Universidade de São Paulo
Instituto de Física

Estudo sobre a produção de entropia e transporte de calor em cadeias harmônicas sujeitas a variações temporais periódicas

Bruno Augusto Naves Akasaki

Orientador: Prof. Dr. Carlos Eduardo Fiore dos Santos

Dissertação de mestrado apresentada ao Instituto de Física da Universidade de São Paulo, como requisito parcial para a obtenção do título de Mestre em Ciências.

Banca Examinadora:
Prof. Dr. Carlos Eduardo Fiore dos Santos - IFUSP
Prof. Dr. Eric de Castro e Andrade - IFSC/USP
Prof. Dr. Karel Proesmans - Simon Fraser Universit

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University of São Paulo
Physics Institute

Entropy production and heat transport in harmonic chains under time-dependent periodic drivings

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Supervisor: Prof. Dr. Carlos Eduardo Fiore dos Santos

Dissertation submitted to the Physics Institute of the University of São Paulo in partial fulfillment of the requirements for the degree of Master of Science.

Examining Committee:
Prof. Dr. Carlos Eduardo Fiore dos Santos (Surpevisor) - IFUSP
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Resumo

Akasaki, B. A. N. **Entropy production and heat transport in harmonic chains under time-dependent periodic drivings.** 2020. Dissertação (Mestrado em Física) - Instituto de Física, Universidade de São Paulo, São Paulo, 2020.

Nesta dissertação de mestrado estudamos as propriedades termodinâmicas de cadeias lineares sujeitas a forças e temperaturas oscilantes no tempo por meio da abordagem termodinâmica estocástica. Os sistemas em questão são descritos pela equação de Fokker-Planck-Kramers e obtivemos o comportamento exato para as propriedades termodinâmicas como funções da frequência e parâmetros do problema. A análise será dividida em duas partes: regime de cadeias curtas e longas. No primeiro caso, obtivemos expressões para a produção de entropia a qual pode ser escrita como uma forma bilinear pelo produto de forças e fluxos termodinâmicos, cujos coeficientes Onsager são calculados para tipos distintos de variações temporais dos parâmetros. O limite de cadeias longas é analisado por meio de um protocolo em que as temperaturas intermediárias são escolhidas de forma auto-consistente e a produção de entropia é decomposta como uma soma de duas contribuições: uma proveniente de banhos reais (colocados nas extremidades da cadeia) e outros de banhos autoconsistentes. Enquanto o primeiro termo devido as temperaturas dos reservatórios térmicos é dominante no regime de cadeias curtas, o último devido as forças variantes no tempo prevalece para os longos. Ainda foi possível constatarmos que o fluxo de calor obedece a lei de Fourier. No caso de duas partículas interagentes, verificamos que o comportamento da produção de entropia com a inclusão de uma defasagem e o comportamento da frequência ótima em relação aos parâmetros do problema.

Palavras-chave: TERMODINÂMICA ESTOCÁSTICA, SISTEMAS FORA DO EQUILÍBRIO, PRODUÇÃO DE ENTROPIA, COEFICIENTES DE ONSAGER

Abstract

We study the properties of interacting linear chains subject to periodic drivings through the framework of stochastic thermodynamics. The systems are described by Fokker-Planck-Kramers equation and exact solutions are obtained as functions of the modulation frequency and strength constants. Analysis will be carried out for short and long chains. In the former case, explicit expressions are derived for a chain of two particles, in which the entropy production is written down as a bilinear function of thermodynamic forces and fluxes, whose associated Onsager coefficients are evaluated for distinct kinds of periodic drivings. The limit of long chains is analyzed by means of a protocol in which the intermediate temperatures are self-consistently chosen and the entropy production is decomposed as a sum of two individual contributions, one coming from real baths (placed at extremities of lattice) and other from self-consistent baths. Whenever the former dominates for short chains, the latter contribution prevails for long ones. It was also possible to verify that the thermal reservoirs leads to a heat flux according to Fourier's law as well as the behavior of the entropy production with a inclusion of a lag and the behavior of the optimal frequency in relation to the problem parameters.

Keywords: STOCHASTIC THERMODYNAMICS, NONEQUILIBRIUM SYSTEMS, ENTROPY PRODUCTION, ONSAGER COEFFICIENTS

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Chapter 1

Introduction

The stochastic approach to equilibrium and nonequilibrium thermodynamics, also known as, stochastic thermodynamics has become one of the main cornestones of modern statistical mechanics and a consistent theory for nonequilibrium thermodynamics [1-29]. It was originated from distinct approaches and pioneer works, such as the seminal work by Onsager and Prigogine who established that close to equilibrium a linear approach can be used to determine the thermodynamic fluxes, such as heat and work. In addition, it has been show that they satisfy general properties, such as Onsager symmetry and the Green-Kubo relations. Other important step in this direction occurred when Schnakenberg [6] introduced the stochastic definition of entropy production rate which has the probabilistic aspect, in addition to the definition of entropy itself introduced by Gibbs [30].

In the last years, stochastic thermodynamics has been put under firmer basis by using Markov dynamics together with the assumption of local detailed balance and leading to a consistent definition of the thermodynamic properties of the system. The stochastic fluxes of the system satisfy general relations such as the Jarzynski equality [58, 59].

Basically, stochastic thermodynamics encompasses two main classes of systems: those described by systems in the continuous and discrete spaces. The former case was used by Einstein [31], Smoluchowski [32], and Langevin [33] to explain Brownian motion. It was generalized to the case of Brownian particles subject to an external force by Fokker [34], Smoluchowski [35], Planck [36], and Ornstein

[37], giving rise to the equation governing the time evolution of the probability distribution became known as the Fokker-Planck equation. Kramers [38] extended the Fokker-Planck equation to the case of a massive particle and studied the escape of a Brownian particle over a potential barrier arriving at the Arrhenius factor. The latter case takes into account discrete state space and has been used in various problems in physics, chemistry and biology. We mention the study of chemical reactions [5, 8, 9, 18, 29], population dynamics and epidemiology [39, 40, 41], and biological systems in general [4, 17, 28, 42, 43, 44, 45, 46, 106]. We wish to mention particularly the stochastic models with many degrees of freedom such as the so-called stochastic lattice models usually used to describe phase transitions and criticality in physics, chemistry, and biology [15, 47, 48, 49, 50, 51, 52, 53, 54].

In all previous examples, the entropy production has played a fundamental role in nonequilibrium statistical physics not only for typifying the irreversibility [62, 63, 64], but also for tackling general considerations about efficiency of heat engines [65], the analysis of (irreversible) phase transition portraits [66, 67, 68], thermodynamic uncertainties relations [60, 61] and others.

A fundamental relation for the entropy production comes from simple entropic arguments in which the system is coupled to a thermal reservoir. Its time entropy variation dS/dt is the difference of two terms

$$\frac{dS}{dt} = \Pi(t) - \Phi(t), \tag{1.1}$$

where $\Pi(t)$ is the entropy production rate and $\Phi(t)$ is the entropy flux rate from/to the system to/from the environment. Since the environment works as a subsystem in equilibrium, $\Pi(t)$ corresponds to the entropy produced inside the system. Eq. (1.1) implies that all entropy spontaneously produced (by the system) has to be delivered to the environment in the steady state regime. When the system is in thermal equilibrium, it follows that $\Pi_s = \Phi_s = 0$, whereas $\Pi_s = \Phi_s > 0$ out of the equilibrium regime. Thereby, entropy production discerns equilibrium and nonequilibrium systems, since it is continuously produced in the latter case. In such case, the steady entropy production rate can alternatively be evaluated through the calculation of the steady entropy flux.

More recently, the stochastic thermodynamics of periodically driven systems [80, 81, 82, 83] has attracted a great deal of interest in part because their thermodynamic properties can be experimentally accessible have attracted a great deal of interest [80, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101]. In addition, some of their remarkable features, such as a general description in the linear regime (in which Onsager coefficients and general reciprocal relations can be achieved), the existence of uncertainties constraints leading to existence of bounds among macroscopic averages and other features have been put under a firmer basis. In other cases, the probability distribution of work for systems described by Langevin equations with time dependent drivings has also been analyzed [78]. However, the more general case of interacting particles subject to distinct time periodic drivings has not been studied thoroughly. In particular, the question of how the inclusion of interaction changes the nonequilibrium trademarks as well as the entropy production properties has not been addressed before.

In this master work, we fill this gap by investigating the thermodynamic properties of interacting chains of Brownian particles subject to (time dependent) periodic forces and temperature drivings. Exact expressions for the thermodynamic quantities, including the dissipated heat, entropy production, heat flux and others are obtained. The limits of short and long particle chains are thoroughly investigated. For the latter case, intermediate temperatures are self-consistently chosen through a protocol taking into account an inner entropy production source. This is meaningfully different from the original approach by Bosterli et al. [104], in which no heat flux is exchanged among the particles and self-consistent baths. Thus, our approach provides us not only to analyze the role of two distinct sources of dissipation, but also establishing which contribution dominates in the limits of short and long chains. Two main findings can be drawn: For the case of two interacting particles, the entropy production is derived as a bilinear function of fluxes and forces for both drivings in forces and temperatures, whose associated Onsager coefficients depend on the interaction parameters and frequency driving. Remarkably, the effect of a phase difference (a lag) between external forces is investigated and the condition for maximum/minimum entropy production is found to depend only on the temperature reservoirs and frequency driving, irrespective of the interaction strength between particles. The effect of oscillating temperature and a comparison with the single (underdamped) the harmonic oscillator will be also considered.

The entropy production of long particle chains can be splitted in two terms: one coming from the thermal reservoirs and the other from the self-consistent ones. This dissertation is organized as follows: In Chapter 2 we give a brief introduction about stochastic thermodynamics and we describe the theoretical background and the exact solution for a case without time dependent drivings in Chapter 3. In Chapter 4 we introduce and thermodynamics properties are evaluated the time dependent force for hamonic chains. In Chapter 5 we focus on the time dependent oscillating temperatures. Conclusions finally are discussed in Chapter 6.

