Estudo de um modelo simples para o diodo térmico

1. Introdução
    1.1. Motivação
    1.2. Fundamentos
2. Modelo matemático
3. Metodologia
    3.1. Análise
    3.2. Métodos Numéricos
4. Resultados
5. Conclusão

1. Introdução

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Solid-State Thermal Rectifier

C. W. Chang,[1,4] D. Okawa,[1] A. Majumdar,[2,3,4] A. Zettl[1,3,4]*

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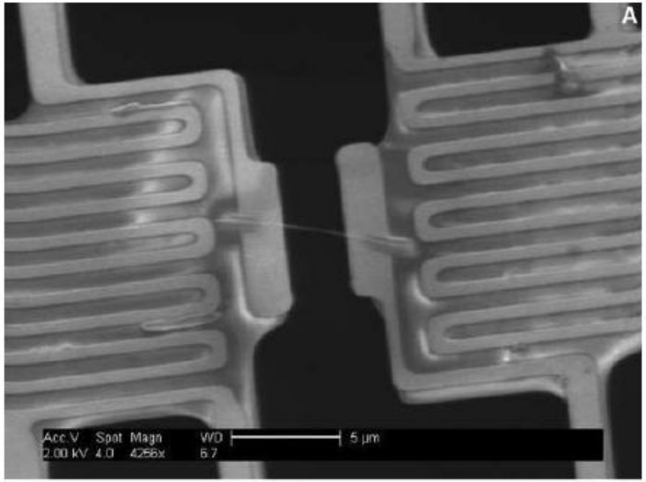

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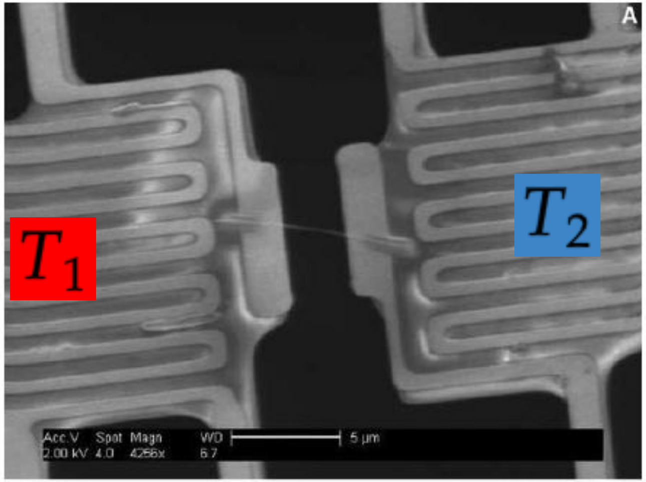

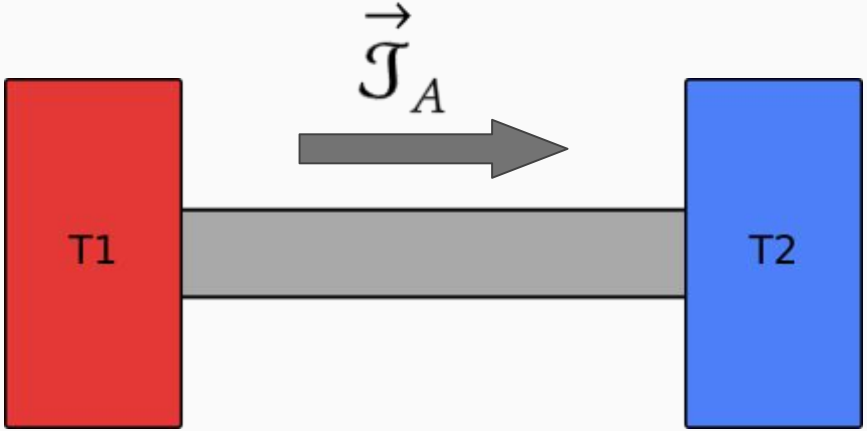

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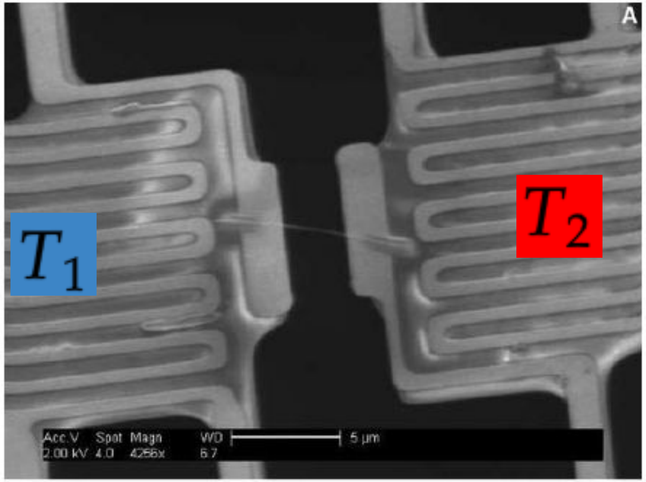

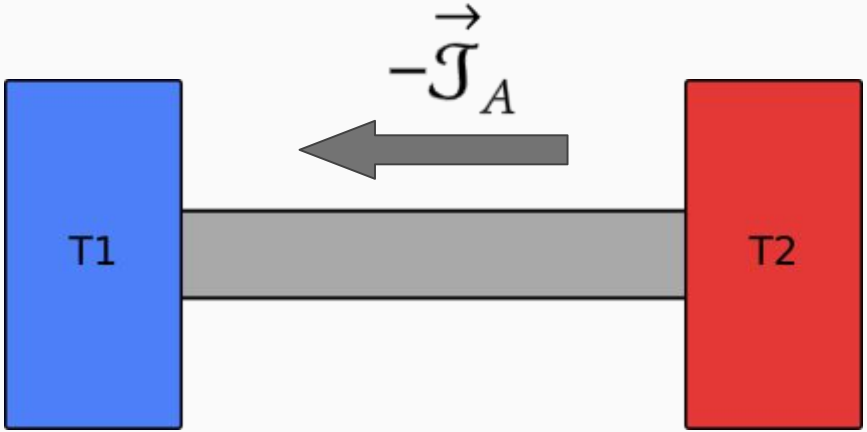

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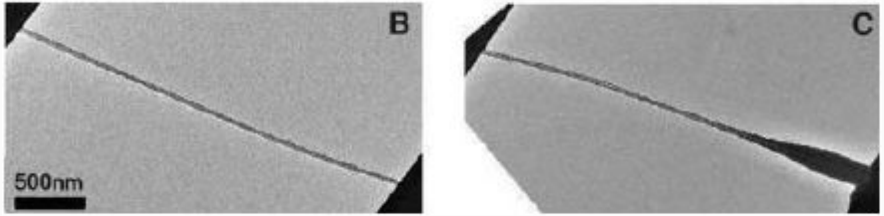

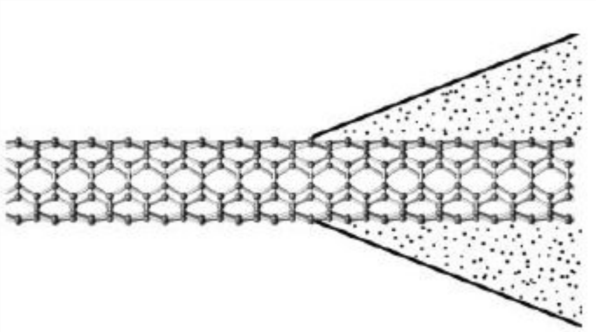

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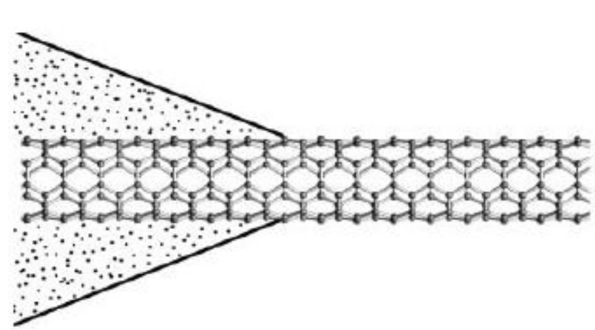

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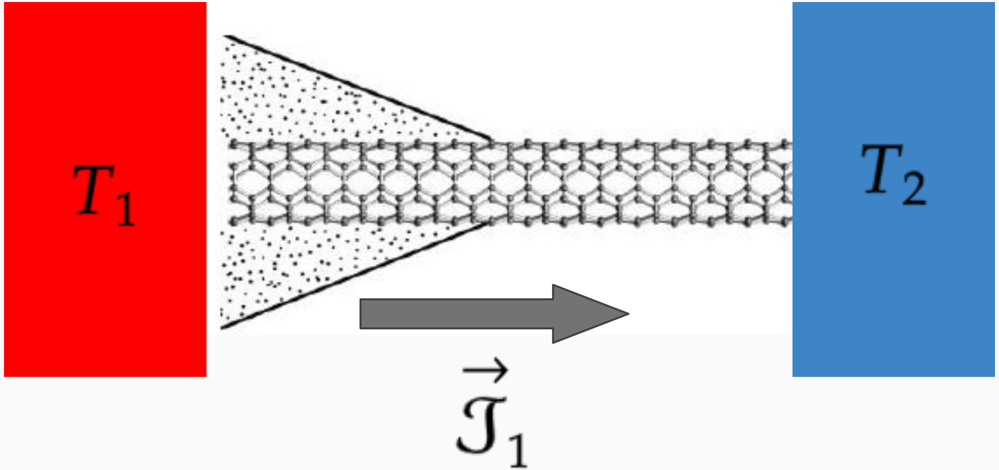

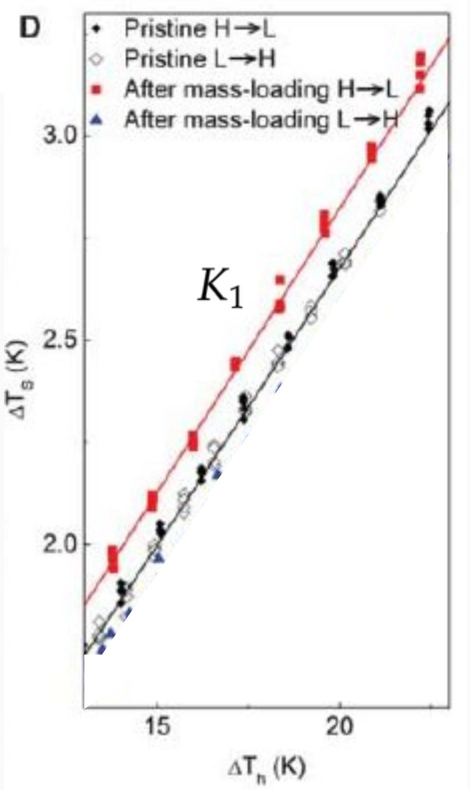

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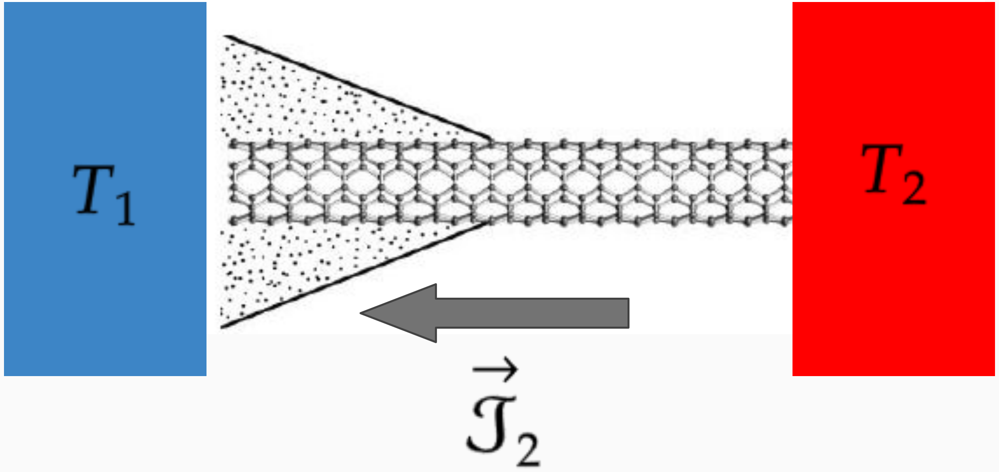

