# Heat and thermal responce in non-equilibrium systems

Schotte Alexis, Vergauwen Bob

Bachelor of Physics, KU Leuven

mei , 2014

# Introduction

## Is heat capacity always positive?

- In equilibrium, it is
- How about non-equilibrium systems?

$$C_j = \frac{\delta\langle Q\rangle}{\partial T_j}\bigg|_{V,T_1,\dots,T_{j-1},T_{j+1},\dots,T_N}$$

## Examples of negative responce

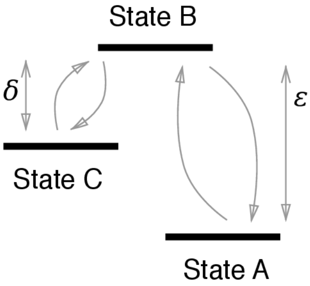
- Stars that emit energy in the form of radiation get hotter.
- Negative compressibility
- Negative resistance

# Outline

# A three state system

## Transition rates

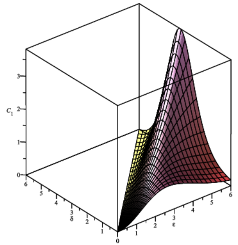
$$
\begin{cases}
k(a,b) = e^{-\beta_1 \epsilon} \\
k(b,a) = 1 \\
k(a,c) = 0 \\
k(c,a) = 0 \\
k(b,c) = 1 \\
k(c,b) = e^{-\beta_2 \delta}
\end{cases}
$$

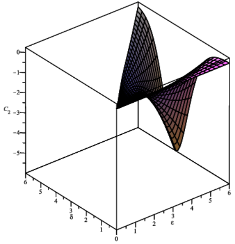


# Analytic results: two transitions

$$\begin{cases} C_1 = \beta_1 \epsilon e^{\beta_1 \epsilon} \dfrac{\epsilon + (\epsilon - \delta) e^{\beta_2 \delta}}{T_1 \left( e^{\beta_1 \epsilon} + 1 + e^{\beta_2 \delta} \right)^2} \\ \\ C_2 = \beta_2 \delta e^{\beta_2 \delta} \dfrac{\delta + (\delta - \epsilon) e^{\beta_1 \epsilon}}{T_2 \left( e^{\beta_1 \epsilon} + 1 + e^{\beta_2 \delta} \right)^2} \end{cases}$$

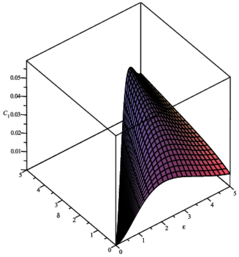
$$C_2 < 0 \Leftrightarrow \delta < \epsilon \frac{e^{\beta_1 \epsilon}}{1 + e^{\beta_1 \epsilon}}$$

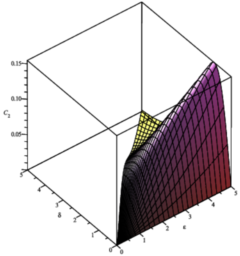




# Analytic results: three transitions

$$
\begin{cases}
C_1 = \dfrac{\epsilon \beta_1 e^{-\beta_1 \epsilon}(e^{-\beta_1 \epsilon}\epsilon + \epsilon + \delta)}{T_1(e^{-\beta_1 \epsilon} + 2)^3(e^{-\beta_2 \delta} + 2)} \\[2ex]
C_2 = \dfrac{\delta \beta_2 e^{-\beta_2 \delta}(e^{-\beta_2 \delta}\delta + \epsilon + \delta)}{T_2(e^{-\beta_1 \epsilon} + 2)(e^{-\beta_2 \delta} + 2)^3}
\end{cases}
$$



# Simulation of discrete system

Two methods have been used to simulate the discrete system.