Chapter 2

Stochastic thermodynamics: fundamental concepts

2.1 Some remarks about entropy production

Classical thermodynamics deals with equilibrium states based on three laws which has been successful in describing systems at the microscopic level, in which local fluctuations are not taken into account. One of the most important findings concerns that total entropy (of an isolated system) never decreases implying that it is always greater than or equal to zero. Stochastic thermodynamics provide some new findings by expanding to nonequilibrium systems with fluctuations, trying to identify on the individual level notions of classical thermodynamics, like the work and heat and the entropy production.

According to the second law of thermodynamics, thermal equilibrium is determined by the principle o maximum entropy. In a equilibrium system, the entropy depends on extensive variables x_k (energy, number of particles, etc). First, let's consider a system composed of two couple subsystems (A and B). By taking into account that the composite system $A + B$ is isolated, we have that

$$x_k^A + x_k^B = \text{constant}, \tag{2.1}$$

and hence

$$dx_k^A = -dx_k^B. \tag{2.2}$$

It is worth mentioning that such above constraints are equivalent to the first law of thermodynamics. Using the additive property of the entropy S

$$S = S_A + S_B, \tag{2.3}$$

its derivative with respect to the x_k^A (or x_k^B) is given by

$$\frac{\partial S}{\partial x_k^A} = \frac{\partial S_A}{\partial x_k^A} + \frac{\partial S_B}{\partial x_k^A}, \tag{2.4}$$

and

$$\frac{\partial S}{\partial x_k^B} = \frac{\partial S_A}{\partial x_k^B} + \frac{\partial S_B}{\partial x_k^B}. \tag{2.5}$$

Taking into account Eq. (2.2), it follows that

$$\frac{\partial S}{\partial x_k^A} = \frac{\partial S_A}{\partial x_k^A} - \frac{\partial S_B}{\partial x_k^B}. \tag{2.6}$$

Due to the second law of thermodynamics, the total entropy is a maximum at the equilibrium and it follows that

$$\frac{\partial S_A}{\partial x_k^A} = \frac{\partial S_B}{\partial x_k^B}, \tag{2.7}$$

where

$$\frac{\partial S_k}{\partial x_k^k} = f_k, \tag{2.8}$$

which f_k represents the intensive thermodynamic variable associated to x_k.

Let us consider the relaxation toward the equilibrium as the two systems A and B are placed in contact with each other. The time evolution of entropy system is given by

$$\frac{dS}{dt} = \sum_k \left(\frac{\partial S_A}{\partial x_k^A} \frac{dx_k^A}{dt} + \frac{\partial S_B}{\partial x_k^B} \frac{dx_k^B}{dt} \right), \tag{2.9}$$

and taking into account the constraint

$$x_k^A + x_k^B = \text{constant}, \tag{2.10}$$

or equivalently

$$\frac{dx_k^A}{dt} = -\frac{dx_k^B}{dt}, \tag{2.11}$$

we have that

$$\frac{dS}{dt} = \sum_k \left(\frac{\partial S_B}{\partial x_k^B} - \frac{\partial S_A}{\partial x_k^A} \right) \frac{dx_k^B}{dt}. \tag{2.12}$$

The first term can be intepreted as the current leaving A and the current entering in B, the last term in the right is the flux associated to the variable x_k^B. Thus

$$\frac{dS}{dt} = \sum_k J_k \left(\frac{\partial S_B}{\partial x_k^B} - \frac{\partial S_A}{\partial x_k^A} \right), \tag{2.13}$$

and

$$\frac{\partial S_B}{\partial x_k^B} - \frac{\partial S_A}{\partial x_k^A} = f_k^B - f_k^A = F_k, \tag{2.14}$$

is a generalized thermodynamic force (affinity). We can interpret $F_k = f_k^B - f_k^A$ as responsible for generating the currents J_k, which is consistent to the thermal equilibrium when the current J_k is zero if no forces exists $f_k^A = f_k^B$. In principle the current J_k at a given time t could depend on the affinities at previous times $t' < t$. We shall assume that the process is close to the equilibrium and systems are large, so that $J_k(t)$ only depends on the affinites at the same time t. Thus, the relation

$$\frac{dS}{dt} = \sum_k F_k J_k, \tag{2.15}$$

reveals that the total entropy is not conserved, but spontaneously produced by the irreversible change of energy/particles. Since $A + B$ is isolated and there is no entropy flux from outside, the change of entropy must be associated with an entropy production. One can rewrite above relation in the case when $F_k = \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$ and $\left(\frac{\mu_2}{T_2} - \frac{\mu_1}{T_1}\right)$, like

$$\frac{dS}{dt} = \sum_k \left(\frac{1}{T_2} - \frac{1}{T_1} \right) J_u + \left(\frac{u_2}{T_2} - \frac{u_1}{T_1} \right) J_N. \tag{2.16}$$

The entropy production is not a property of A or B, but a global property of the joint system $A+B$. There is one case where one can give a different interpretation. Let us consider the system $B \gg A$ (B acts as a thermal reservoir case). Then, we can assume that

$$\frac{\partial S_B}{\partial x_k^B} = f_k^B = \text{const}, \tag{2.17}$$

since B will always remain closed to the equilibrium and f_k^B will not change due to the contact with A. In such case, we can assume that there is not entropy production due to the subsystem B, since its dynamics is always reversible and thereby the entropy production is only due to the subsystem A. Thus, from Eq. (2.13) the term

$$\frac{dS_B}{dt} = \sum_k f_k^B J_k, \tag{2.18}$$

can be interpreted as an entropy flux Φ (e.g., the entropy contribution coming from the reservoir).

The terms in the right side of Eq. (2.13) can be rewritten as

$$\frac{dS_B}{dt} = \sum_k f_k^B J_k, \tag{2.19}$$

$$\frac{dS_A}{dt} = -\sum_k f_k^A J_k, \tag{2.20}$$

respectively. Hence,

$$\frac{dS}{dt} = \frac{dS_B}{dt} + \frac{dS_A}{dt}, \tag{2.21}$$

and

$$\frac{dS_A}{dt} = \frac{dS}{dt} - \frac{dS_B}{dt} = \Pi - \Phi. \tag{2.22}$$

In other words: the time variation of the entropy of A is the difference of two terms. The entropy production and an entropy flux from/to the environment. Such relation will be obtained in the next chapter from stochastic arguments. An exemplification is

$$\Phi = \sum_k f_k^B J_K = \frac{J_u}{T}, \tag{2.23}$$

if $k = u$ and T is the both temperature.

2.1.1 Linear responsive theory

Linear stochastic thermodynamics is commonly the starting point for a nonequilibrium thermodynamics theory. In the case of systems A and B are quite close to the equilibrium and that the affinites (forces) $F_k = f_k^B - f_k^A$ are small. Then, we can expand the currents in Taylor series in F_k up to first order, it becomes

$$J_k = \sum_l L_{k,l} F_l, \tag{2.24}$$

where $L_{k,l}$ are Onsager coefficients. For example for K and l being the μ and N, we have that

$$J_u = L_{u,u} F_u + L_{u,N} F_N \tag{2.25}$$

and

$$J_N = L_{N,u} F_u + L_{N,N} F_N. \tag{2.26}$$

According to Onsager, the cross coefficients are equal $L_{u,n} = L_{n,u}$. In particular, the main result by Onsager was to show that the matrix L is positive semi-definite $L \geq 0$.

Above finding is a typical structure of a linear responsive theory: it means that when the stimulus is small, the corresponding response will be linear on it. Let us return to the entropy production, according to the previous relations

$$\Pi = \frac{dS}{dt} = \sum_k f_k J_k, \tag{2.27}$$

In the regime of linear response, we may substitute and we get

$$\Pi = \sum_k \sum_l L_{k,l} F_k F_l. \tag{2.28}$$

Since $\Pi \geq 0$ it follows that

$$4 L_{ll} L_{kk} - (L_{lk} + L_{kl})^2 \geq 0 \tag{2.29}$$

Such features about Onsager coefficients will be verified in the next chapter for a chain of two interacting particles.

Chapter 3

Continuous variable systems approach

3.1 Langevin equation

Brownian motion plays a fundamental role in statistical physics, since several insights about dynamics of macroscopic systems can be achieved and corroborated by it main features. It corresponds to the random movement of fluid-immersed particles due to the collision with fluid molecules. Its general description was established by Robert Brown (1773-1858) in 1828, who studied the movement of the pollen particles and observed an agitated and irregular movement. In the nineteenth century, it was found the dependence of the Brownian motion with several physical parameter, such as diameter, temperature and viscosity.

Afterwards, in 1905 Albert Einstein (1879-1955) developed a quantitative description of the Brownian motion. In particular, he realized that an underlying atomic bath was required for providing fluctuations for the erratic motion of particles, giving rise to the random walk. Thus, in quantitative terms, Brownian motion corresponds to a random motion subject to two forces, the first being dissipative and the second a random due to the collision between particles and molecules fluid. For simplicity, we assume that the dissipative frictional force is proportional to its velocity and a random force, which comes from independent impacts.

The motion equation fulfilling these properties is called a Langevin equation and it is given by

$$m\frac{dv}{dt} = -\alpha v + F_a(t), \tag{3.1}$$

and

$$\frac{dx}{dt} = v, \tag{3.2}$$

where v is the particle velocity, x the particle position and α the coefficient of friction, respectively. The dissipative force is represented by the first term in the right side of the equation (3.1), whereas the random force is given by $F_a(t)$, which has the following properties:

$$\langle F_a(t)\rangle = 0, \tag{3.3}$$

and

$$\left\langle F_a(t)F_a(t^{'})\right\rangle = B\delta(t-t^{'}), \tag{3.4}$$

implying that on average the force due to impacts with the molecules is zero and collisions are independent. The random force that satisfies such above conditions is called white noise. By dividing both terms of the equation (3.1) by the mass m, we have that

$$\frac{dv}{dt} = -\gamma v + \zeta(t), \tag{3.5}$$

where $\gamma = \frac{\alpha}{m}$ e $\zeta(t) = \frac{F_a(t)}{m}$ is a stochastic variable that has the following properties:

$$\langle \zeta(t)\rangle = 0, \tag{3.6}$$

and

$$\left\langle \zeta(t)\zeta(t^{'})\right\rangle = \Gamma\delta(t-t^{'}), \tag{3.7}$$

where $\Gamma = \frac{B}{m^2}$.

