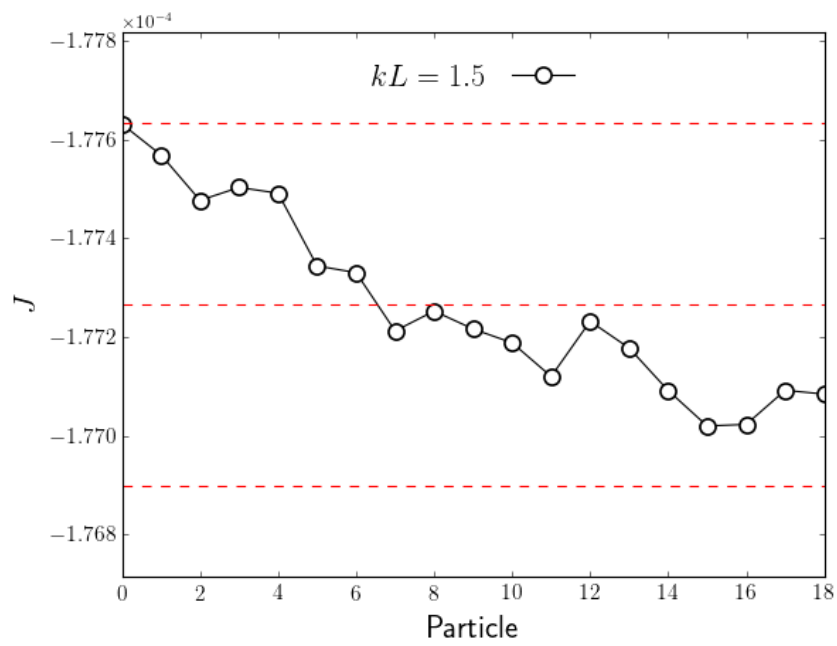
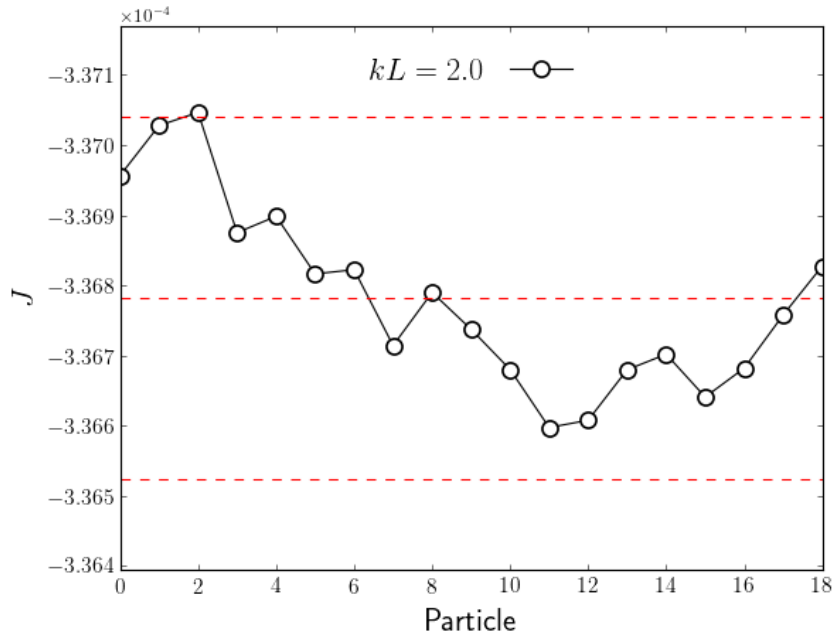


Figure 4.8: Heat along the chain $kL=0.5$

Figure 4.9: Heat along the chain $kL=1.0$ Figure 4.10: Heat along the chain $kL=1.5$

Figure 4.11: Heat along the chain $kL=2.0$

4.1.1.3

FK-diode varying dT

Simulation parameters:

- Number of samples: 100
- Number of particles: 20
- Time step: 0.001
- Total simulation time: 300000.0
- Transient time: 100000.0
- Mean temperature: 0.09
- Temp diff: [varying]
- chain ratio $\lambda = 0.2$,
- spring constant between segments 0.05,
- power law coefficient $\mu = 2.0$,
- amplitude of the potential on the left $V_L = 5$,
- chain spring constant on the left 1.0,
- drag coefficient, $\gamma = 1.0$,

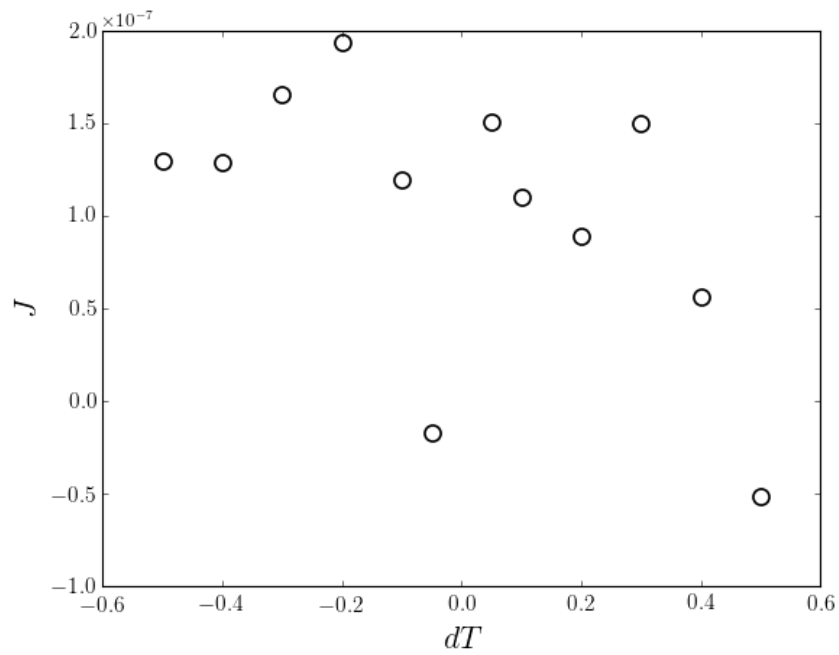
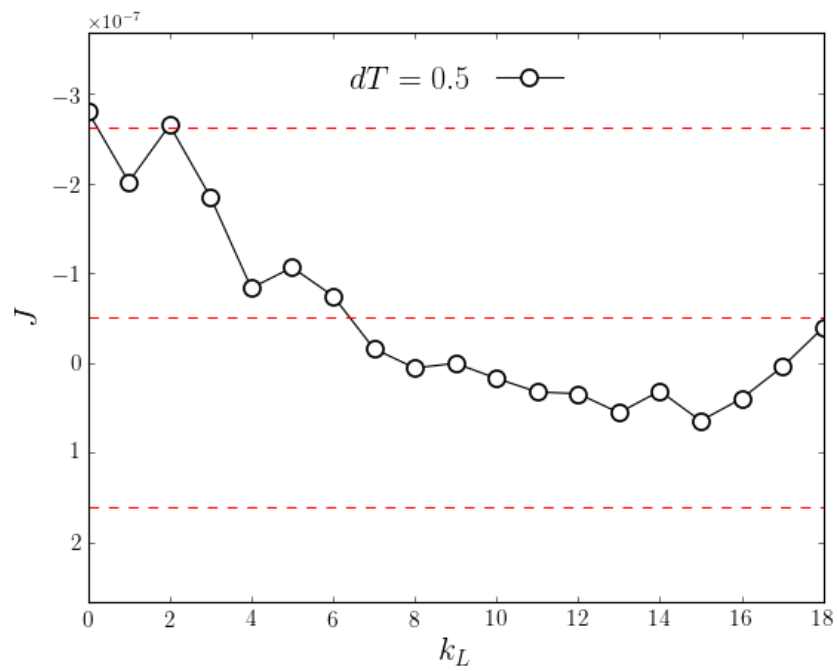
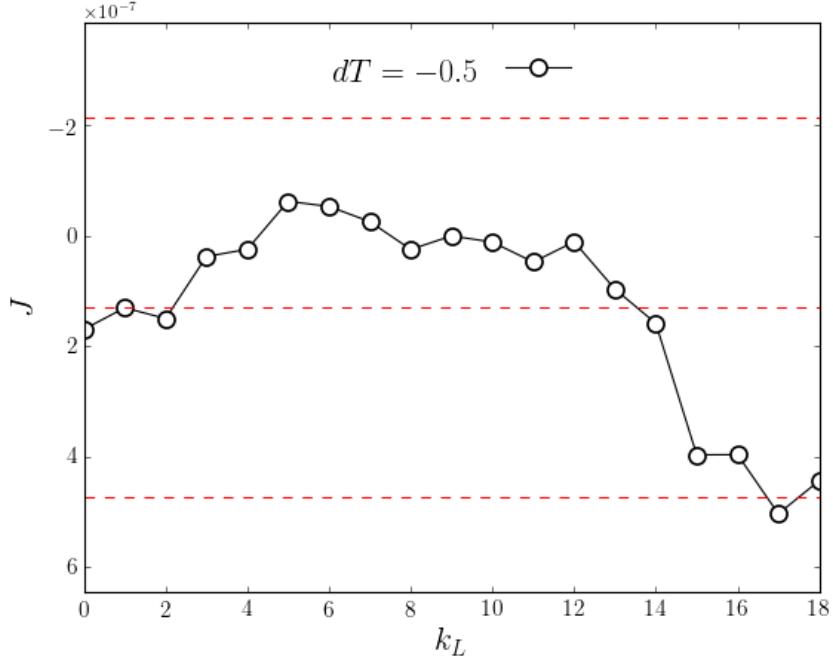