## Deterministic methode

- Uses the Markov framework
- Transition matrix
- Fast
- Easy to implement
- No direct physics involved, just mathematics
- Can be speed up by linearisation

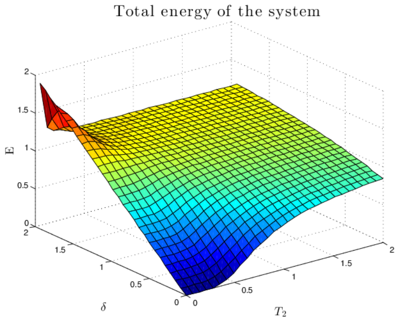
## Stochastic methode

- Uses the a jump process
- The outcome is random
- One jump at the time
- Slow
- Represents the physical system very good
- Can produce more stochastic information

# Deterministic method

## Algorithme

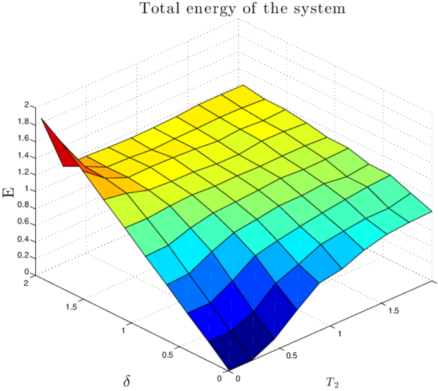
- Create a transition matrix $M(T)$
- Chose an initial distribution $\rho_0$
- Update the distribution $\rho(t) = \rho_0 e^{Mt}$
- Calculate the energy $E$
- Change the temperature by a small fraction
- repeat this process



# Stochastic method

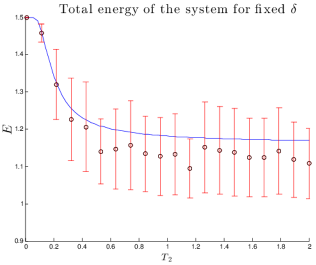
## Algorithme

- Pick a random starting position
- Let the particle jump for some steps
- Calculate the energy
- Repeat this for a good result
- Change the temperature by a small fraction
- repeat this process

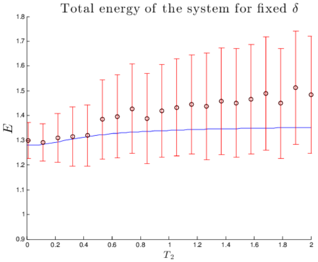


# Comparison of the two results

## Two transitions



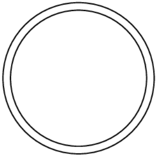

## Three transitions



# Langevin dynamics

$$\ddot{x} = F - \nabla U - \gamma \dot{x} + \sqrt{2T\gamma}\,\xi_t$$

- constant force $F$
- force caused by periodic potential $U$
- friction, proportional to the velocity
- Brownian motion



## Underdamped

Particle needs infinite time to reach its final velocity

## Overdamped

Very high friction $\rightarrow$ particle instantaneously reaches its final velocity $v_f$

$$\gamma v_f = F - \nabla U + \sqrt{2T\gamma}\,\xi_t$$

# The Fokker-Planck equation

$$\frac{\partial \mu_t(x)}{\partial t} + \nabla j_{\mu_t}(x) = 0, \qquad j_{\mu_t} = \frac{1}{\gamma}\mu_t\left(F - \nabla U\right) - \frac{\nabla \mu_t}{\beta\gamma}$$

## Solution

- $\boxed{F = 0}$ $\rightarrow$ equilibrium $\qquad \rho(x) = \frac{1}{\mathcal{Z}} e^{-\beta U(x)}, \ \mathcal{Z} = \int_0^1 e^{-\beta U} \mathrm{d}x$
- $\boxed{F \neq 0}$ and $\int_0^1 F \mathrm{d}x \neq 0 \rightarrow$ no equilibrium

$$\rho(x) = \frac{1}{\mathcal{Z}} \int_0^1 \beta\gamma e^{\beta W(y,x)} \mathrm{d}y, \qquad \mathcal{Z} = \int_0^1 \int_0^1 \beta\gamma e^{\beta W(y,x)} \mathrm{d}y\mathrm{d}x$$

$$W(y,x) = U(y) - U(x) + \begin{cases} \int_y^x F \mathrm{d}z & \text{for } y \leq x \\ \int_y^1 F \mathrm{d}z + \int_0^x F \mathrm{d}z & \text{for } y > x \end{cases}$$