We can easily find a generic solution for the Langevin equation (3.5) for any noise $\zeta(t)$, by integrating equation (3.1):

$$v(t) = v_0 e^{-\gamma t} + e^{-\gamma t}\int_0^t e^{\gamma t^{'}}\zeta(t^{'})dt^{'}, \tag{3.8}$$

where v_0 is the particle velocity at time $t = 0$.

The average velocity can be given using the expression (3.8) and by using the properties of white noise given by Eq. (3.6) e (3.7), we have that

$$\langle v \rangle = v_0 e^{-\gamma t}, \tag{3.9}$$

meaning that on the average the particle velocities exponentially vanishes, as expected for a particle subject to a viscous force. In particular, the velocity variance can be evaluated in a simular way, whose expression reads

$$\left\langle v^2 \right\rangle_{cv} = \left\langle v^2 \right\rangle - \langle v \rangle^2 = \frac{\Gamma}{2\gamma}\left(1 - e^{-2\gamma t}\right). \tag{3.10}$$

Note that for long times, $\langle v^2 \rangle \to \frac{\Gamma}{2\gamma}$. This can be understood by recalling that the kinetic energy of a particle with mass m moving at a velocity v is

$$E_{\text{kin}} = \frac{1}{2} m v^2, \tag{3.11}$$

and the principle of equipartition energy ensures that in thermal equilibrium the particles have the same average kinetic energy for a given temperature. So that, for a particle moving in a fluid at a temperature T, it follows that

$$\langle E_{\text{cin}} \rangle = \frac{1}{2} k_B T \quad \Rightarrow \quad \frac{1}{2} m \left\langle v^2 \right\rangle = \frac{1}{2} k_B T. \tag{3.12}$$

Substituting Eq. (3.10) in this last equation for long times, we get

$$\Gamma = \frac{2\gamma k_B T}{m}, \tag{3.13}$$

and

$$B = 2\alpha k_B T. \tag{3.14}$$

Thus, the parameter B is related to the system temperature through relation $\Gamma = \frac{B}{m^2}$.

3.2 Fokker-Planck equation

Let us take again the above set of Langevin equations for a set of N particles. Each particle, i is then given by the equations,

$$\frac{dx_i}{dt} = f_i(x) + \zeta_i(t), \qquad \begin{cases} \langle \zeta_i(t) \rangle = 0 \\ \left\langle \zeta_i(t),\zeta_i(t^{`}) \right\rangle = \Gamma_i \delta_{ij} \delta(t - t^{`}), \end{cases} \tag{3.15}$$

where i attempts for the ith particle ranged from $i = 1,\ldots,N$. Above equation describes the overdamped case, in which it has the following Fokker-Planck equations (or Smoluchowski equations)

$$\frac{\partial}{\partial t} P(x,t) = -\sum_{i=1}^{N} \frac{\partial}{\partial x} \left[f_i(x) P(x,t) \right] + \sum_{i=1}^{N} \frac{\Gamma_i}{2} \frac{\partial^2}{\partial x_i^2} P(x,t), \tag{3.16}$$

where $P(x,t)$ denotes the probability distribution of the $x = x_1, \ldots, x_N$. The Fokker-Planck equation can be conveniently rewritten as a continuity equation

$$\frac{\partial}{\partial t} P(x,t) = -\sum_{i=1}^{N} \frac{\partial J_i(x,t)}{\partial x_i}, \tag{3.17}$$

where the i -th component of the probability flow $J_i(x,t)$ is given by

$$J_i(x,t) = f_i(x) P(x,t) - \frac{\Gamma_i}{2} \frac{\partial P(x,t)}{\partial x_i}. \tag{3.18}$$

In the first analysis, we obtained its steady state solution in which $\frac{\partial}{\partial t} P(x,t) = 0$, implying that the probability density is independent on the time $P(x,t) = P(x)$. The equation (3.17) then reads

$$0 = \sum_{i=1}^{N} \frac{\partial J_i(x)}{\partial x_i}, \tag{3.19}$$

which also implies that $J_i(x)$ is time independent and constant. When each current vanishes $J_i(x) = 0$, we have the microscopic reversibility and steady state corresponds to the thermodynamic equilibrium. Hence, Eq. (3.18), can be rewritten as

$$\frac{\partial}{\partial x_i}\ln P(x) = \frac{2}{\Gamma_i} f_i(x), \tag{3.20}$$

and when forces f_i are conservative for all i ($f_i = -\frac{\partial V}{\partial x_i}$) and all of them are in the same temperature ($\Gamma_i = \Gamma$), it follows that by finding the probability $P(x)$ has the Boltzmann-Gibbs form given by

$$P(x) = Ae^{-2V(x)/\Gamma}, \tag{3.21}$$

where A is a probability normalization constant related to the partition function.

Thereby, when forces are conservative and the microscopic reversibility is satisfied, the probability distribution is Boltzmann-Gibbs and the system is in thermodynamic equilibrium, in which it is in contact with a thermal reservoir at a temperature proportional to Γ. When $J_i(x) \neq 0$, the system will evolve to a nonequilibrium state. This is indeed the case of temperatures being different and/or not conservative forces.

3.2.1 Entropy and entropy production

The entropy S of a system described by a probability distribution $P(x,t)$ is defined by

$$S(t) = -k_B \int P(x,t) \ln P(x,t) dx, \tag{3.22}$$

which $dx = dx_1 dx_2 \cdots dx_N$.

We can determine the temporal variation of entropy by the Fokker-Planck Eq. (3.17) (for $k_B = 1$)

$$\frac{dS}{dt} = -\sum_{i=1}^{N} \int J_i \frac{\partial \ln P}{\partial x_i} dx, \tag{3.23}$$

By using Eq. (3.18), we can rewrite the above equation in the following way

$$\frac{dS}{dt} = -\sum_{i=1}^{N} \frac{2}{\Gamma_i} \int f_i J_i dx + \sum_{i=1}^{N} \frac{2}{\Gamma_i} \int \frac{J_i^2}{P} dx, \tag{3.24}$$

and hence the time variation of the entropy is given in the form introduced by

Prigonine and deduced previously through entropy arguments

$$\frac{dS}{dt} = \Pi - \Phi. \tag{3.25}$$

The first term in the right side of Eq. (3.24) is the flux from/to the system to/from the reservoir. Plugin Eq. (3.18) into Eq. (3.24), we can simplify the entropy flux for a more intuitive expression, given by

$$\Phi = \sum_{i=1}^{N} \left(\frac{2}{\Gamma_i} \left\langle f_i^2 \right\rangle + \left\langle \frac{\partial f_i}{\partial x_i} \right\rangle \right). \tag{3.26}$$

Note that above expression depends on the averages of forces and its derivatives and can be evaluated under a simpler way. Conversely, the second term in the right side of Eq. (3.24) represents the entropy production rate Π, given by

$$\Pi = \sum_{i=1}^{N} \frac{2}{\Gamma_i} \int \frac{J_i^2}{P} dx, \tag{3.27}$$

and it depends on currents J_i's and it is always greater than 0, as should be. In the steady state regime, $\frac{dS}{dt} = 0$, we have that $\Pi = \Phi$, in such a way that all entropy produced by the system has to be delivered to the reservoir.

Once again from Eq. (3.24), we can realize that both the entropy production and the entropy flux depends on the current J_i. In other words, when there is microscopic reversibility $J_i = 0$ is fulfilled it leads to thermodynamic equilibrium steady state.

3.3 Kramers equation

The two-variable Fokker-Planck equation is called the Kramers equation. It described the "underdamped" Brownian motion represented by the Langevin Equation (3.1) which has a dissipative force, a force depending on the position, apart from the random force. In this case, we will consider a system with N particles subject to a force $F(x)$ that depends only on position x and random forces. Newton's equations are given by

$$m\frac{dv_i}{dt} = -\alpha v_i + F_i(x) + F_i^a(t), \tag{3.28}$$

and

$$\frac{dx_i}{dt} = v_i, \tag{3.29}$$

where $i = 1,2,\ldots,N$, $x = (x_1,\ldots,x_N)$ and $v = (v_1,\ldots,v_N)$ are the set of positions and velocities, respectively, $F_i(x)$ is the force, α the coefficient of friction and $F_i^a(t)$ the dissipative random force.

As stated previously, the random noise $F_a(t)$ also has the following properties:

$$\langle F_i^a(t)\rangle = 0, \tag{3.30}$$

and

$$\left\langle F_i^a(t)F_i^a(t^{'})\right\rangle = B_i\delta_{ij}\delta(t-t^{'}), \tag{3.31}$$

respectively. We can conveniently divide both terms of the equation (3.28) by the mass m, reading

$$\frac{dv_i}{dt} = -\gamma v_i + f_i(x) + \zeta_i(t), \qquad \begin{cases} \langle \zeta_i(t)\rangle = 0 \\ \left\langle \zeta_i(t),\zeta_i(t^{`})\right\rangle = \Gamma_i\delta_{ij}\delta(t-t^{`}) \end{cases} \tag{3.32}$$

which $\gamma = \frac{\alpha}{m}$, $f_i(x) = \frac{F_i(x)}{m}$, $\zeta_i(t) = \frac{F_i^a(t)}{m}$ and $\Gamma_i = \frac{B_i}{m^2}$.