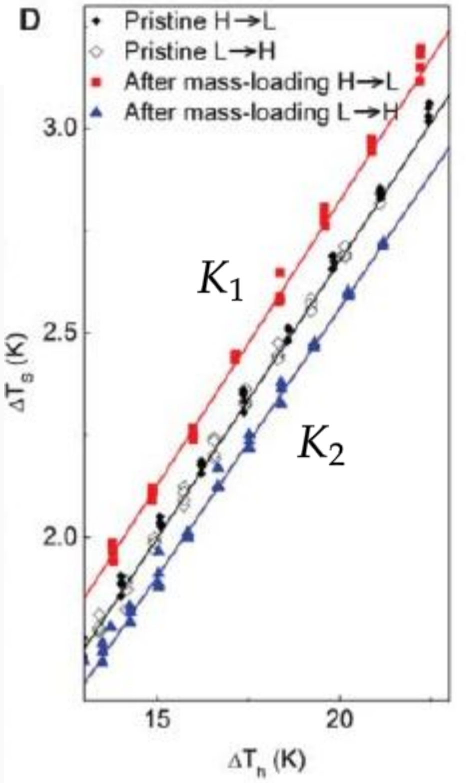

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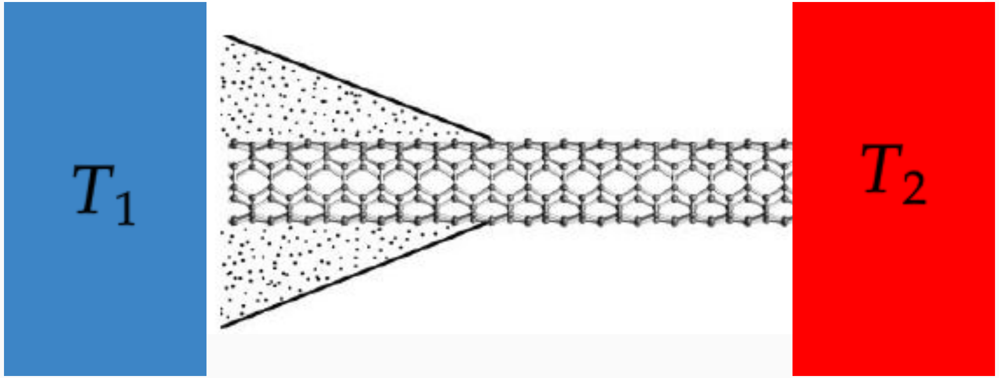
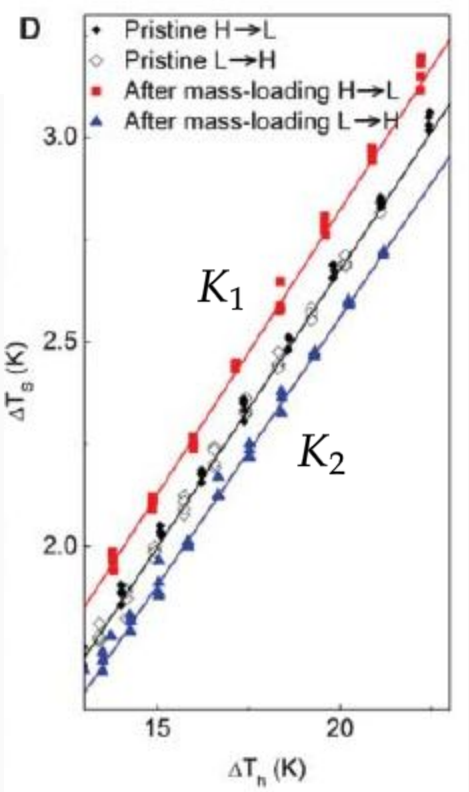


$$\frac{K_1 - K_2}{K_2} \approx 7\%$$



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Maria José Martínez-Pérez, Antonio Fornieri and Francesco Giazotto*

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PUBLISHED ONLINE: 23 FEBRUARY 2015 | DOI: 10.1038/NNANO.2015.11

Equação do Calor

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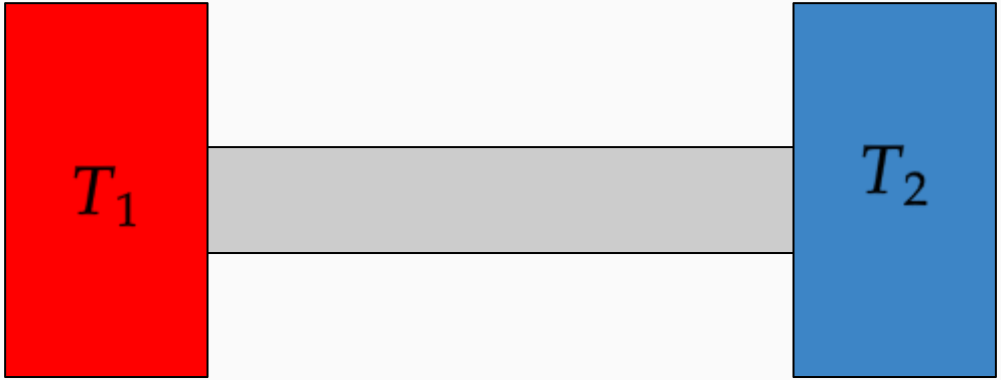

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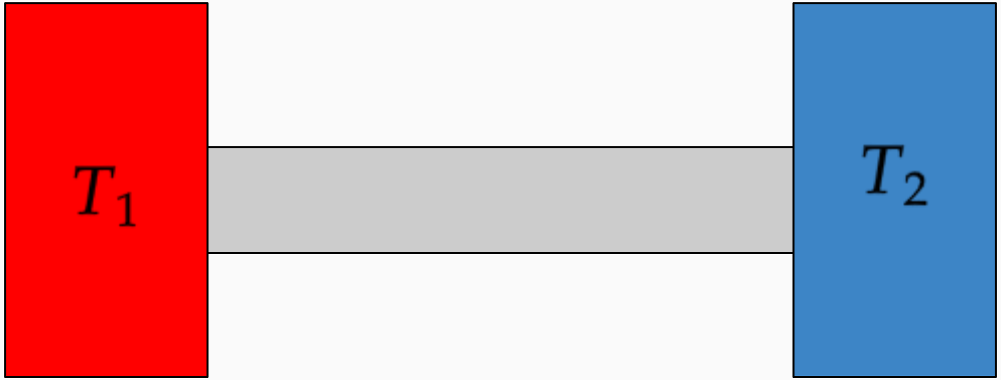

1ª lei da termodinâmica → Equação da Continuidade

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

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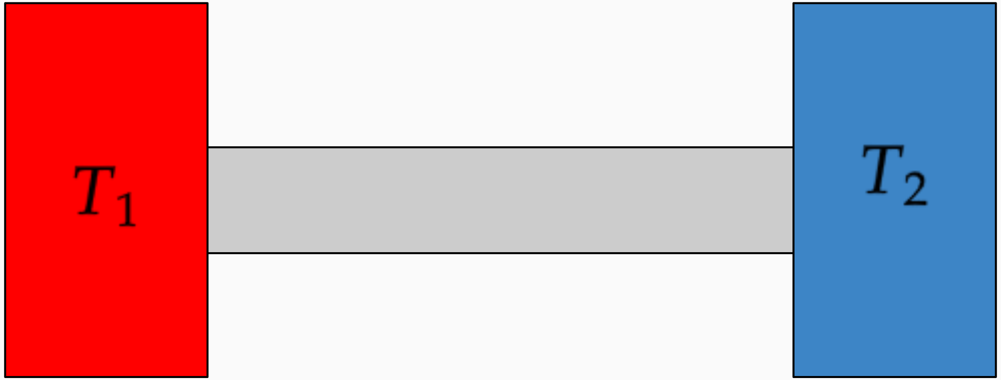

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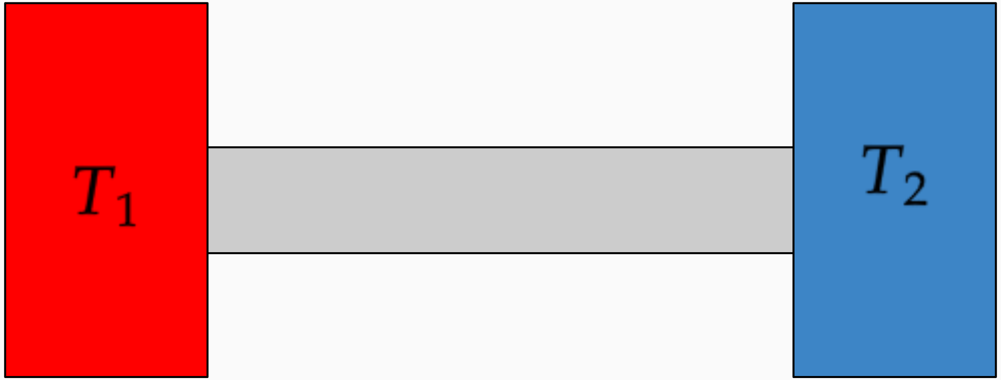

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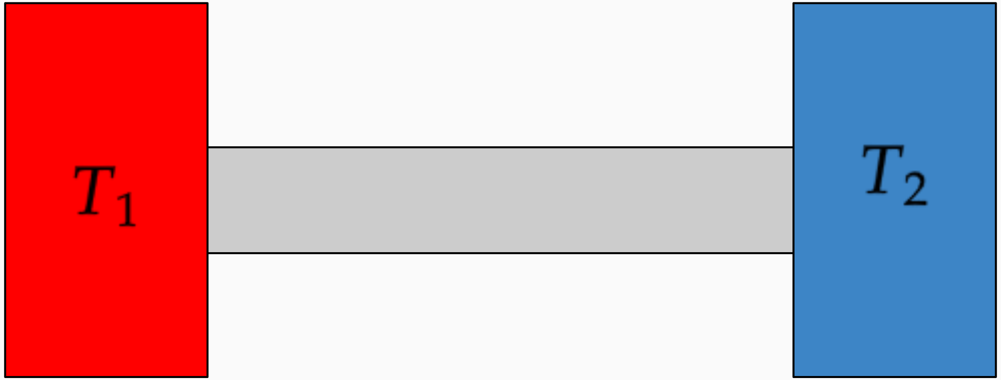

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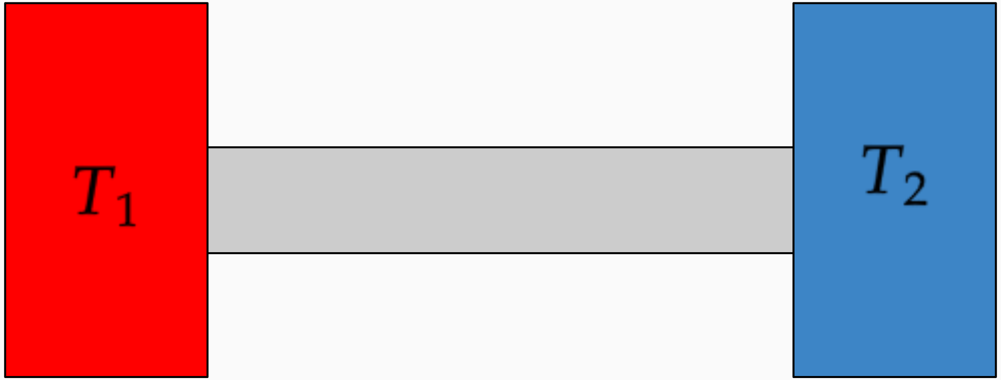

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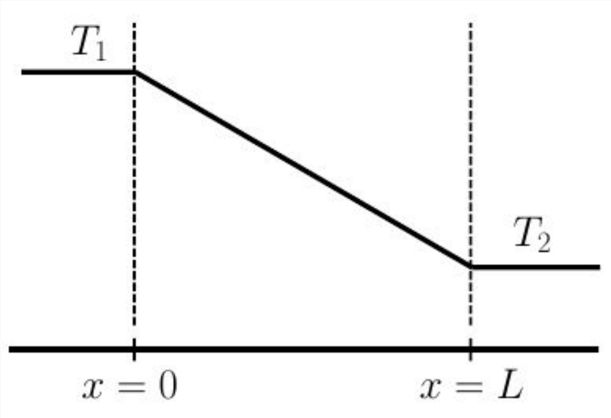
Estado Estacionário

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



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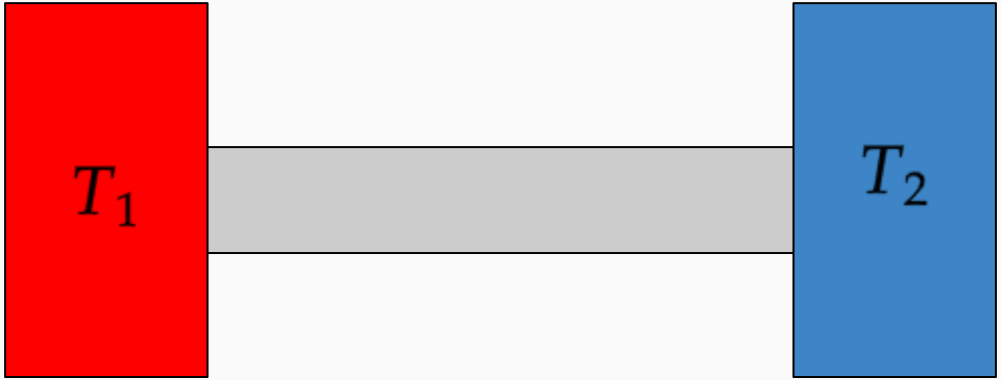