# The Fokker-Planck equation

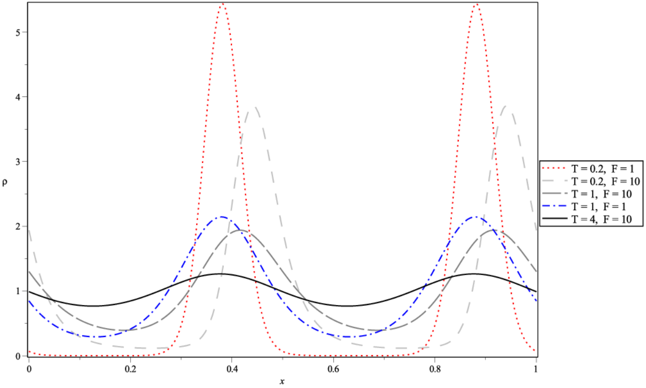



Figure : $\rho(T)$ with $U = \sin(4\pi x)$, $k_b = 1$, $\gamma = 1$

# Simulation of the Langevin equation

Two possible approximation methods.

## Overdamped

$$\dot{v} = F - \nabla U - \gamma v + \sqrt{2T\gamma}\xi_t$$

- This is the most general method

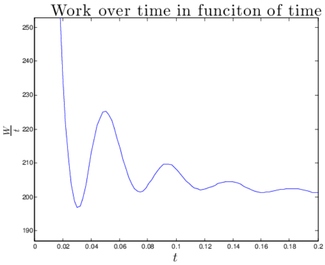
## Underdamped

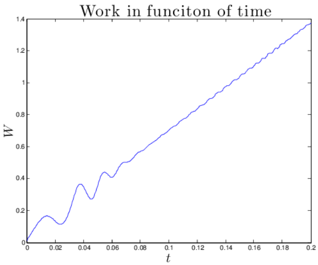
$$\gamma v_f = F - \nabla U + \sqrt{2T\gamma}\xi_t$$

- Particle reaches terminal velocity after each step

# Results

The result for both methods gave the same numerical result.



# Discrete system

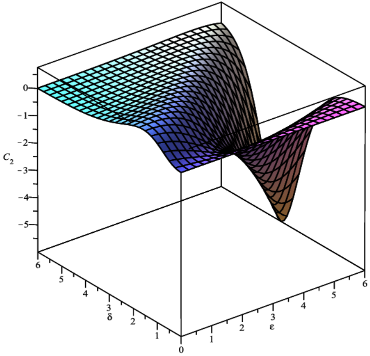



Figure : Result calculated using analytic calculations

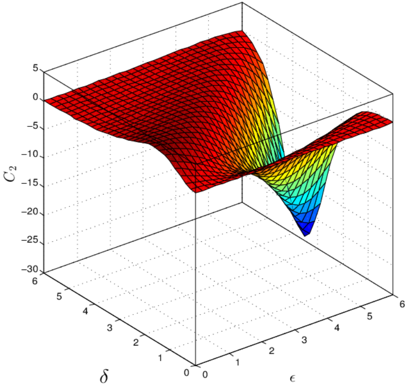



Figure : Data calculated using the stochastic method

# Langevin equation

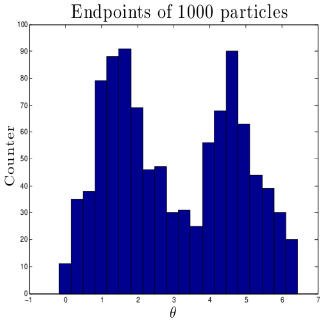



Figure : Simulated data

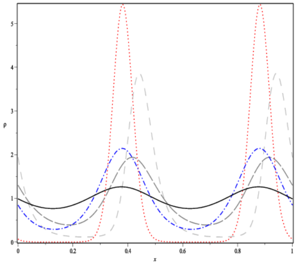


Figure : Analytic solution

# Open questions

- Can we use the theory of the discrete systems for the ring?
- What is the heat capacity of this ring?
- How does the system change when the ring has a temperature in function of its position?

*"The best thing about learning about equilibrium, is that nothing changes"*

*Anonymous*