Above set of equations has the probability distribution $P(x,v,t)$ associated to the Kramers equation

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x_i}\left(v_i P\right) - \frac{\partial}{\partial v_i}\left[\left(f_i - \gamma v_i\right)P\right] + \frac{\Gamma_i}{2}\frac{\partial^2 P}{\partial v_i^2}. \tag{3.33}$$

As performed previously, we can write the Kramers equation (3.33) in the form of a continuity equation given by

$$\frac{\partial}{\partial t}P(x,v,t) = -\sum_{i=1}^{n}\frac{\partial J_i^x}{\partial x_i} - \sum_{i=1}^{n}\frac{\partial J_i^v}{\partial v_i}, \tag{3.34}$$

where

$$J_i^x = v_i P, \tag{3.35}$$

and

$$J_i^v = \left(f_i - \gamma v_i\right) P - \frac{\Gamma}{2}\frac{\partial P}{\partial v_i}, \tag{3.36}$$

denote the components of the probability stream. J_i^x represents a probability current in the direction x_i and J_i^v represents a probability current in the direction v_i. At the steady state regime the Kramers equation becomes

$$\frac{\partial J_i^x}{\partial x_i} + \frac{\partial J_i^v}{\partial v_i} = 0. \tag{3.37}$$

Microscopic reversibility is expressed by the following conditions:

$$J_i^x(x, -v) = -J_i^x(x,v), \tag{3.38}$$

$$J_i^v(x, -v) = -J_i^v(x,v), \tag{3.39}$$

respectively.

3.3.1 Entropy and entropy production

By defining the system entropy $S(t)$ in the following way

$$S(t) = -k_B \int P(x,v,t) \ln P(x,v,t) dx dv, \tag{3.40}$$

where $dx = dx_1 dx_2 \cdots dx_N$ and $dv = dv_1 dv_2 \cdots dv_N$ and taking its time derivative we have that

$$\frac{dS}{dt} = -k_B \int \frac{dP(x,v,t)}{dt} \left(\ln P(x,v,t) + 1\right) dx\ dv. \tag{3.41}$$

By setting $k_B = 1$ and by using the Eq. (3.34), integrating by parts and by imposing that the probability distribution and their derivatives vanishes the boundaries of a R region of the *space*(x, v), the temporal variation of entropy reads

$$\frac{dS}{dt} = -\sum_{i=1}^{N} \int J_i^x \frac{\partial \ln P}{\partial x_i} dx dv - \sum_{i=1}^{N} \int J_i^v \frac{\partial \ln P}{\partial v_i} dv dx. \tag{3.42}$$

Setting the current $J_i(x,v)$ as given by

$$J_i = -\gamma v_i P - \frac{\Gamma_i}{2}\frac{\partial P}{\partial v_i}, \tag{3.43}$$

we can rewrite the components of the probability as follows

$$J_i^x = v_i P, \tag{3.44}$$

$$J_i^v = f_i P + J_i, \tag{3.45}$$

and by substituting in the temporal variation of entropy and integrating by parts, the entropy time variation is once again given by

$$\frac{dS}{dt} = \Pi - \Phi, \tag{3.46}$$

where the entropy production rate Π is given by

$$\Pi = \sum_{i=1}^{N}\left(\frac{2}{\Gamma_i}\int \frac{J_i^2}{P} dx dv\right), \tag{3.47}$$

and the entropy flux Φ is given by

$$\Phi = \sum_{i=1}^{N}\left(\frac{2\gamma^2}{\Gamma_i}\left\langle v_i^2\right\rangle - \gamma\right). \tag{3.48}$$

As stated before, If f_i is conservative, each current J_i vanishes and $\Phi = 0 = \Pi$ in the steady state regime.

3.4 Example: particles in contact with different reservoirs

As an example, we will obatin some nonequilibrium properties of a system of two mass m particles in contact with thermal reservoirs at different temperatures and interacting through a harmonic force. This system was solved in Ref. [72] and it will be used in the next chapters. The motion equation are given by the following

Langevin equations:

$$m\frac{dv_1}{dt} = F_1 - \alpha v_1 + \mathcal{F}_1(t), \tag{3.49}$$

and

$$m\frac{dv_2}{dt} = F_2 - \alpha v_2 + \mathcal{F}_2(t), \tag{3.50}$$

respectively, where i = 1,2, x_i and $v_i = \frac{dx_i}{dt}$ denote position and velocity of the ith particle, respectively. The stochastic variable for each particle has white noise properties:

$$\langle \mathcal{F}_i(t) \rangle = 0, \tag{3.51}$$

$$\left\langle \mathcal{F}_i(t)\mathcal{F}_j(t^{'}) \right\rangle = 2\alpha T_i \delta_{ij} \delta(t - t^{'}), \tag{3.52}$$

the particles are subject to the following forces

$$F_i = -k\left(x_i - x_j\right) - k^{'} x_i \qquad \text{for} \quad i \neq j. \tag{3.53}$$

The time evolution of the probability distribution $P(x, v, t)$ associated with this equation of motion is given by the Kramers equation.

$$\begin{aligned}\frac{\partial P}{\partial t} = &-\frac{\partial}{\partial x_1}\left(v_1 P\right) - \frac{\partial}{\partial x_2}\left(v_2 P\right) - \frac{\partial}{\partial v_1}\left[\left(\frac{F_1}{m} - \gamma v_2\right) P\right] - \frac{\partial}{\partial v_2}\left[\left(\frac{F_2}{m} - \gamma v_1\right) P\right] \\ &+ \frac{\Gamma_1}{2}\frac{\partial^2 P}{\partial v_1^2} + \frac{\Gamma_2}{2}\frac{\partial^2 P}{\partial v_2^2}\end{aligned} \tag{3.54}$$

where $\gamma = \frac{\alpha}{m}$ and $\Gamma_i = \frac{2\alpha T_i}{m^2}$.

Although equivalent, the properties can be alternatively obtained by solving the equations for the averages, instead of solving Eq. (3.54). In particular, the time evolution of a generic average of type $\langle g \rangle = \int g(x{,}v)P(x{,}v{,}t)dxdv$ is obtained through expression

$$\frac{d}{dt}\langle g \rangle = \int g(x{,}v)\frac{\partial P}{\partial t}dxdv, \tag{3.55}$$

and by inserting Eq. (4.9) in Eq. (3.55) and by performing appropriate partial integrations, an explicit equation for the time evolution of $\langle g \rangle$ is evaluated in terms of correlations associated to the positions and velocities.

For example, for $g = x_1^2,\, x_2^2,\, x_1,\, x_2,\, x_1 v_1,\, ...$ their associate motion equations reads

$$\frac{d}{dt}\left\langle x_1^2 \right\rangle = 2\left\langle v_1 x_1 \right\rangle , \tag{3.56}$$

$$\frac{d}{dt}\left\langle x_2^2 \right\rangle = 2\left\langle v_2 x_2 \right\rangle , \tag{3.57}$$

$$\frac{d}{dt}\left\langle x_1 x_2 \right\rangle = \left\langle v_1 x_2 \right\rangle + \left\langle v_2 x_1 \right\rangle , \tag{3.58}$$

$$\frac{d}{dt}\left\langle x_1 v_1 \right\rangle = \left\langle v_1^2 \right\rangle - K\left\langle x_1^2 \right\rangle + L\left\langle x_1 x_2 \right\rangle - \gamma\left\langle x_1 v_1 \right\rangle , \tag{3.59}$$

$$\frac{d}{dt}\left\langle x_2 v_2 \right\rangle = \left\langle v_2^2 \right\rangle - K\left\langle x_2^2 \right\rangle + L\left\langle x_2 x_1 \right\rangle - \gamma\left\langle x_2 v_2 \right\rangle , \tag{3.60}$$

$$\frac{d}{dt}\left\langle x_1 v_2 \right\rangle = \left\langle v_1 v_2 \right\rangle - K\left\langle x_1 x_2 \right\rangle + L\left\langle x_1^2 \right\rangle - \gamma\left\langle x_1 v_2 \right\rangle , \tag{3.61}$$

$$\frac{d}{dt}\left\langle x_2 v_1 \right\rangle = \left\langle v_2 v_1 \right\rangle - K\left\langle x_2 x_1 \right\rangle + L\left\langle x_2^2 \right\rangle - \gamma\left\langle x_2 v_1 \right\rangle , \tag{3.62}$$

$$\frac{d}{dt}\left\langle v_1^2 \right\rangle = -2K\left\langle v_1 x_1 \right\rangle + 2L\left\langle x_2 v_1 \right\rangle - 2\gamma\left\langle v_1^2 \right\rangle + \Gamma_1, \tag{3.63}$$

$$\frac{d}{dt}\left\langle v_2^2 \right\rangle = -2K\left\langle v_2 x_2 \right\rangle + 2L\left\langle x_1 v_2 \right\rangle - 2\gamma\left\langle v_2^2 \right\rangle + \Gamma_2, \tag{3.64}$$

and

$$\frac{d}{dt}\left\langle v_1 v_2 \right\rangle = -K\left\langle x_1 v_2 \right\rangle + L\left\langle x_2 v_2 \right\rangle - K\left\langle x_2 v_1 \right\rangle + L\left\langle x_1 v_1 \right\rangle - 2\gamma\left\langle v_1 v_2 \right\rangle ,$$

where $K = \left(\frac{k+k^{'}}{m}\right)$ and $L = \frac{k}{m}$. Since we are interested in the steady state properties, it follows that

$$\langle v_1 x_1 \rangle = \langle v_2 x_2 \rangle = \langle v_1 v_2 \rangle = 0, \tag{3.65}$$

$$\langle v_1 x_2 \rangle + \langle v_2 x_1 \rangle = 0, \tag{3.66}$$

$$\left\langle v_1^2 \right\rangle - \left(\frac{k+k^{'}}{m}\right) \left\langle x_1^2 \right\rangle + \frac{k}{m} \langle x_1 x_2 \rangle - \gamma \langle x_1 v_1 \rangle = 0, \tag{3.67}$$

$$\left\langle v_2^2 \right\rangle - \left(\frac{k+k^{'}}{m}\right) \left\langle x_2^2 \right\rangle + \frac{k}{m} \langle x_2 x_1 \rangle - \gamma \langle x_2 v_2 \rangle = 0, \tag{3.68}$$

$$-\left(\frac{k+k^{'}}{m}\right) \langle x_1 x_2 \rangle + \frac{k}{m} \left\langle x_1^2 \right\rangle - \gamma \langle x_1 v_2 \rangle = 0, \tag{3.69}$$

$$-\left(\frac{k+k^{'}}{m}\right) \langle x_2 x_1 \rangle + \frac{k}{m} \left\langle x_2^2 \right\rangle - \gamma \langle x_2 v_1 \rangle = 0, \tag{3.70}$$

$$2\left(\frac{k+k^{'}}{m}\right) \langle v_1 x_1 \rangle + 2\frac{k}{m} \langle x_2 v_1 \rangle - 2\gamma \left\langle v_1^2 \right\rangle + \Gamma_1 = 0, \tag{3.71}$$

and

$$-2\left(\frac{k+k^{'}}{m}\right) \langle v_2 x_1 \rangle + 2\frac{k}{m} \langle x_1 v_2 \rangle - 2\gamma \left\langle v_2^2 \right\rangle + \Gamma_2 = 0. \tag{3.72}$$