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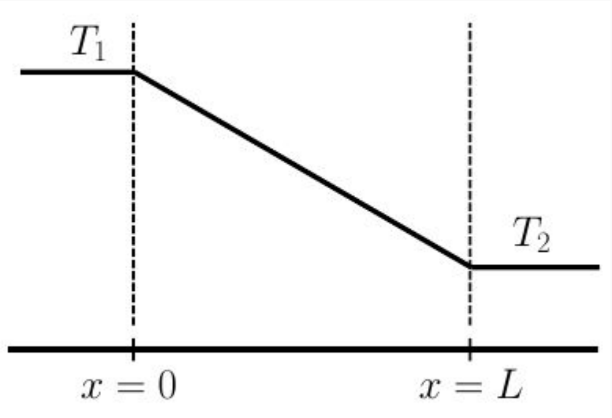

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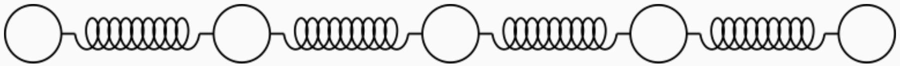
Sólidos



$$H = \sum_n \frac{m}{2}v^2 + \frac{K}{2}(u_n - u_{n+1})^2$$

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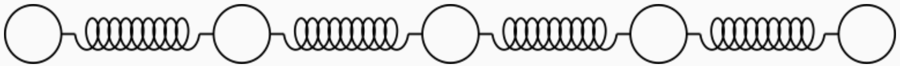

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Condutores | Isolantes

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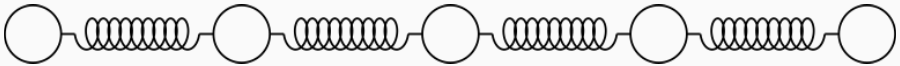

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1. Introdução

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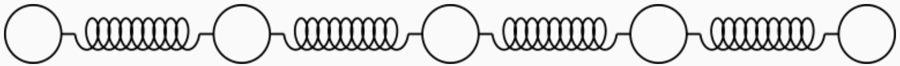

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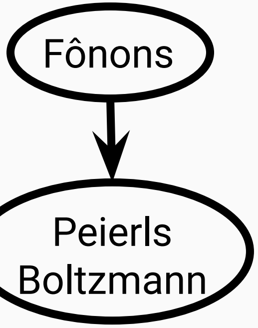

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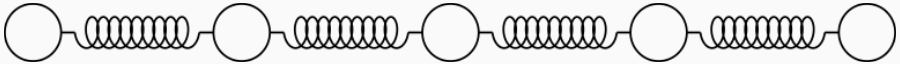

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- Resistividade elétrica ☑
- Calor específico ☑
- Condutividade térmica ☒

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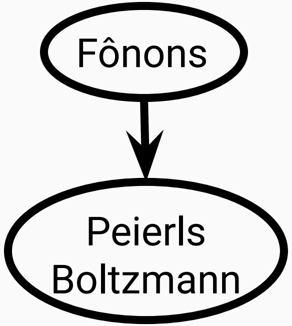

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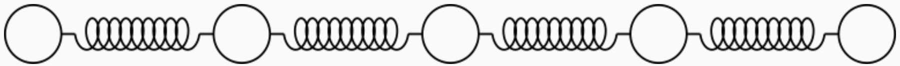

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- Resistividade elétrica ☑
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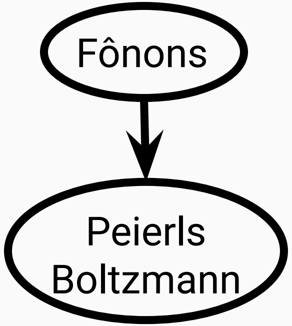
$$U^{anh} = \sum_{i,j,k} \frac{1}{3!} \frac{\partial^3 U}{\partial u_i \partial u_j \partial u_k}\bigg|_{\mathbf{u}=0} \cdot u_i u_j u_k + \sum_{i,j,k,l} \frac{1}{4!} \frac{\partial^4 U}{\partial u_i \partial u_j \partial u_k \partial u_l}\bigg|_{\mathbf{u}=0} \cdot u_i u_j u_k u_l + \ldots$$

Condutores | Isolantes



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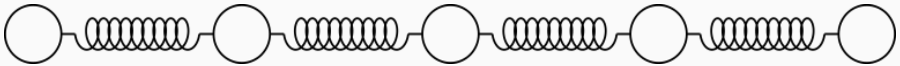

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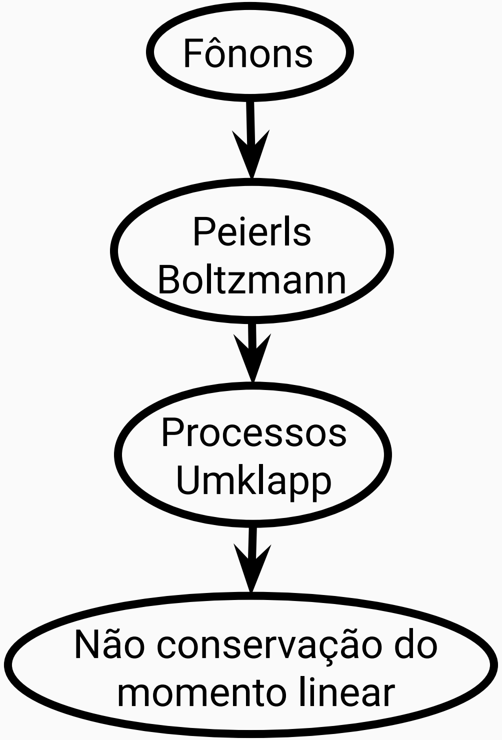

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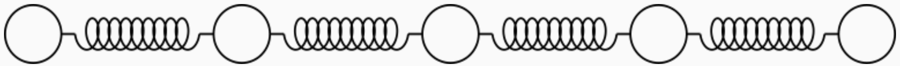

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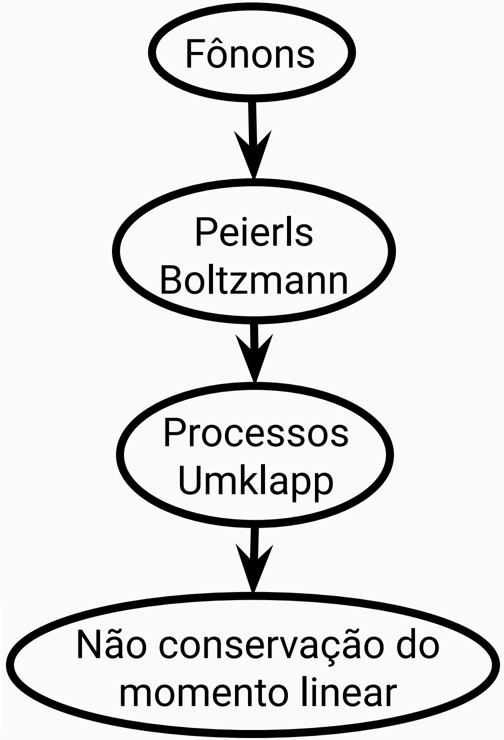

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cálculo da **condutividade térmica**

X

relaxação para o estado estacionário

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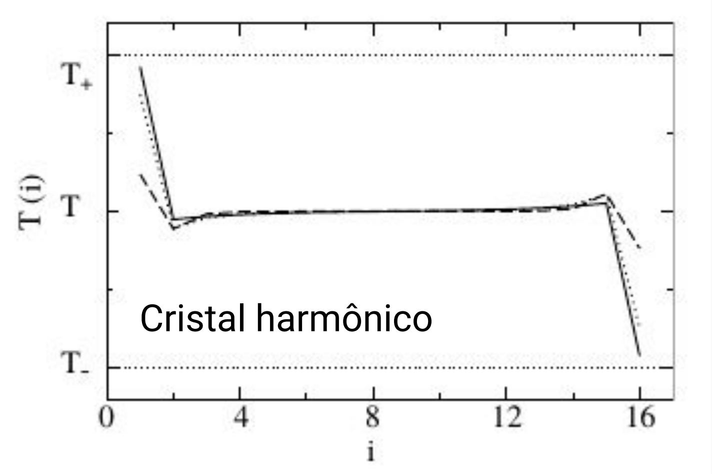

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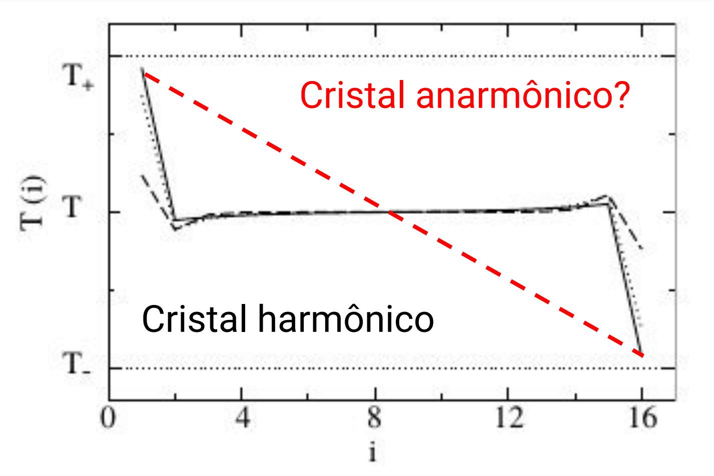

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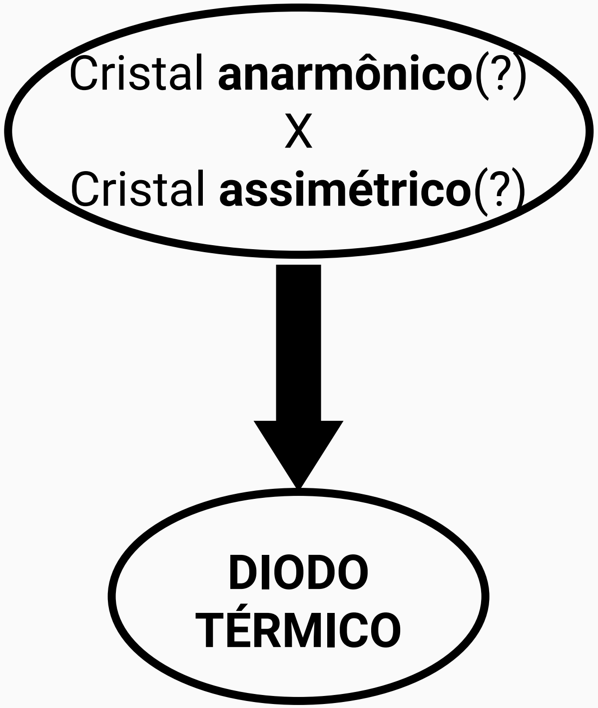

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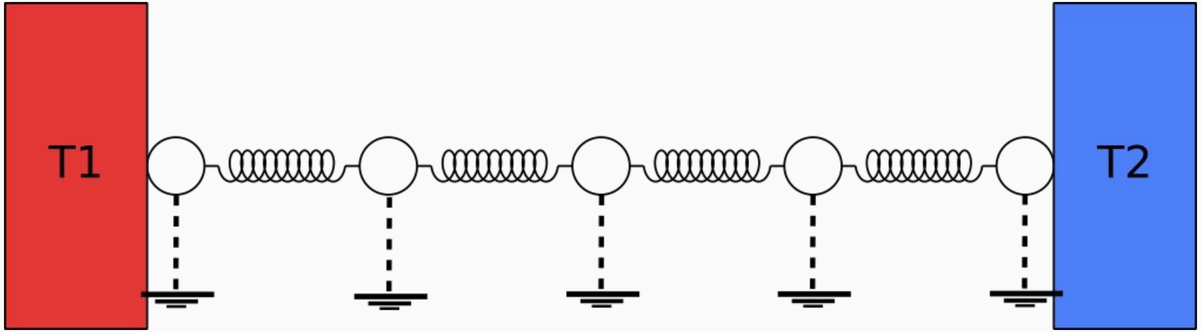