Figure 4.12: Heat current for different temp difference

Figure 4.13: Heat current along the chain $dT=0.5$

Figure 4.14: Heat current along the chain $dT=-0.5$

4.1.2

The ϕ^4 model

In the case of the ϕ^4 model, we get for the momenta of the particles in contact with the baths

$$\begin{aligned}\frac{dp_1}{dt} &= -k_L(2q_1 - q_0 - q_2) - V_L q_1^3 - \gamma p_1 + 2\gamma k_B T_L \epsilon_1(t), \\ \frac{dp_N}{dt} &= -k_R(2q_N - q_{N-1} - q_{N+1}) - V_R q_N^3 - \gamma p_N + 2\gamma k_B T_R \epsilon_2(t),\end{aligned}$$

where $\epsilon_1(t)$ and $\epsilon_2(t)$ are again white noises with zero mean and unit variances, for the interphase particles the equations will now be

$$\begin{aligned}\frac{dp_{\frac{N}{2}}}{dt} &= -k_L(q_{\frac{N}{2}} - q_{\frac{N}{2}-1}) - k_\mu \frac{|q_{\frac{N}{2}} - q_{\frac{N}{2}+1}|^\mu}{q_{\frac{N}{2}} - q_{\frac{N}{2}+1}} - V_L q_{\frac{N}{2}}^3, \\ \frac{dp_{\frac{N}{2}+1}}{dt} &= -k_R(q_{\frac{N}{2}+1} - q_{\frac{N}{2}+2}) - k_\mu \frac{|q_{\frac{N}{2}+1} - q_{\frac{N}{2}}|^\mu}{q_{\frac{N}{2}+1} - q_{\frac{N}{2}}} - V_R q_{\frac{N}{2}+1}^3,\end{aligned}$$

while the rest of the particles will have, for their momenta,

$$\begin{aligned}\frac{dp_n}{dt} &= -k_L(2q_n - q_{n-1} - q_{n+1}) - V_n q_n^3, \\ n &= 2, 3, \dots, \frac{N}{2} - 1, \frac{N}{2} + 2, \frac{N}{2} + 3, \dots, N - 1,\end{aligned}$$

where as before we have $V_n = V_L, n = 2, 3, \dots, N/2 - 1$ and $V_n = V_R, n = N/2 + 2, N/2 + 3, \dots, N - 1$ for the right chain particles.