Since such equations are linear, their solutions can be found and given by

$$\left\langle v_1^2 \right\rangle = \frac{\Gamma_1 + \Gamma_2}{4\gamma} + \frac{K\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma\right)}, \tag{3.73}$$

$$\left\langle v_1^2 \right\rangle = \frac{\Gamma_1 + \Gamma_2}{4\gamma} - \frac{K\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma\right)}, \tag{3.74}$$

$$\left\langle x_1 v_2 \right\rangle = -\left\langle x_2 v_1 \right\rangle = \frac{L\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma\right)}, \tag{3.75}$$

$$\left\langle x_1^2 \right\rangle = \frac{K\left(\Gamma_1 + \Gamma_2\right)}{4\gamma\left(K^2 - L^2\right)} + \frac{\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma^2\right)}, \tag{3.76}$$

$$\left\langle x_2^2 \right\rangle = \frac{K\left(\Gamma_1 + \Gamma_2\right)}{4\gamma\left(K^2 - L^2\right)} - \frac{\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma^2\right)}, \tag{3.77}$$

and

$$\left\langle x_1 x_2 \right\rangle = \frac{L\left(\Gamma_1 + \Gamma_2\right)}{4\gamma\left(K^2 - L^2\right)}, \tag{3.78}$$

where $K = \left(\frac{k+k'}{m}\right)$ and $L = \frac{k}{m}$. Since $\Pi = \Phi$ in the steady state regime, it follows that

$$\Phi = \frac{2\gamma^2}{\Gamma_1}\left\langle v_1^2 \right\rangle + \frac{2\gamma^2}{\Gamma_2}\left\langle v_2^2 \right\rangle - 2\gamma, \tag{3.79}$$

and we finally arrive at the following

$$\Phi = \frac{\left(\Gamma_1 - \Gamma_2\right)^2}{2\Gamma_1\Gamma_2}\frac{\gamma L^2}{L^2 + K\gamma^2}, \tag{3.80}$$

or even

$$\Pi = \frac{\left(T_1 - T_2\right)^2}{2T_1T_2}\frac{\alpha k^2}{2\left(mk^2 + \left(k + k'\right)\alpha^2\right)}. \tag{3.81}$$

Note that $\Phi > 0$ and it vanishes when will be $T_1 = T_2$. This result will be used in the next chapter where two particles are also subject to periodic drivings.

Chapter 4

Linear chains in the presence of external force

4.1 Fokker-Planck-Kramers equation

As stated previously, we shall analyze some nonequilibrium properties of a system of N particles subject to a force that depends only on the position $F(x)$ in the presence of a time dependent external thermal force $F^{\text{ext}}(t)$. A given ith particle is described by the motion equations:

$$m\frac{dv}{dt} = \tilde{F}_i - \alpha v + \mathcal{F}_i(t), \tag{4.1}$$

$$v_i = \frac{dx_i}{dt}, \tag{4.2}$$

which $i = 1,2,\ldots,N$, $x = (x_1,\ldots,x_N)$ is the set of positions, $v = (v_1,\ldots,v_N)$ is the set of velocities, $\tilde{F}_i = F_i(x) + F_i^{\text{ext}}(t)$ the total external force, α the coefficient of friction and $\mathcal{F}_i(t)$ the random force. Also $F_i(t)$ fulfills the conditions:

$$\langle \mathcal{F}_i(t) \rangle = 0, \tag{4.3}$$

$$\left\langle \mathcal{F}_i(t)\mathcal{F}_i(t^{'}) \right\rangle = 2\alpha T_i \delta_{ij}\delta(t - t^{'}). \tag{4.4}$$

By dividing both sides of the equation (4.1) by the mass m, we have that

$$\frac{dv_i}{dt} = -\gamma v_i + \tilde{f}_i(x) + \zeta_i(t), \tag{4.5}$$

where

$$\langle \zeta_i(t) \rangle = 0, \tag{4.6}$$

$$\left\langle \zeta_i(t)\zeta_i(t^{'}) \right\rangle = \Gamma_i \delta_{ij} \delta(t-t^{'}), \tag{4.7}$$

where $\gamma = \frac{\alpha}{m}$, $\tilde{f}_i = f_i(x) + f_i^{\text{ext}}(t) = \frac{F_i(x)}{m} + \frac{F_i^{\text{ext}}(t)}{m}$, $\zeta_i(t) = \frac{\mathcal{F}_i(t)}{m}$ e $\Gamma_i = \frac{2\alpha T_i}{m^2}$.

Here we rederive the main expressions in the presence of external forces. Let $P(x,v,t) \equiv P(x_1,..,x_N,v_1,...,v_N,t)$ be the joint probability distribution at time t, where x and v denote the collection of particle positions x_i and velocities v_i, respectively. As described previously, its time evolution is described by the Fokker-Planck-Kramers (FPK) equation [57, 72, 63]

$$\frac{\partial P}{\partial t} = -\sum_i \left(\frac{\partial}{\partial x_i}(v_i P) - \frac{\partial}{\partial v_i}\left[\left(\tilde{f}_i - \gamma v_i \right) P \right] + \frac{\Gamma}{2}\frac{\partial^2 P}{\partial v_i^2} \right), \tag{4.8}$$

that conveniently can be rewritten in the form of a continuity equation

$$\frac{\partial P}{\partial t} = -\sum_i \left(v_i \frac{\partial P}{\partial x_i} + [f_i + f_i^{ext}(t)]\frac{\partial P}{\partial v_i} + \frac{\partial J_i}{\partial v_i} \right), \tag{4.9}$$

where

$$J_i = -\gamma v_i P - \frac{\gamma k_{\text{B}} T_i}{m}\frac{\partial P}{\partial v_i}. \tag{4.10}$$

If the temperatures of all particles T_i are the same and the external forces are null, the probability distribution approaches for large times the Gibbs equilibrium distribution,

$$P^e(x,v) = \frac{1}{Z} e^{-E/k_{\text{B}}T}, \tag{4.11}$$

where $E = mv^2/2 + V$ is the energy of the system. This result shows that the FPK Eq. (4.9) indeed describes the contact of a system with a heat reservoir at a temperature T. On the other hand, this will not be the case of the system in contact with distinct reservoirs and/or when it is subject to time oscillating forces or temperatures. In such case, the system dissipates heat and continuously produce entropy.

The present stochastic approach for nonequilibrium thermodynamics also reproduces the first law of thermodynamics. For instance, let us take the definition of mean total energy given by

$$u = \langle E \rangle = \int (T + V)\, P dx dv \tag{4.12}$$

so deriving from time

$$\frac{du}{dt} = \int (T + V)\, \frac{\partial P}{\partial t} dx dv \tag{4.13}$$

From the FK equation, we can rewrite the time variation of the energy $U = \langle E \rangle$ as

$$\frac{dU}{dt} = -\sum_{i=1}^{N} (\Phi_{\mathrm{q}}^{(i)} + \Phi_{\mathrm{w}}^{(i)}), \tag{4.14}$$

where the heat flux $\Phi_{\mathrm{q}}^{(i)}$ from the system to the environment (thermal bath) is expressed as [72, 63]

$$\Phi_{\mathrm{q}}^{(i)} = \gamma(m\langle v_i^2 \rangle - k_{\mathrm{B}} T_i), \tag{4.15}$$

whose first and second terms can be understood as the heating power and the power of heat losses, respectively. The term $\Phi_{\mathrm{w}}^{(i)}$ can be interpreted as the work per unity of time given by

$$\Phi_{\mathrm{w}}^{(i)} = -m\langle v_i \rangle f_i^{ext}(t). \tag{4.16}$$

In the absence of external forces all heat flux comes from/goes to the thermal bath.

4.1.1 Entropy and entropy production

As stated before the construction of stochastic thermodynamics requires the definition of an entropy function.

The entropy S of the system is determined from the Gibbs expression

$$S = -k_{\mathrm{B}} \int P(x,v,t) \ln P(x,v,t) dx dv. \tag{4.17}$$

By appealing to the definition, its time derivative is (again) given by the sum of two terms:

$$\frac{dS}{dt} = \Pi - \Phi, \tag{4.18}$$

where the first is identified as the rate of entropy production given by [72, 63]

$$\Pi = k_{\mathrm{B}} \sum_{i=1}^{N} \frac{1}{\Gamma_i} \int \frac{J_i^2}{P} dx dv. \tag{4.19}$$

Once again, $\Pi \geq 0$ (as expected). Conversely, the second term corresponds to the flux of entropy given by

$$\Phi = -\sum_{i=1}^{N} \frac{2\gamma k_{\mathrm{B}}}{\Gamma_i} \int v_i J_i dx dv, \tag{4.20}$$

or even rewritten as

$$\Phi = k_{\mathrm{B}} \sum_{i=1}^{N} \frac{\Phi_{\mathrm{q}}^{(i)}}{T_i}. \tag{4.21}$$

As mentioned previously, Eq. (4.21) can be alternatively used for evaluated the steady production of entropy, since it depends only on averages $\langle v_i^2 \rangle$ and on the temperatures T_i.