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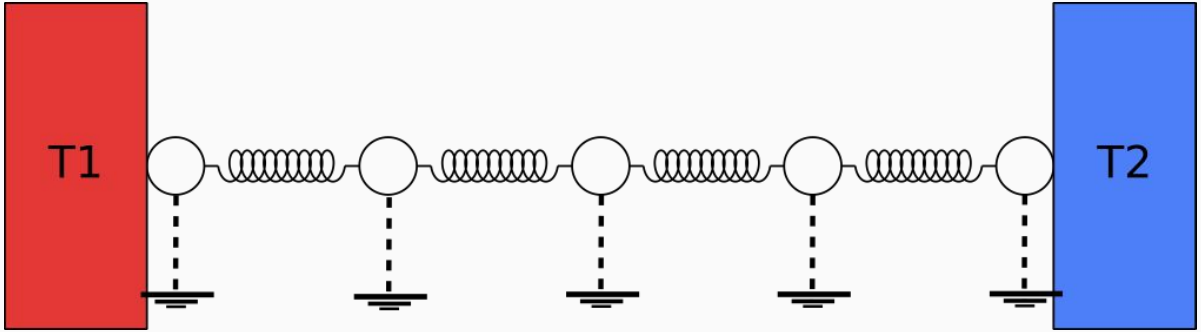

$$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + U_{int}(x_{i+1}, x_i) + U_{ext,\,i}(x_i)$$

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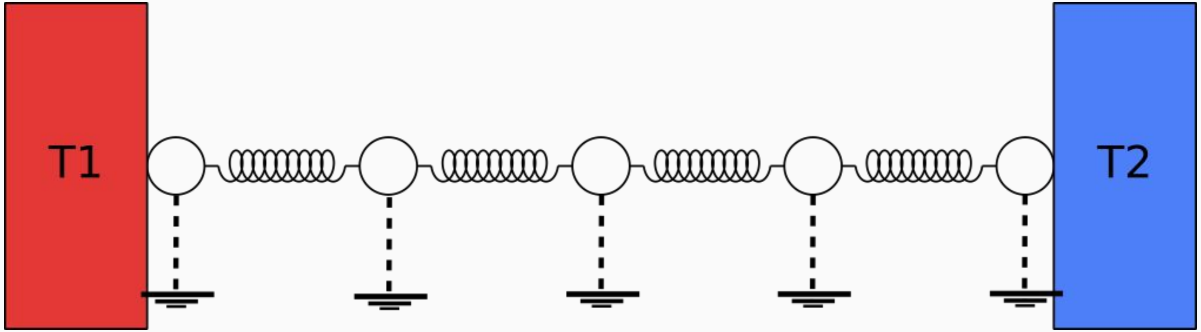

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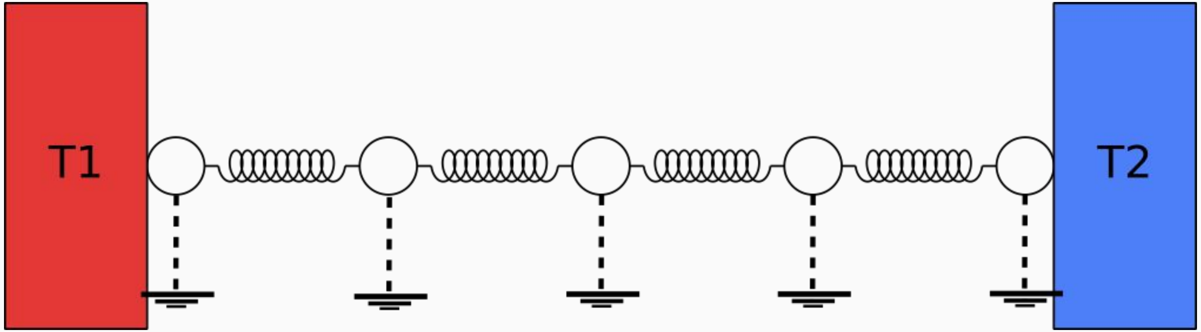
Banho Térmico?



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Banho Térmico?

Alterações nas equações de movimento para as partículas 1 e N

2. Modelo matemático

Como interpretar o modelo em termos “termodinâmicos”?

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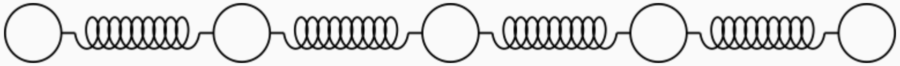
$$T_j = \left\langle \frac{p_j^2}{m} \right\rangle$$



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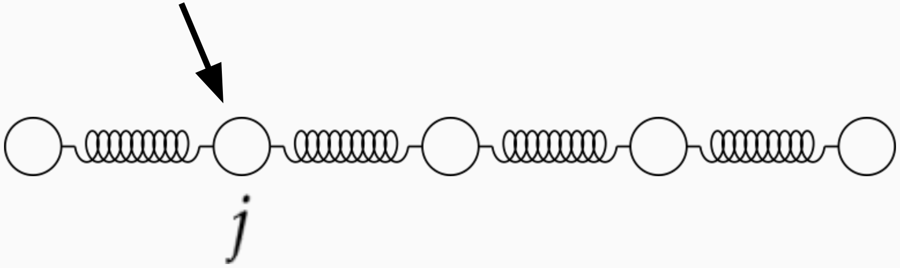

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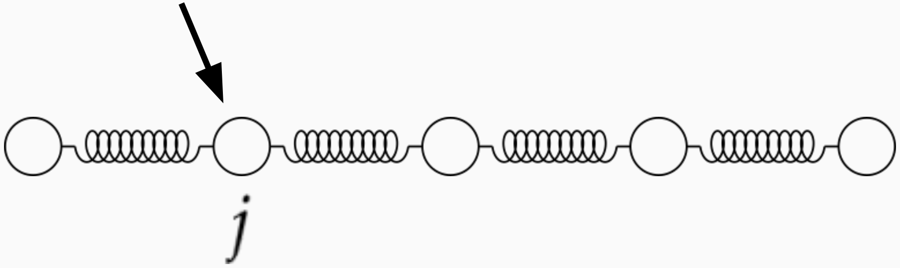
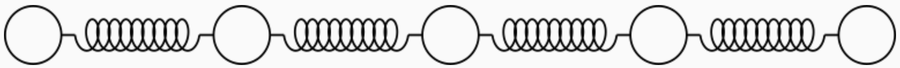


Fluxo de Calor

$$\mathcal{J}_n = \frac{1}{2}(\dot{x}_{n+1} + \dot{x}_n) \cdot F(x_{n+1} - x_n)$$

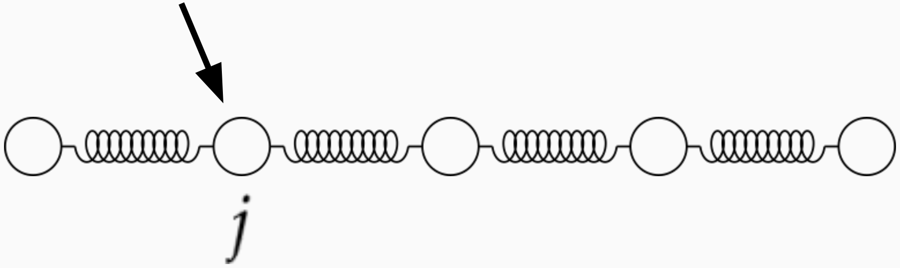


2. Modelo matemático

Como interpretar o modelo em termos "termodinâmicos"?

Temperatura "Cinética"

$$T_j = \left\langle \frac{p_j^2}{m} \right\rangle$$



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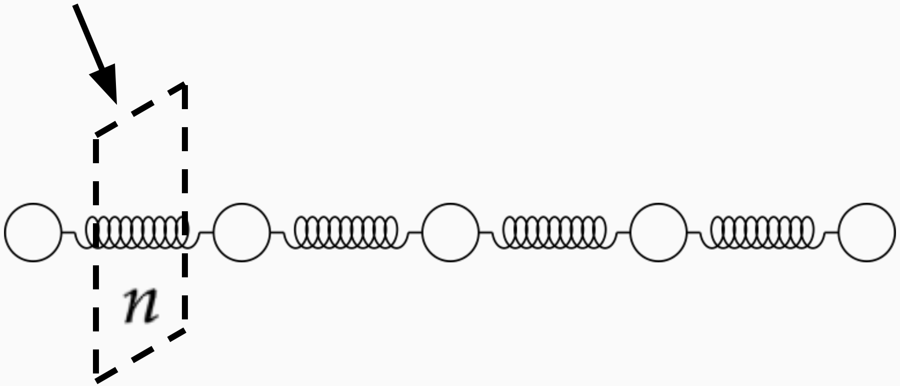
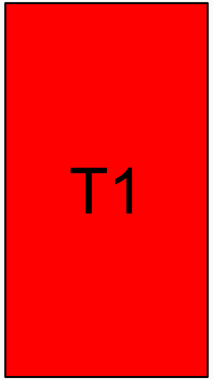


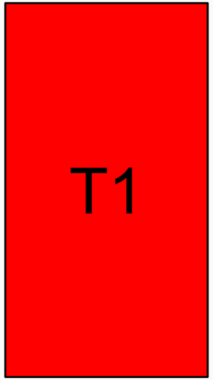
2. Modelo matemático

Banho Térmico



2. Modelo matemático

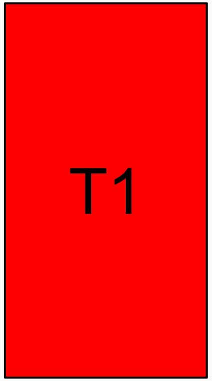
Banho Térmico



Como descrever um banho térmico?

2. Modelo matemático

Banho Térmico

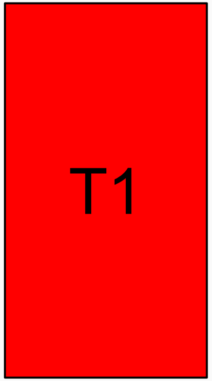


Temperatura constante ⇒ Ensemble canônico ⇒ Distribuição de Maxwell-Boltzmann

Como descrever um banho térmico?

2. Modelo matemático

Banho Térmico

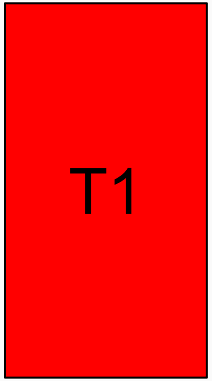


Como descrever um banho térmico?

Distribuição de Maxwell-Boltzmann

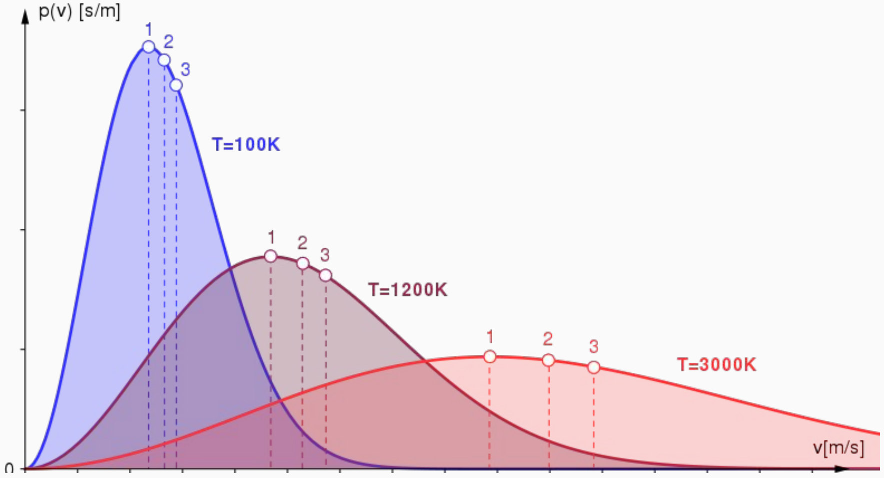
2. Modelo matemático

Banho Térmico



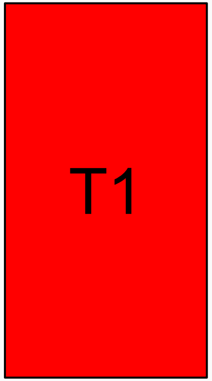
Como descrever um banho térmico?