The particle's displacements read the exact same as before,

$$\frac{dq_n}{dt} = p_n, n = 1, 2, \dots, N,$$

along with the initial conditions $q_n(0) = p_n(0) = 0$.

[Reproduction of Fourier's law]

[Thermal diode changing Number of Particles in the chain]

4.1.2.1

phi4-varying mu and dT

Simulation parameters:

- Number of samples: 200
- Number of particles: 4
- Time step: 0.001
- Total simulation time: 100000.0
- Transient time: 1000.0
- Mean temperature: 1.0
- Temp diff: [varying]
- chain ratio $\lambda = 5.0$,
- spring constant between segments 0.1,
- power law coefficient [varying],
- amplitude of the potential on the left $V_L = 1$,
- chain spring constant on the left 1.0,
- drag coefficient, $\gamma = 1.0$,

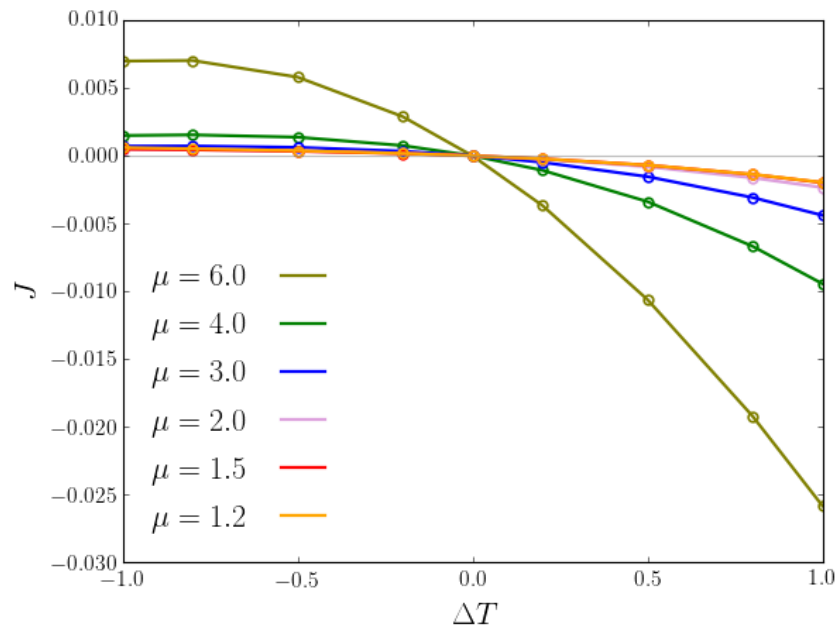


Figure 4.15: capt

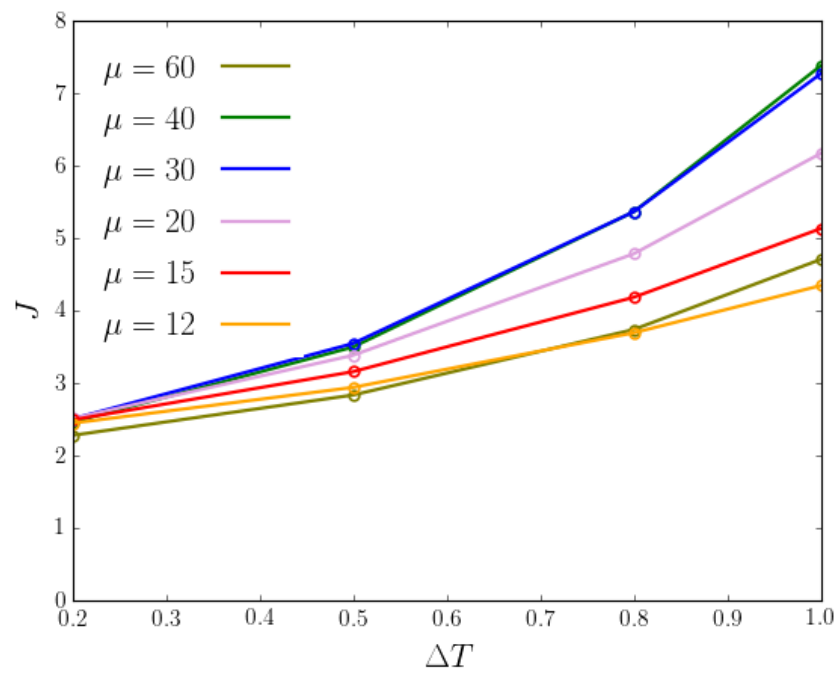


Figure 4.16: capt2

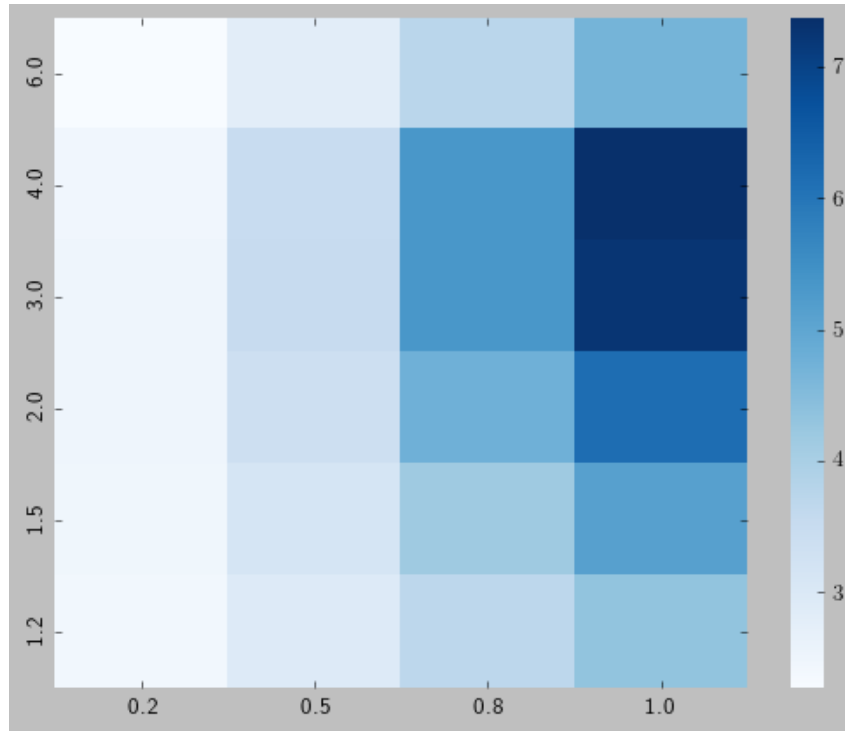


Figure 4.17: capt3

4.1.2.2

phi4-varying mu and kint

Simulation parameters:

- Number of samples: 200
- Number of particles: 4
- Time step: 0.001
- Total simulation time: 100000.0
- Transient time: 1000.0
- Mean temperature: 1.0
- Temp diff: 1.0
- chain ratio $\lambda = 5.0$,
- spring constant between segments [varying],
- power law coefficient [varying],
- amplitude of the potential on the left $V_L = 1$,
- chain spring constant on the left 1.0,
- drag coefficient, $\gamma = 1.0$,