4.2 Exact solution for time dependent periodic drivings

Now we are in position for presenting the (original) results that consists of obtaining the nonequilibrium properties of "brownian particles" in the presence of time dependent periodic drivings.

For simplifying matters, from now on we shall adopt $k_{\mathrm{B}} = 1$. Except in Chapter. 5, all analysis will restrict to the case of a chain of N particles interacting to its nearest neighbors by means of harmonic forces and also subject to individual and external forces. The expression for the force of i-th particle f_i^* then reads

$$f_i^* = -\frac{k}{m}(x_i - x_{i+1}) - \frac{k^*}{m} x_i + f_i^{\mathrm{ext}}(t), \tag{4.22}$$

$$f_i^* = -\frac{k}{m}\left(x_i - x_{i-1}\right) - \frac{k^*}{m}x_i + f_i^{\text{ext}}(t), \tag{4.23}$$

for particles placed at extremities, $i = 1$ and N, respectively, and

$$f_i^* = -\frac{k}{m}\left(2x_i - x_{i-1} - x_{i+1}\right) - \frac{k^*}{m}x_i + f_i^{\text{ext}}(t), \tag{4.24}$$

for the intermediate ones. Quantities k^* and k are spring constants characterizing individual harmonic forces and the coupling between neighboring particles, respectively. Each particle is subject to an external force $f_i^{\text{ext}}(t)$. Above expressions can be conveniently rewritten as

$$f_i^* = -Kx_i + Lx_{i+1} + f_i^{\text{ext}}(t), \tag{4.25}$$

$$f_i^* = -Kx_i + Lx_{i-1} + f_i^{\text{ext}}(t), \tag{4.26}$$

and, for $i = 1$ and $i = N$, respectively, and

$$f_i^* = -\left(K + L\right)x_i + L\left(x_{i+1} + x_{i-1}\right) + f_i^{\text{ext}}(t), \tag{4.27}$$

respectively, where $L = k/m$ and $K = (k + k^*)/m$ for $i \neq 1$ and $i \neq N$.

Performed in the previous chapter, the time evolution of a generic average of type $\langle g \rangle = \int g(x,v)P(x,v,t)dxdv$ is obtained through expression

$$\frac{d}{dt}\langle g \rangle = \int g(x,v)\frac{\partial P}{\partial t}dxdv, \tag{4.28}$$

and by inserting Eq. (4.9) in Eq. (4.28) and performing appropriate partial integrations, an explicit equation for the time evolution of $\langle g \rangle$ is evaluated in terms of correlations associated to the positions and velocities. Now, due to the time dependence on the external forces, the evaluation of averages like $\langle g \rangle$ becomes cumbersome. However, the calculations become quite simpler by rewriting the motion equations in terms of their associate covariances. For instance, let us take for example a generic average $\langle g \rangle = \left\langle v_i^l x_j^m \right\rangle$ (with $l \geq 1$ and $m \geq 1$) with covariance given by $\left\langle v_i^l x_j^m \right\rangle_{cv} \equiv \langle v_i^l x_j^m \rangle - \langle v_i^l \rangle \langle x_j^m \rangle$. Unlike the time evolution of $\langle v_i^l x_j^m \rangle$, the time equation for $d\left\langle v_i^l x_j^m \right\rangle_{cv}/dt = d\langle v_i^l x_j^m\rangle/dt - \langle x_j^m\rangle d\langle v_i^l\rangle/dt - \langle v_i^l\rangle d\langle x_j^m\rangle/dt$ does not depend explicitly on t. Since the equations for all covariances are linear and time independent, the exact solution is possible for all system sizes N. Finally, having the covariances $\langle v_i^2\rangle_{cv}$ and the averages $\langle v_i\rangle$, the entropy flux can be directly evaluated from the usage of Eqs. (4.15) and (4.21).

Below we derive explicit expressions for distinct covariances between the i th and $i+1$-th particles for a generic chain of N sites.

$$\frac{d}{dt}\left\langle x_i^2\right\rangle_{cv} = 2\left\langle v_i x_i\right\rangle_{cv}, \tag{4.29}$$

$$\frac{d}{dt}\left\langle x_i x_{i+1}\right\rangle_{cv} = \left\langle v_i x_{i+1}\right\rangle_{cv} + \left\langle v_i x_{i+1}\right\rangle_{cv}, \tag{4.30}$$

$$\frac{d}{dt}\left\langle x_i v_i\right\rangle_{cv} = \left\langle v_i^2\right\rangle_{cv} - K\left\langle x_i^2\right\rangle_{cv} + L\left\langle x_i x_{i+1}\right\rangle_{cv} - \gamma\left\langle x_i v_i\right\rangle_{cv}, \tag{4.31}$$

$$\frac{d}{dt}\left\langle x_i v_{i+1}\right\rangle_{cv} = \left\langle v_i v_{i+1}\right\rangle_{cv} - K\left\langle x_i x_{i+1}\right\rangle_{cv} + L\left\langle x_i^2\right\rangle_{cv} - \gamma\left\langle x_i v_{i+1}\right\rangle_{cv}, \tag{4.32}$$

$$\frac{d}{dt}\left\langle v_i^2\right\rangle_{cv} = -2K\left\langle v_i x_i\right\rangle_{cv} + 2L\left\langle x_{i+1} v_i\right\rangle_{cv} - 2\gamma\left\langle v_i^2\right\rangle_{cv} + \Gamma_i, \tag{4.33}$$

$$\frac{d}{dt}\left\langle v_i v_{i+1}\right\rangle_{cv} = -K\left\langle x_i v_{i+1}\right\rangle_{cv} + L\left\langle x_{i+1} v_{i+1}\right\rangle_{cv} - K\left\langle x_{i+1} v_i\right\rangle_{cv} + L\left\langle x_i v_i\right\rangle_{cv} - 2\gamma\left\langle v_i v_{i+1}\right\rangle_{cv}. \tag{4.34}$$

Here we introduced the rescaled temperature Γ_i defined by $\Gamma_i = 2\gamma T_i/m$ and thereby for fixed Γ_i's, the achievement of $\langle v_i^2\rangle_{cv}$'s reduces to systems of linear equations.

The time evolution of single averages $\langle v_i\rangle$ and $\langle x_i\rangle$ are also required for obtaining

$\langle v_i^2 \rangle$, whose expressions read

$$\frac{d}{dt}\langle v_i \rangle = -(K+L)\langle x_i \rangle + L(\langle x_{i+1} \rangle + \langle x_{i-1} \rangle) - \gamma \langle v_i \rangle + f_i^{ext}(t), \tag{4.35}$$

for $i \neq 1{,}N$ and

$$\frac{d}{dt}\langle v_i \rangle = -K\langle x_i \rangle + L\langle x_{i+1} \rangle - \gamma \langle v_i \rangle + f_i^{ext}(t), \tag{4.36}$$

$$\frac{d}{dt}\langle v_i \rangle = -K\langle x_i \rangle + L\langle x_{i-1} \rangle - \gamma \langle v_i \rangle + f_i^{ext}(t), \tag{4.37}$$

for $i = 1$ and N, respectively and from Eq. (3.50), the time evolution of $\langle x_i \rangle$ reads

$$\frac{d}{dt}\langle x_i \rangle = \langle v_i \rangle. \tag{4.38}$$

Although the previous procedure does not depend on the shape of external forces, from now on we will restrict our analysis to harmonic external forces given by

$$f_i^{ext}(t) = f_{0i}\cos(\omega t + \phi), \tag{4.39}$$

with ω and ϕ being its frequency and phase difference (lag), respectively. By assuming that each $\langle x_i \rangle$ has solution of type

$$\langle x_i \rangle = A_{0i} + A_{1i}\cos\omega t + A_{2i}\sin\omega t, \tag{4.40}$$

The mean velocity $\langle v_i \rangle$ then becomes

$$\langle v_i \rangle = \omega \Big[A_{2i}\cos(\omega t) - A_{1i}\sin(\omega t) \Big] \tag{4.41}$$

By inserting above solutions in Eqs. (4.35) [or Eq. (4.36)/(4.37)] and (4.38), the coefficients A_{1i} and A_{2i} are obtained.

We shall start the analysis of chains of two particles and further we are going to generalize for long chain of an arbitrary system.

4.3 Two particles case

We have defined a non-equilibrium theory for external forces affecting the system with two sections. Defining that these efforts have oscillatory behavior, so that

$$\begin{cases} f_1^{\text{ext}} = f_{01}\cos\omega t, \\ f_2^{\text{ext}} = f_{02}\cos(\omega t + \phi). \end{cases}$$

The motion equations are the same as in Eq. (4.5). In addition, random noise has the same properties (4.6) and (4.6) and particles are subject to the following forces

$$F_i = -k\left(x_i - x_j\right) - k^{'} x_i \qquad i \neq j, \tag{4.42}$$

which can be conveniently rewritten as

$$f_i^* = -K x_i + L x_j \qquad i \neq j, \tag{4.43}$$

respectively, where $L = k/m$ and $K = (k + k^*)/m$.