Distribuição de Maxwell-Boltzmann



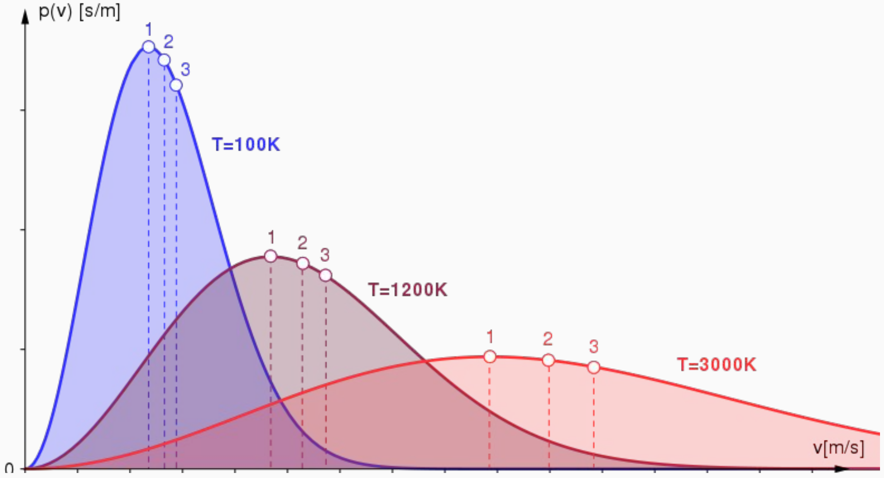
2. Modelo matemático

Banho Térmico



Como descrever um banho térmico?

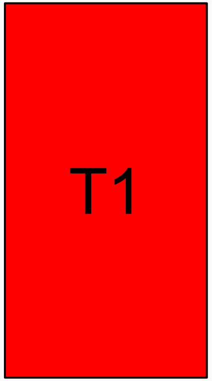
Distribuição de Maxwell-Boltzmann



$$p(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$

2. Modelo matemático

Banho Térmico



Distribuição de Maxwell-Boltzmann

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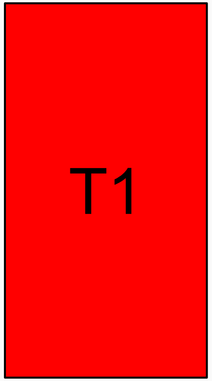
2. Modelo matemático

Banho Térmico



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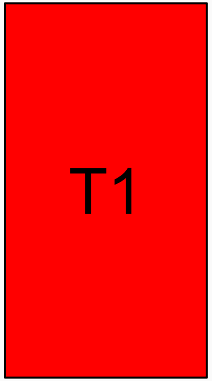
Modelo determinístico

Termostato de
Nosè-Hoover

2. Modelo matemático

Banho Térmico



Distribuição de Maxwell-Boltzmann

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Modelo determinístico

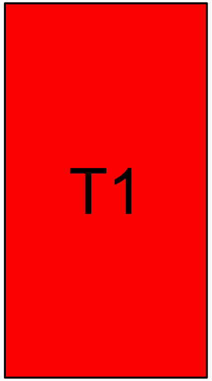
Termostato de
Nosè-Hoover

Modelo estocástico

Banho de Langevin

2. Modelo matemático

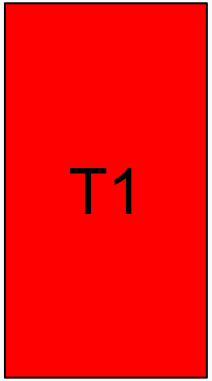
Banho Térmico



Termostato Nosè-Hoover

$$H_N = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m_i s^2} + \phi(\mathbf{q}) \right) + g k_B T \cdot \ln(s) + \frac{p_s^2}{2Q} \quad ; \quad \begin{aligned} Q &= 3N k_B T \tau^2 \\ g &= 3N \end{aligned}$$

Banho Térmico



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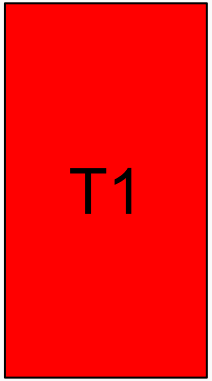
$$\begin{aligned} \frac{d\mathbf{q}_i}{dt} &= \frac{\mathbf{p}_i}{m} \\ \frac{d\mathbf{p}_i}{dt} &= \mathbf{F}_i - \xi \mathbf{p}_i \\ \frac{d\xi}{dt} &= \frac{1}{\tau^2}\left[\frac{1}{mk_B TN}\sum_{i=1}^{N}\mathbf{p}_i^2 - 1\right] \end{aligned}$$

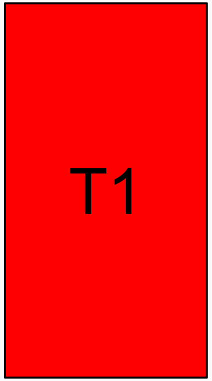
Banho Térmico



Banho de Langevin

$$m\frac{d\dot{q}}{dt} = -\gamma\dot{q} + \eta(t) \quad ; \quad \begin{aligned} \langle \eta(t) \rangle &= 0 \\ \langle \eta(t)\eta(t') \rangle &= \Gamma\delta(t-t') \end{aligned}$$

Banho Térmico



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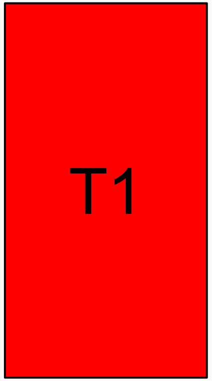
Graus de liberdade rápidos

Graus de liberdade lentos

Banho Térmico



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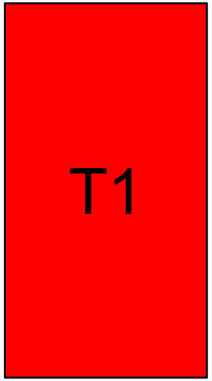
2. Modelo matemático

Banho Térmico



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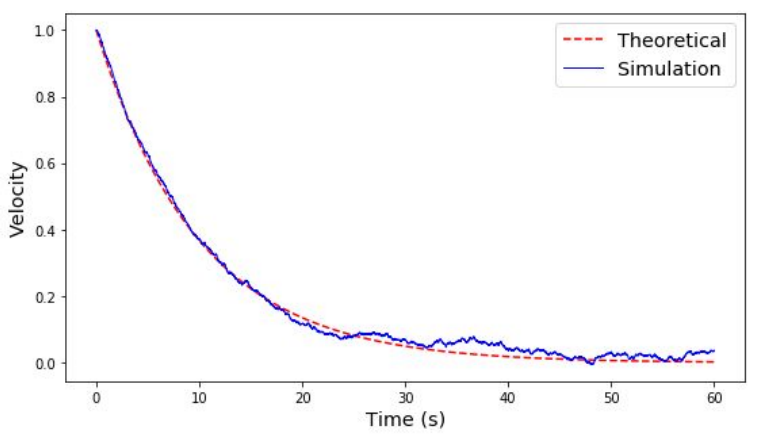
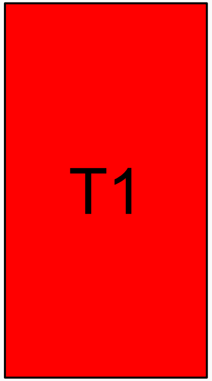
$$\langle \dot{q} \rangle = v_0 e^{-\gamma t}$$



2. Modelo matemático

Banho Térmico



Banho de Langevin

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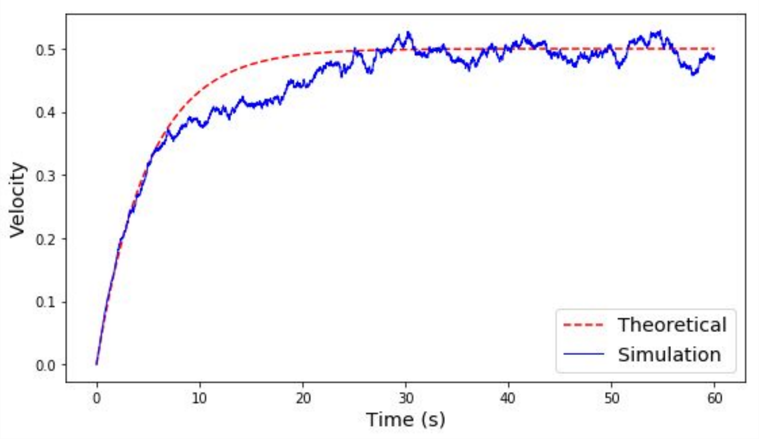
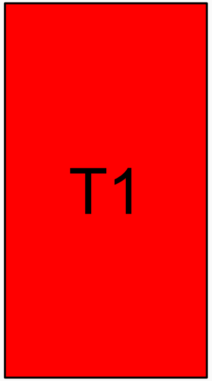
$$\langle \dot{q}^2 \rangle - \langle \dot{q} \rangle^2 = \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right)$$



2. Modelo matemático

Banho Térmico



Banho de Langevin

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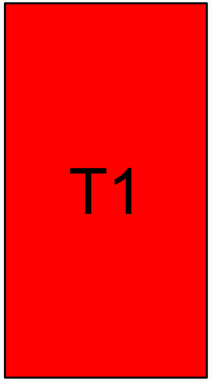
$$\Gamma = \frac{2\gamma k_B T}{m}$$

2. Modelo matemático

Banho Térmico



Banho de Langevin

$$m\frac{d\dot{q}}{dt} = -\gamma\dot{q} + \frac{2\gamma k_B T}{m}\epsilon(t) \quad ; \quad \begin{aligned} \langle\epsilon(t)\rangle &= 0 \\ \langle\epsilon(t)\epsilon(t')\rangle &= \delta(t-t') \end{aligned}$$

$$\langle\dot{q}\rangle = v_0 e^{-\gamma t}$$

$$\langle\dot{q}^2\rangle - \langle\dot{q}\rangle^2 = \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right)$$

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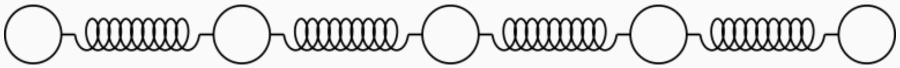
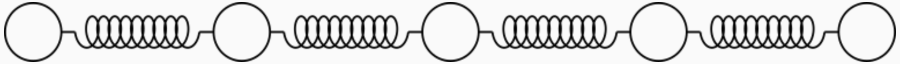
2. Modelo matemático

Cadeia de Partículas



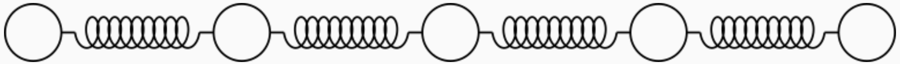
2. Modelo matemático

Cadeia de Partículas



2. Modelo matemático

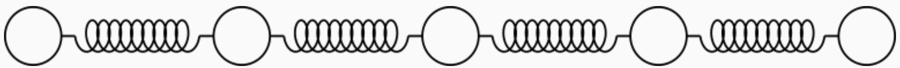
Cadeia de Partículas



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

2. Modelo matemático

Cadeia de Partículas



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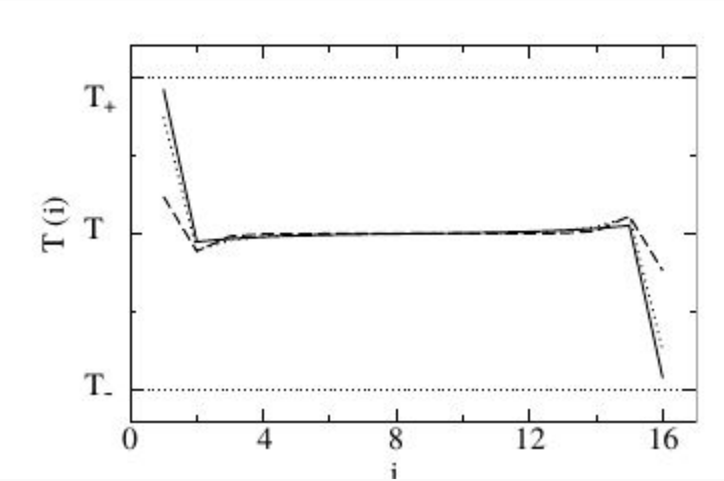
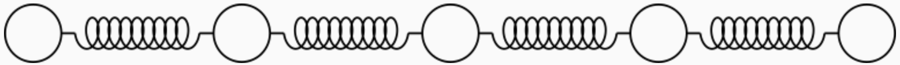
Modelo harmônico