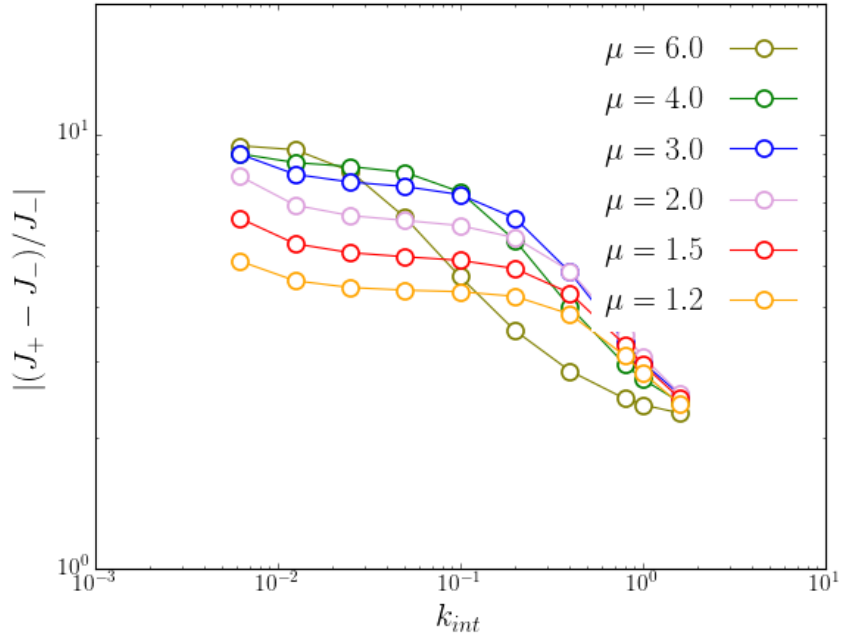


Figure 4.18: cpt

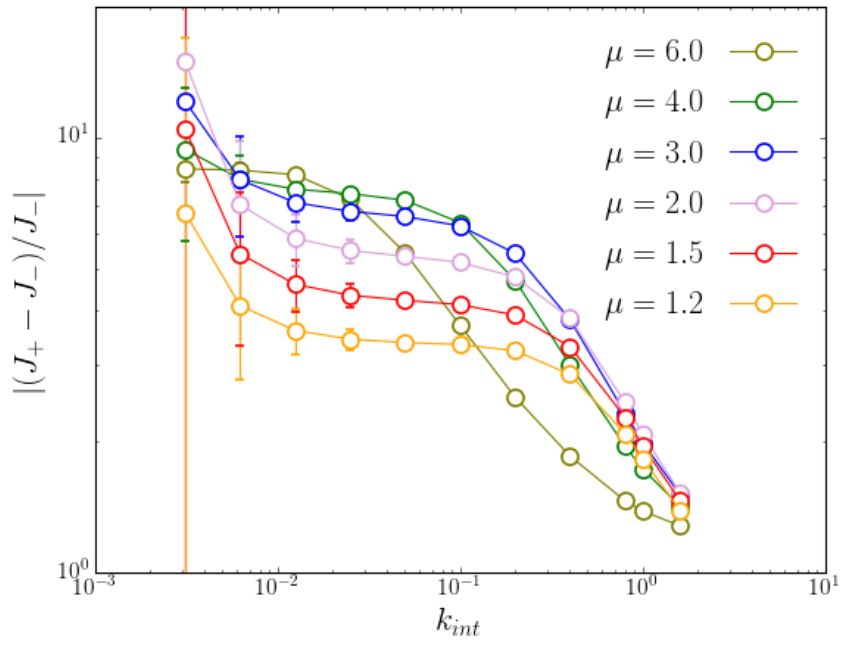


Figure 4.19: cpt

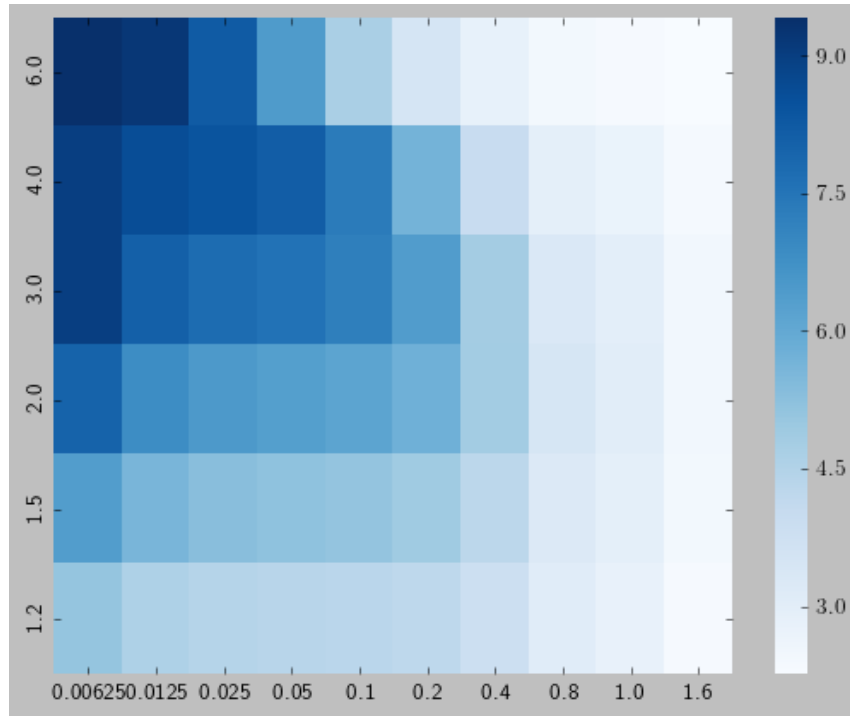


Figure 4.20: cpt

4.1.2.3

phi4-varying Tm

Simulation parameters:

- Number of samples: 200
- Number of particles: 4
- Time step: 0.001
- Total simulation time: 100000.0
- Transient time: 1000.0
- Mean temperature: [varying]
- Temp diff: 1.0