As we noted in previous chapters for calculating entropy yields it is necessary to calculate averages of type $\langle x_i x_j \rangle$, $\langle x_i v_j \rangle$ and $\langle v_i v_j \rangle$. We can find the averages using the Kramers equations and through a system of equations for the temporal evolution of these averages.

$$\frac{d}{dt}\left\langle x_1^2 \right\rangle = 2\left\langle v_1 x_1 \right\rangle, \tag{4.44}$$

$$\frac{d}{dt}\left\langle x_2^2 \right\rangle = 2\left\langle v_2 x_2 \right\rangle, \tag{4.45}$$

$$\frac{d}{dt}\left\langle x_1 x_2 \right\rangle = \left\langle v_1 x_2 \right\rangle + \left\langle v_2 x_1 \right\rangle, \tag{4.46}$$

$$\frac{d}{dt}\left\langle x_1 v_1\right\rangle = \left\langle v_1^2\right\rangle - K\left\langle x_1^2\right\rangle + L\left\langle x_1 x_2\right\rangle - \gamma\left\langle x_1 v_1\right\rangle + f_1^{\text{ext}}\left\langle x_1\right\rangle , \tag{4.47}$$

$$\frac{d}{dt}\left\langle x_2 v_2\right\rangle = \left\langle v_2^2\right\rangle - K\left\langle x_2^2\right\rangle + L\left\langle x_2 x_1\right\rangle - \gamma\left\langle x_2 v_2\right\rangle + f_2^{\text{ext}}\left\langle x_2\right\rangle , \tag{4.48}$$

$$\frac{d}{dt}\left\langle x_1 v_2\right\rangle = \left\langle v_1 v_2\right\rangle - K\left\langle x_1 x_2\right\rangle + L\left\langle x_1^2\right\rangle - \gamma\left\langle x_1 v_2\right\rangle + f_2^{\text{ext}}\left\langle x_1\right\rangle , \tag{4.49}$$

$$\frac{d}{dt}\left\langle x_2 v_1\right\rangle = \left\langle v_2 v_1\right\rangle - K\left\langle x_2 x_1\right\rangle + L\left\langle x_2^2\right\rangle - \gamma\left\langle x_2 v_1\right\rangle + f_1^{\text{ext}}\left\langle x_2\right\rangle , \tag{4.50}$$

$$\frac{d}{dt}\left\langle v_1^2\right\rangle = -2K\left\langle v_1 x_1\right\rangle + 2L\left\langle x_2 v_1\right\rangle - 2\gamma\left\langle v_1^2\right\rangle + \Gamma_1\cos\omega t + 2f_1^{\text{ext}}\left\langle v_1\right\rangle , \tag{4.51}$$

$$\frac{d}{dt}\left\langle v_2^2\right\rangle = -2K\left\langle v_2 x_2\right\rangle + 2L\left\langle x_1 v_2\right\rangle - 2\gamma\left\langle v_2^2\right\rangle + \Gamma_2\cos\omega t + 2f_2^{\text{ext}}\left\langle v_2\right\rangle , \tag{4.52}$$

and

$$\begin{aligned}\frac{d}{dt}\left\langle v_1 v_2\right\rangle = &-K\left\langle x_1 v_2\right\rangle + L\left\langle x_2 v_2\right\rangle - K\left\langle x_2 v_1\right\rangle + L\left\langle x_1 v_1\right\rangle - 2\gamma\left\langle v_1 v_2\right\rangle + \\ &+ f_1^{\text{ext}}\left\langle v_2\right\rangle + f_2^{\text{ext}}\left\langle v_1\right\rangle \qquad ,\end{aligned}$$

where $K = \left(\frac{k+k'}{m}\right)$ and $L = \frac{k}{m}$. As exposed in the last section, there are components $f_i^{\text{ext}}\left\langle x_i\right\rangle$, $f_j^{\text{ext}}\left\langle x_i\right\rangle$, $f_i^{\text{ext}}\left\langle v_i\right\rangle$ and $f_j^{\text{ext}}\left\langle v_i\right\rangle$ for $i \neq j$ in the equations above differently from Ref. [63].

The time evolution for the covariances is then given by

$$\frac{d}{dt}\left\langle x_1^2\right\rangle_{cv} = 2\left\langle v_1 x_1\right\rangle_{cv} , \tag{4.53}$$

$$\frac{d}{dt}\left\langle x_2^2\right\rangle_{cv} = 2\left\langle v_2 x_2\right\rangle_{cv} , \tag{4.54}$$

$$\frac{d}{dt}\left\langle x_1 x_2\right\rangle_{cv} = \left\langle v_1 x_2\right\rangle_{cv} + \left\langle v_2 x_1\right\rangle_{cv}, \tag{4.55}$$

$$\frac{d}{dt}\left\langle x_1 v_1\right\rangle_{cv} = \left\langle v_1^2\right\rangle_{cv} - K\left\langle x_1^2\right\rangle_{cv} + L\left\langle x_1 x_2\right\rangle_{cv} - \gamma\left\langle x_1 v_1\right\rangle_{cv}, \tag{4.56}$$

$$\frac{d}{dt}\left\langle x_2 v_2\right\rangle_{cv} = \left\langle v_2^2\right\rangle_{cv} - K\left\langle x_2^2\right\rangle_{cv} + L\left\langle x_2 x_1\right\rangle_{cv} - \gamma\left\langle x_2 v_2\right\rangle_{cv}, \tag{4.57}$$

$$\frac{d}{dt}\left\langle x_1 v_2\right\rangle_{cv} = \left\langle v_1 v_2\right\rangle_{cv} - K\left\langle x_1 x_2\right\rangle_{cv} + L\left\langle x_1^2\right\rangle_{cv} - \gamma\left\langle x_1 v_2\right\rangle_{cv}, \tag{4.58}$$

$$\frac{d}{dt}\left\langle x_2 v_1\right\rangle_{cv} = \left\langle v_2 v_1\right\rangle_{cv} - K\left\langle x_2 x_1\right\rangle_{cv} + L\left\langle x_2^2\right\rangle_{cv} - \gamma\left\langle x_2 v_1\right\rangle_{cv}, \tag{4.59}$$

$$\frac{d}{dt}\left\langle v_1^2\right\rangle_{cv} = -2K\left\langle v_1 x_1\right\rangle_{cv} + 2L\left\langle v_1 x_2\right\rangle_{cv} - 2\gamma\left\langle v_1^2\right\rangle_{cv} + \Gamma_1, \tag{4.60}$$

$$\frac{d}{dt}\left\langle v_2^2\right\rangle_{cv} = -2K\left\langle v_2 x_2\right\rangle_{cv} + 2L\left\langle v_2 x_1\right\rangle_{cv} - 2\gamma\left\langle v_2^2\right\rangle_{cv} + \Gamma_2, \tag{4.61}$$

and

$$\frac{d}{dt}\left\langle v_1 v_2\right\rangle_{cv} = -K\left\langle x_1 v_2\right\rangle_{cv} + L\left\langle x_2 v_2\right\rangle_{cv} - K\left\langle x_2 v_1\right\rangle_{cv} + L\left\langle x_1 v_1\right\rangle_{cv} - 2\gamma\left\langle v_1 v_2\right\rangle_{cv}. \tag{4.62}$$

At the steady state we have a set of equations are similar to those found for the averages of a system with zero external forces of the application in the last chapter, and hence it gives the following solutions for the variances.

$$\left\langle v_1^2\right\rangle_{cv} = \frac{\Gamma_1 + \Gamma_2}{4\gamma} + \frac{K\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma^2\right)}, \tag{4.63}$$

and

$$\left\langle v_2^2\right\rangle_{cv} = \frac{\Gamma_1 + \Gamma_2}{4\gamma} - \frac{K\gamma\left(\Gamma_1 - \Gamma_2\right)}{4\left(L^2 + K\gamma^2\right)}, \tag{4.64}$$

respectively. The system entropy flux (4.20) can be written as

$$\Phi = \frac{2\gamma^2}{\Gamma_1}\Big(\left\langle v_1^2\right\rangle_{cv} + \left\langle v_1\right\rangle^2\Big) + \frac{2\gamma^2}{\Gamma_2}\Big(\left\langle v_2^2\right\rangle_{cv} + \left\langle v_2\right\rangle^2\Big) - 2\gamma. \tag{4.65}$$

That is, it is possible to determine the entropy production by evaluating $\left\langle v_i\right\rangle^2$ and $\langle v_i^2\rangle_{cv}$. Using the motion equations of the system, we can get a set of equations for their expected values.

$$\frac{d}{dt}\left\langle x_1\right\rangle = \left\langle v_1\right\rangle, \tag{4.66}$$

$$\frac{d}{dt}\left\langle x_2\right\rangle = \left\langle v_2\right\rangle, \tag{4.67}$$

$$\frac{d}{dt}\left\langle v_1\right\rangle = -K\left\langle x_1\right\rangle + L\left\langle x_2\right\rangle + f_1^{\text{ext}} - \gamma\left\langle v_1\right\rangle, \tag{4.68}$$

and

$$\frac{d}{dt}\left\langle v_2\right\rangle = -K\left\langle x_2\right\rangle + L\left\langle x_1\right\rangle + f_2^{\text{ext}} - \gamma\left\langle v_2\right\rangle, \tag{4.69}$$

respectively. Since the external forces are periodic, one assumes that $\langle x_i\rangle$'s and $\langle v_i\rangle$'s changes into the time in the following way

$$\left\langle x_1\right\rangle = A_0^{(\text{x1})} + A_1^{(\text{x1})}\cos\omega t + A_2^{(\text{x1})}\sin\omega t, \tag{4.70}$$

and

$$\left\langle x_2\right\rangle = A_0^{(\text{x2})} + A_1^{(\text{x2})}\cos\omega t + A_2^{(\text{x2})}\sin\omega t, \tag{4.71}$$

respectively. By inserting Eq. (4.70) into (4.66), we have that

$$\frac{d}{dt}\left\langle x_1\right\rangle = \left\langle v_1\right\rangle = -\omega A_1^{(\text{x1})}\sin\omega t + \omega A_2^{(\text{x1})}\cos\omega t, \tag{4.72}$$

by inserting Eq. (4.71) into (4.67), we have that

$$\frac{d}{dt}\langle x_2\rangle = \langle v_2\rangle = -\omega A_1^{(\mathrm{x2})}\sin\omega t + \omega A_2^{(\mathrm{x2})}\cos\omega t. \tag{4.73}$$