2. Modelo matemático

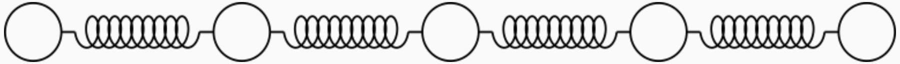
Cadeia de Partículas



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

2. Modelo matemático

Cadeia de Partículas



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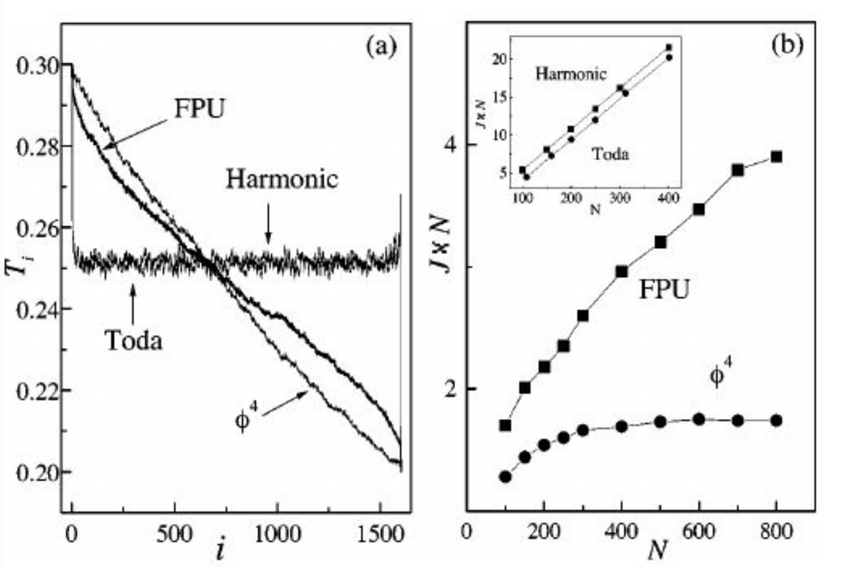
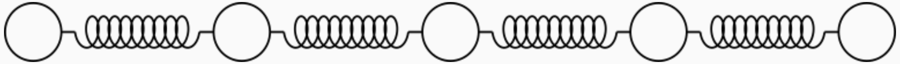


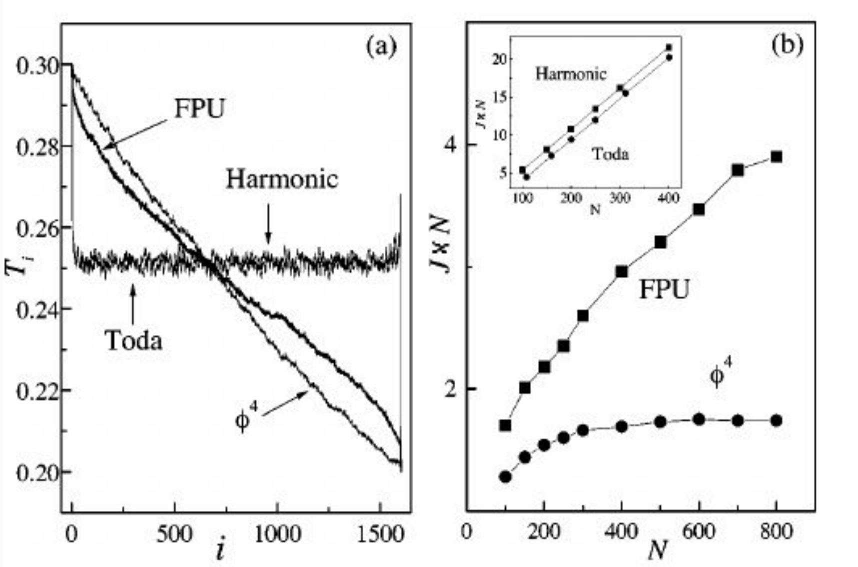
2. Modelo matemático

Cadeia de Partículas



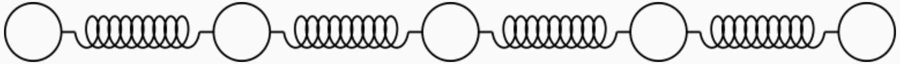
Toda

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



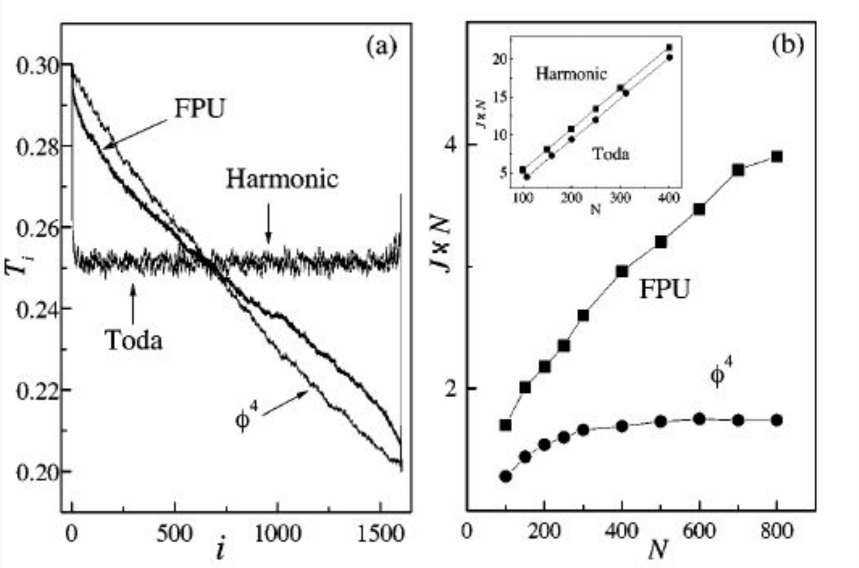
2. Modelo matemático

Cadeia de Partículas



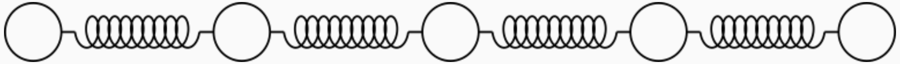
Toda $$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \exp(-(x_{i+1} - x_i)) + (x_{i+1} - x_i) - 1$$

FPUT $$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{k}{2}(x_i - x_{i+1})^2 + \frac{k'}{4}(x_i - x_{i+1})^4$$



2. Modelo matemático

Cadeia de Partículas



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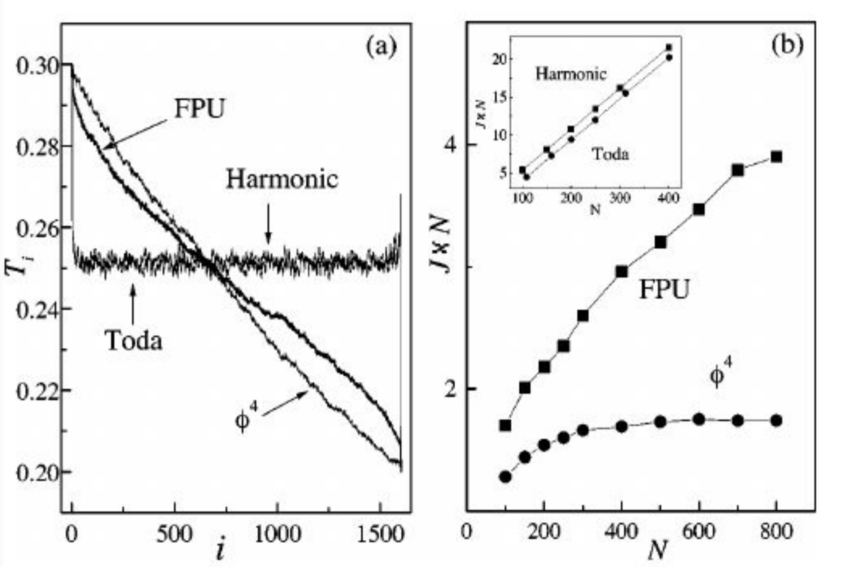
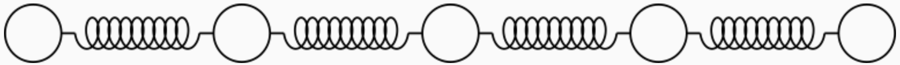
ϕ^4 $$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{k}{2}(x_i - x_{i+1})^2 + \frac{k''}{4}x_i^4$$



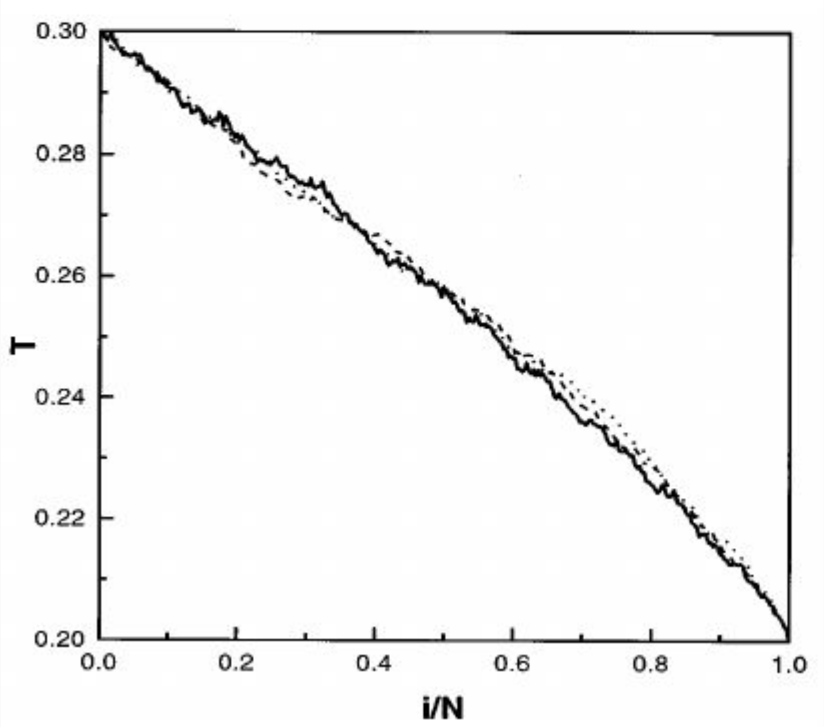
2. Modelo matemático

Cadeia de Partículas

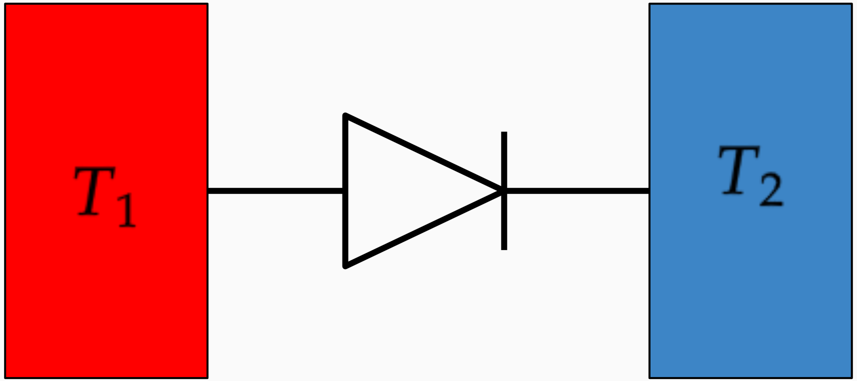


Frenkel-Kontorova

$$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{k}{2}(x_i - x_{i+1})^2 + \frac{k'}{4}(x_i - x_{i+1})^4$$