- chain ratio $\lambda = 5.0$,
- spring constant between segments 0.1,
- power law coefficient 2.0,
- amplitude of the potential on the left $V_L = 1$,
- chain spring constant on the left 1.0,
- drag coefficient, $\gamma = 1.0$,

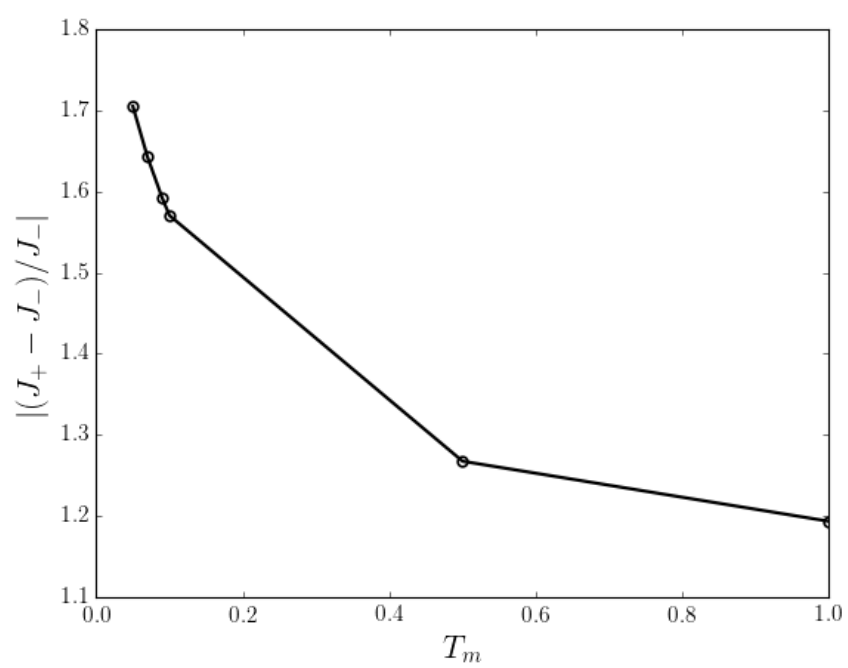


Figure 4.21: capt

5

Conclusions

The conclusions are what we conclude.

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