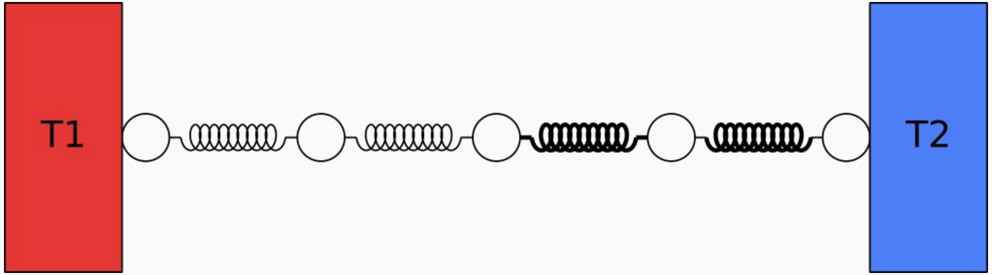


Diodo Térmico



2. Modelo matemático

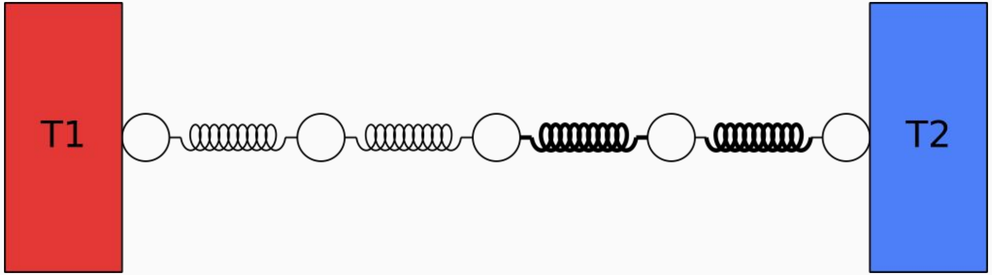
Diodo Térmico



2. Modelo matemático

Diodo Térmico

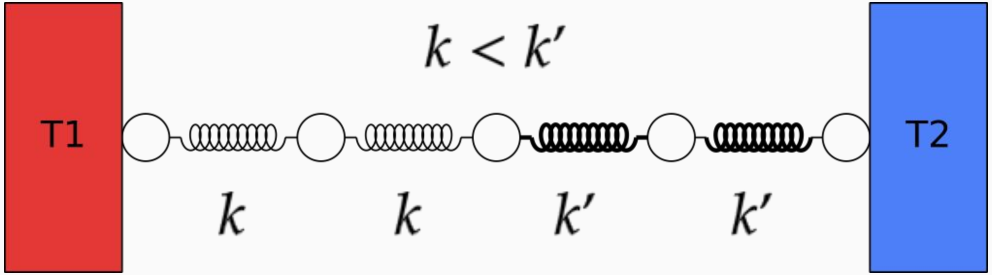
Assimetria



2. Modelo matemático

Diodo Térmico

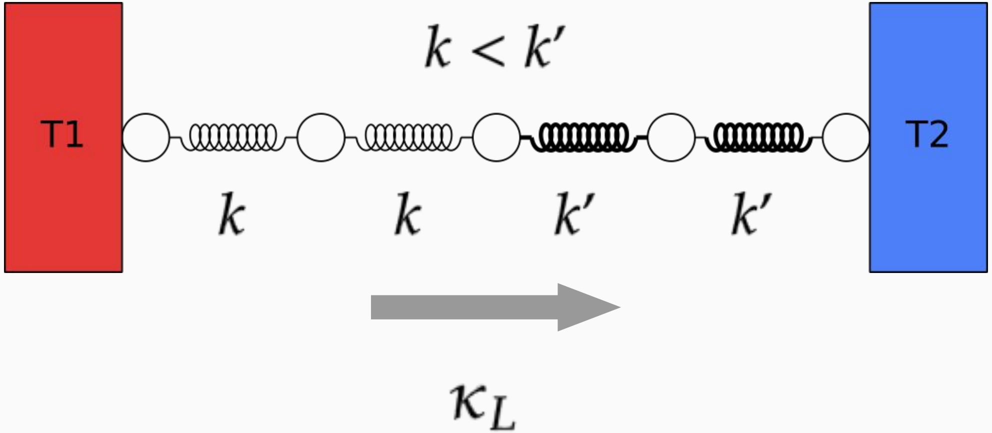
Assimetria



2. Modelo matemático

Diodo Térmico

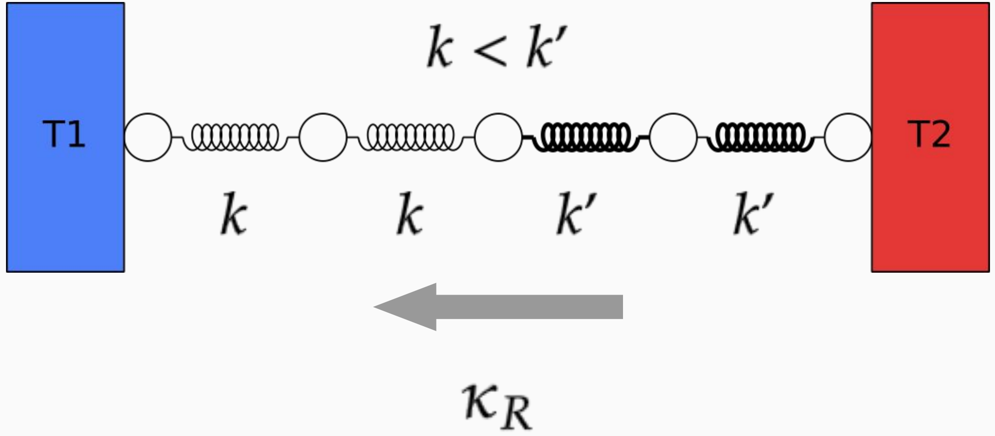
Assimetria



2. Modelo matemático

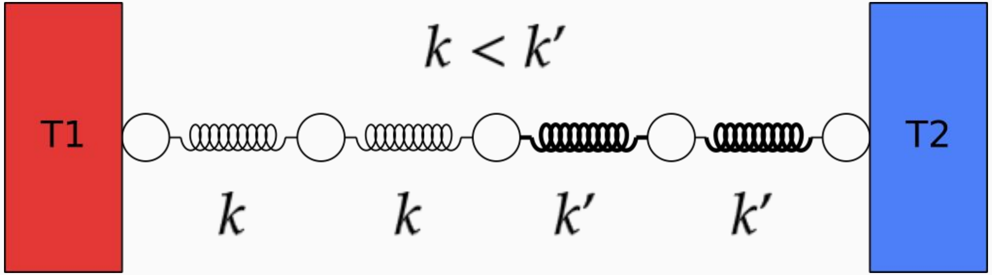
Diodo Térmico

Assimetria



Diodo Térmico

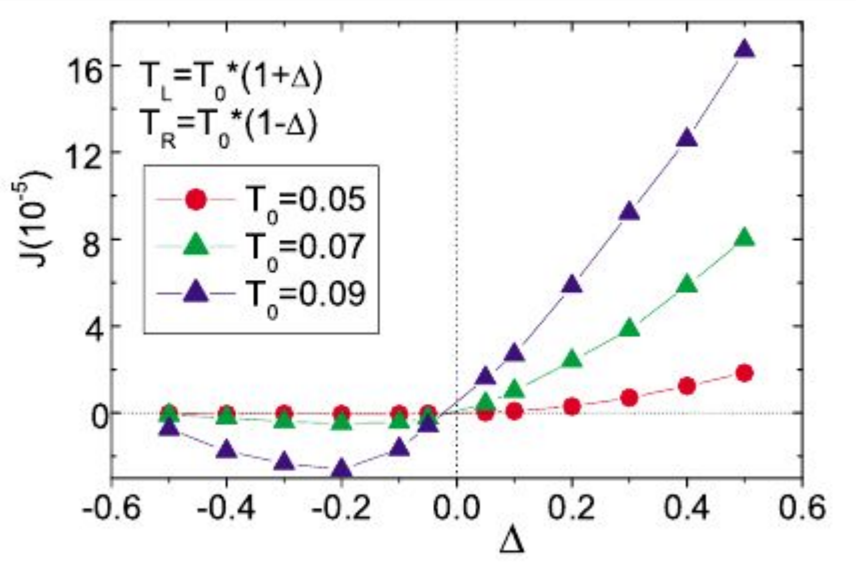
Assimetria



$$R = \frac{\kappa_R - \kappa_L}{\kappa_L}$$

2. Modelo matemático

Diodo Térmico



3. Metodologia

3. Metodologia

Métodos Numéricos Estocásticos

Processo Ornstein-Uhlenbeck => Cálculo Estocástico => Revisar nossos métodos numéricos

Pulo do Gato: Variar só um pouco os determinísticos pra obter os estocásticos. É mais fácil.

B.2
Integração numérica de equações diferenciais estocásticas

Para uma equação diferencial estocástica da forma

$$\frac{dx}{dt} = a(x,t) + b(x,t)\xi(t), \tag{B-5}$$

não existe uma adaptação simples dos métodos numéricos de equações diferencias ordinárias [22] e isto é porque a idealização do ruido é não diferenciável. Portanto, a solução

$$x(t) = x_0 + \int_{t_0}^{t} a(x(s))ds + \int_{t_0}^{t} b(x(s))dW(s), \tag{B-6}$$

3. Metodologia

o qual permite usar os métodos de integração numérica usuais e acrescentar o termo do ruído a cada passo de tempo.

3. Metodologia

Euler

The Euler's Method consists of approaching the evolution of the system by a Taylor series truncated at the linear terms at each step

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

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

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

3. Metodologia

Verlet

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

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. Metodologia

Runge Kutta

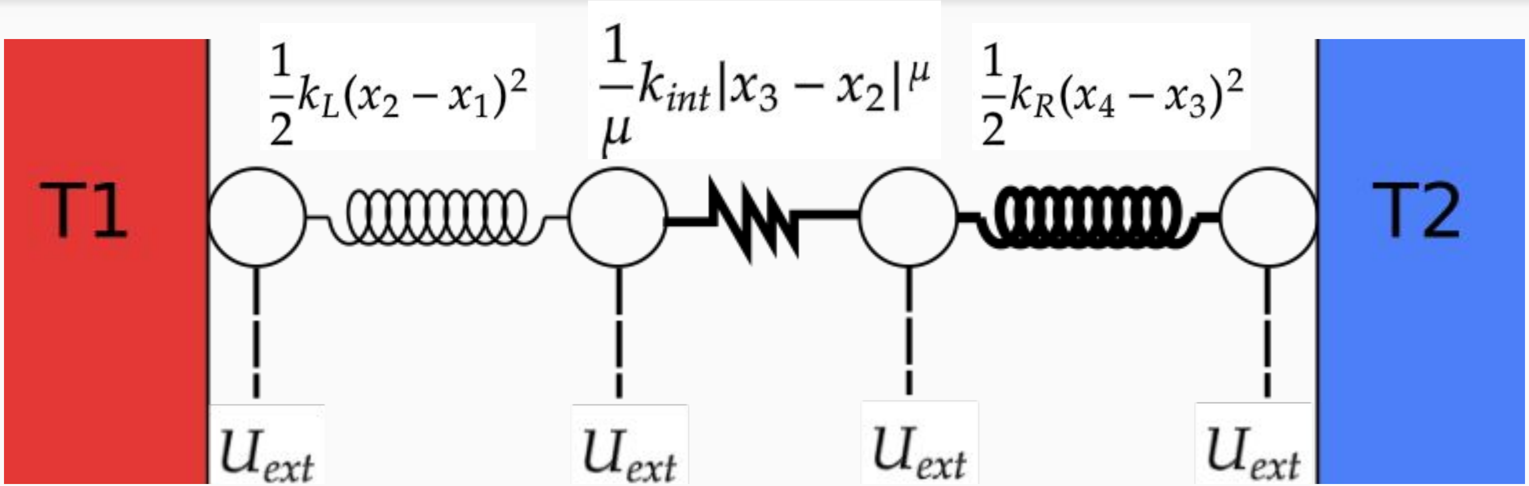
Runge Kutta

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.

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

4. Resultados

4. Resultados



Modelo de Frenkel-Kontorova

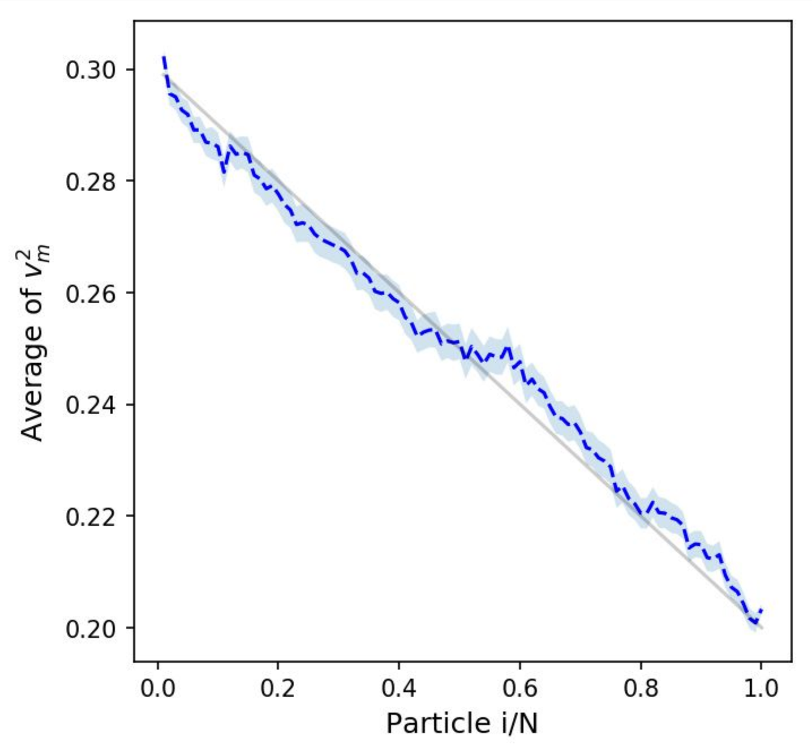
$$U_{ext}(x_i) = A \cdot \left(1 - \cos\left(\frac{2\pi x_i}{a_S}\right)\right)$$

Modelo ϕ^4

$$U_{ext}(x_i) = A \cdot x_i^4$$

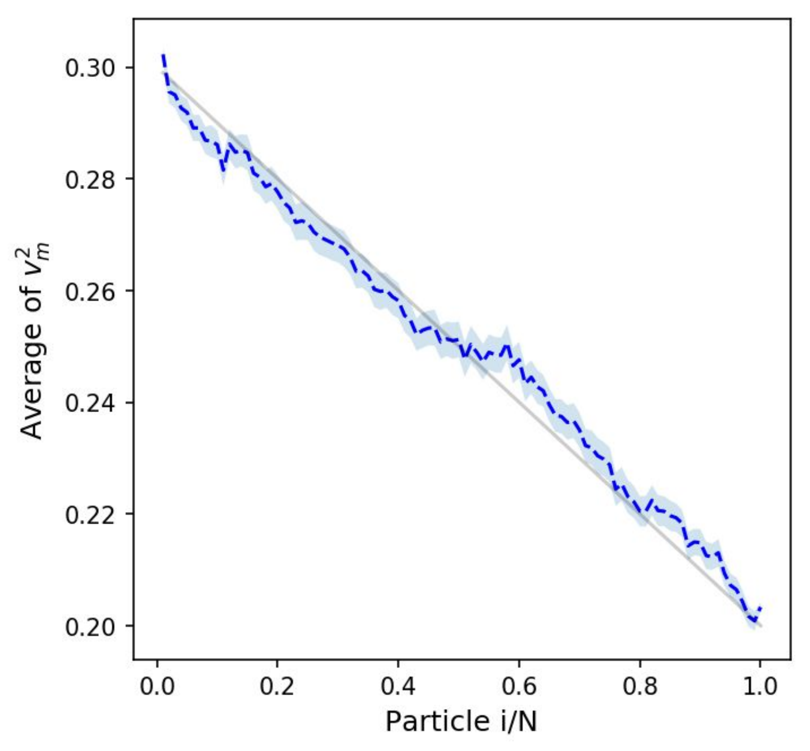
4. Resultados

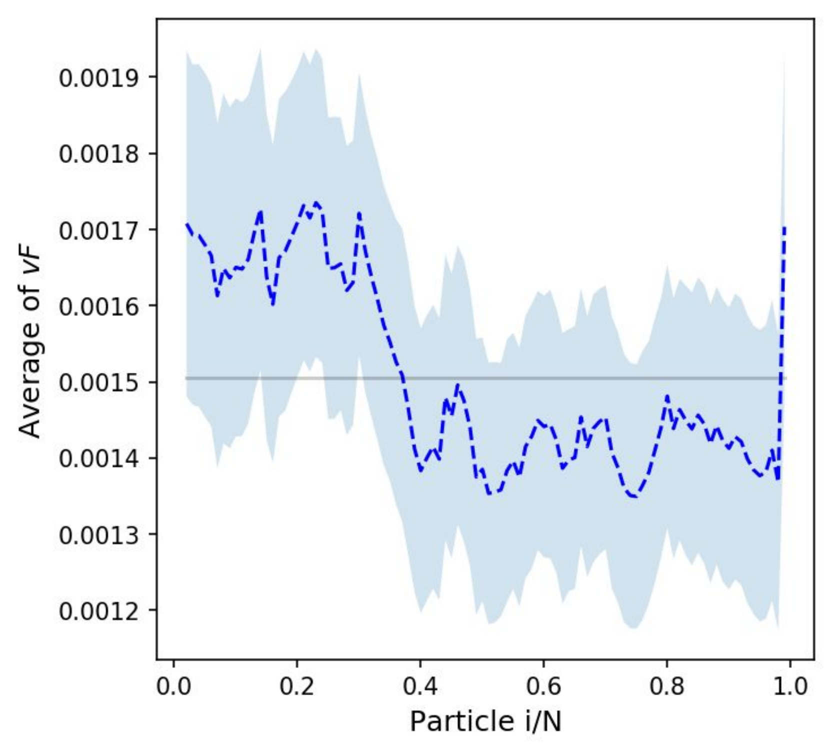
Modelo Frenkel-Kontorova



4. Resultados

Modelo Frenkel-Kontorova

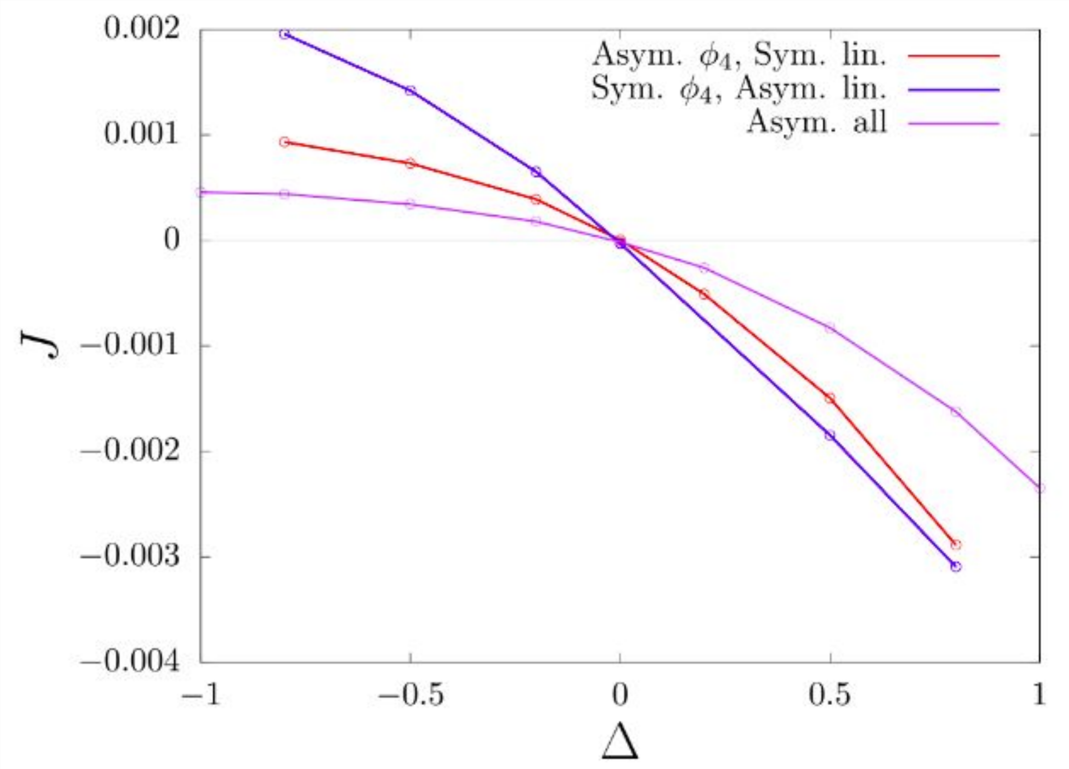




Modelo Frenkel-Kontorova x Modelo ϕ^4

Dificuldade do modelo Frenkel Kontorova para convergência

Modelo ϕ^4



Asym. ϕ_4, Sym. lin.
Sym. ϕ_4, Asym. lin.
Asym. all
J
Δ
0.002
0.001
0
−0.001
−0.002
−0.003
−0.004
−1
−0.5
0
0.5
1

4. Resultados

Número de amostras: 200
Número de partículas na cadeia: 4
Potencial:

Passo de tempo: 0.001
Tempo total da simulação: 100,000.0
Tempo transiente: 1,000.0

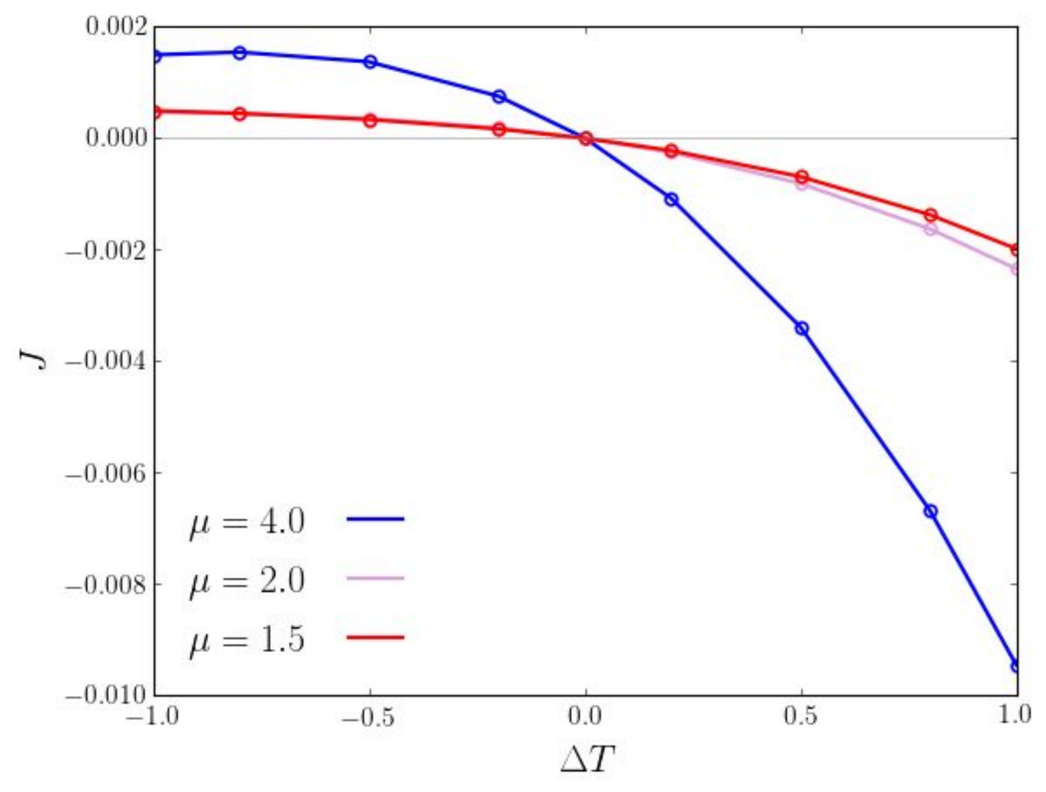
Temperatura média: 1.0
Constante elástica da esquerda: 1.0
Amplitude do potencial esquerdo: 1.0
Constante elástica da direita: 5.0
Amplitude do potencial direita: 5.0
Coeficiente de arraste: 1.0
Constante elástica da interfase: 0.1

A razão k/A fica constante na esquerda e na direita.

> Variar mu
> Variar dT ou k_int

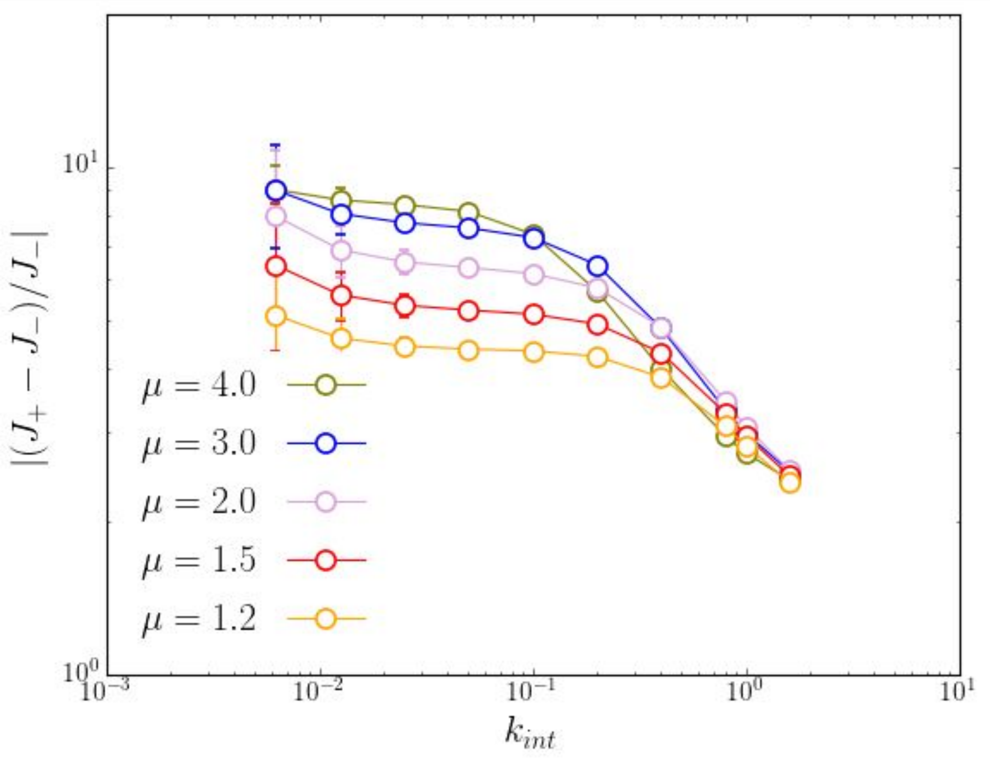
4. Resultados

Diodo Térmico



4. Resultados

Eficiência



5. Conclusão

5. Conclusões

Discussão de resultados

- Mu: um tipo de interação de interfase. Quanto maior, melhor.

5. Conclusões

Novos trabalhos

- Tempo até estacionaridade

REFERÊNCIAS

Obrigado!

1. Introdução