By deriving Eq. (4.72) and Eq. (4.73) relative to time we have

$$\frac{d}{dt}\langle v_1\rangle = -\omega^2 A_1^{(\mathrm{x1})}\cos\omega t - \omega^2 A_2^{(\mathrm{x1})}\sin\omega t, \tag{4.74}$$

and

$$\frac{d}{dt}\langle v_2\rangle = -\omega^2 A_1^{(\mathrm{x2})}\cos\omega t - \omega^2 A_2^{(\mathrm{x2})}\sin\omega t \tag{4.75}$$

respectively, by replacing Eq. (4.74) into (4.68), finally have that

$$\begin{aligned}
0 = &\Big(- KA_0^{(\mathrm{x1})} + LA_0^{(\mathrm{x2})}\Big) + \\
&+ \Big(- KA_1^{(\mathrm{x1})} + LA_1^{(\mathrm{x2})} - \gamma\omega A_2^{(\mathrm{x1})} + f_{01} + \omega^2 A_1^{(\mathrm{x1})}\Big)\cos\omega t + \\
&+ \Big(- KA_2^{(\mathrm{x1})} + LA_2^{(\mathrm{x2})} + \gamma\omega A_1^{(\mathrm{x1})} + \omega^2 A_2^{(\mathrm{x1})}\Big)\sin\omega t.
\end{aligned}$$

By replacing Eq. (4.75) into (4.69), we have that

$$\begin{aligned}
0 = &\Big(- KA_0^{(\mathrm{x2})} + LA_0^{(\mathrm{x1})}\Big) + \\
&+ \Big(+ LA_1^{(\mathrm{x1})} - \gamma\omega A_2^{(\mathrm{x2})} + f_{02}\cos\phi + \big(-K + \omega^2\big) A_1^{(\mathrm{x2})}\Big)\cos\omega t + \\
&+ \Big(+ LA_2^{(\mathrm{x1})} + \gamma\omega A_1^{(\mathrm{x2})} + f_{02}\sin\phi + \big(-K + \omega^2\big) A_2^{(\mathrm{x2})}\Big)\sin\omega t.
\end{aligned}$$

Separating the constant terms, cosines and sines from the two equations and equaling zero, we get the following equations

- **Constants**

$$- KA_0^{(\mathrm{x1})} + LA_0^{(\mathrm{x2})} = 0 \tag{4.76}$$

and

$$-KA_0^{(\mathrm{x2})}+LA_0^{(\mathrm{x1})}=0. \tag{4.77}$$

- **Sines**

$$-KA_2^{(\mathrm{x1})}+LA_2^{(\mathrm{x2})}+\gamma\omega A_1^{(\mathrm{x1})}+\omega^2A_2^{(\mathrm{x1})}=0, \tag{4.78}$$

and

$$LA_2^{(\mathrm{x1})}+\gamma\omega A_1^{(\mathrm{x2})}+f_{02}\sin\phi+\left(-K+\omega^2\right)A_2^{(\mathrm{x2})}=0. \tag{4.79}$$

- **Cosines**

$$-KA_1^{(\mathrm{x1})}+LA_1^{(\mathrm{x2})}-\gamma\omega A_2^{(\mathrm{x1})}+f_{01}+\omega^2A_1^{(\mathrm{x1})}=0, \tag{4.80}$$

and

$$LA_1^{(\mathrm{x1})}-\gamma\omega A_2^{(\mathrm{x2})}+f_{02}\cos\phi+\left(-K+\omega^2\right)A_1^{(\mathrm{x2})}=0. \tag{4.81}$$

Solving these systems of equations, we get

$$A_0^{(\mathrm{x2})}=A_0^{(\mathrm{x1})}=0, \tag{4.82}$$

$$A_1^{(\mathrm{x1})}=\frac{f_{01}\left(K-\omega^2\right)\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2-L^2\right)+f_{02}L\left(-\omega^2\left(\gamma^2+2K\right)+K^2-L^2+\omega^4\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}, \tag{4.83}$$

$$A_2^{(\mathrm{x1})}=\frac{\gamma\omega\left(f_{01}\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2+L^2\right)+2f_{02}L\left(K-\omega^2\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}, \tag{4.84}$$

$$A_1^{(\mathrm{x2})}=\frac{f_{01}L\left(-\omega^2\left(\gamma^2+2K\right)+K^2-L^2+\omega^4\right)+f_{02}\left(K-\omega^2\right)\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2-L^2\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}, \tag{4.85}$$

and

$$A_2^{(\mathrm{x2})} = \frac{\gamma\omega\left(2f_{01}L\left(K-\omega^2\right)+f_{02}\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2+L^2\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}. \tag{4.86}$$

Replacing these solutions in Eq. (4.72), we have

$$\begin{aligned}\langle v_1\rangle = \omega\Bigg[&\frac{\gamma\omega\cos(t\omega)\left(f_{01}\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2+L^2\right)+2f_{02}L\left(K-\omega^2\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}+\\ &-\frac{\sin(t\omega)\left(f_{01}\left(K-\omega^2\right)\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2-L^2\right)+f_{02}L\left(-\omega^2\left(\gamma^2+2K\right)+K^2-L^2+\omega^4\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}\Bigg].\end{aligned}$$

Replacing these solutions in Eq. (4.73), we have

$$\begin{aligned}\langle v_2\rangle = \omega\Bigg[&\frac{\gamma\omega\cos(t\omega)\left(f_{01}\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2+L^2\right)+2f_{02}L\left(K-\omega^2\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}+\\ &-\frac{\sin(t\omega)\left(f_{01}\left(K-\omega^2\right)\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2-L^2\right)+f_{02}L\left(-\omega^2\left(\gamma^2+2K\right)+K^2-L^2+\omega^4\right)\right)}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}\Bigg].\end{aligned}$$

Thereby, having obtained $\langle v_1\rangle$ and $\langle v_2\rangle$ the entropy flux $\Phi(t)$ in the steady state regime can be obtained.

4.3.1 Entropy production

So for a chain of two interacting particles subject to harmonic forces without phase difference (laglesscase, $\phi = 0$). From the solution of linear set of equations described before, we can describe the expressions for the covariances as:

$$\left\langle v_1^2\right\rangle_{cv} = \frac{\Gamma_1+\Gamma_2}{4\gamma}+\frac{K\gamma\left(\Gamma_1-\Gamma_2\right)}{4\left(L^2+K\gamma^2\right)}, \tag{4.87}$$

and

$$\left\langle v_2^2\right\rangle_{cv} = \frac{\Gamma_1+\Gamma_2}{4\gamma}-\frac{K\gamma\left(\Gamma_2-\Gamma_1\right)}{4\left(L^2+K\gamma^2\right)}. \tag{4.88}$$

Taking into account that $\langle v_i^2 \rangle = \langle v_i^2 \rangle_{cv} + \langle v_i \rangle^2$ (for $i = 1$ and 2), we see that the entropy flux can be splitted in two parts,

$$\Phi(t) = \Phi_T + \Phi_f(t), \tag{4.89}$$

where Φ_T and $\Phi_f(t)$ read

$$\Phi_T = \frac{2\gamma^2}{\Gamma_1} \left\langle v_1^2 \right\rangle_{cv} + \frac{2\gamma^2}{\Gamma_2} \left\langle v_2^2 \right\rangle_{cv} - 2\gamma, \tag{4.90}$$

and

$$\Phi_f(t) = \frac{2\gamma^2}{\Gamma_1} \langle v_1 \rangle^2 + \frac{2\gamma^2}{\Gamma_2} \langle v_2 \rangle^2 , \tag{4.91}$$

respectively. The former term can be identified as the entropy flux coming from the thermal reservoirs, whereas the latter is associated to the entropy flux coming from the oscillating forces.

Above expressions can be simplified, acquiring the following form

$$\Phi_T = \frac{\gamma L^2}{2\left(L^2 + K\gamma^2\right)} \frac{\left(\Gamma_1 - \Gamma_1\right)^2}{\Gamma_1 \Gamma_2}, \tag{4.92}$$

and

$$\Phi_f(t) = 2\gamma^2\omega^2 \sum_i \left(\frac{(A_{2i}\cos\omega t - A_{1i}\sin\omega t)^2}{\Gamma_i} \right), \tag{4.93}$$

respectively, whose coefficients A_{1i} and A_{2i} are shown in Appendix 7.1. Since we are interested in the steady state regime, we shall appeal to Eq. (1.1) and referring the first and second terms as the entropy production rates $\Pi_T \equiv \Phi_T$ and defining the average over a cycle as

$$\overline{\Pi} \equiv \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \Phi_f(t) dt, \tag{4.94}$$

respectively. Once again, $\Pi_T \equiv \Phi_T$ solely depends on the difference of temperatures and are similar to the case with no external forces [72], whereas $\bar{\Pi}$ is related to the time dependent forces averaged over a oscillation period and it is given by

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left[\Gamma_1\left(A_{12}^2 + A_{22}^2\right) + \Gamma_2\left(A_{11}^2 + A_{21}^2\right)\right]}{\Gamma_1\Gamma_2}. \tag{4.95}$$

By substituting the expressions for A_{1i}'s and A_{2i}'s we finally arrive at the following expression:

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left\{f_{01}^2\left[\Gamma_2\left(\gamma^2\omega^2 + \left(K-\omega^2\right)^2\right) + L^2\Gamma_1\right] + 2f_{01}f_{02}L\left(K-\omega^2\right)\left(\Gamma_1+\Gamma_2\right) + f_{02}^2\left[\Gamma_1\left(\gamma^2\omega^2 + \left(K-\omega^2\right)^2\right) + L^2\Gamma_2\right]\right\}}{\Gamma_1\Gamma_2\left[\gamma^2\omega^2 + (K+L-\omega^2)^2\right]\left[\gamma^2\omega^2 + (-K+L+\omega^2)^2\right]}. \tag{4.96}$$

This is the one of main results of this section, and we pause to make some few comments: First, from Eq. (4.95) it follows that $\overline{\Pi}$ is always greater than 0, vanishing when $f_{01} = f_{02} = 0$ and/or $\omega = 0$. Second, in the limit of slow or fast oscillations, $\omega << 1$ or $\omega >> 1$, $\overline{\Pi}$ behaves as

$$\overline{\Pi} \sim \frac{\gamma^2\Big[\Gamma_1(f_{01}K + f_{02}L)^2 + \Gamma_2(f_{01}L + f_{02}K)^2\Big]\omega^2}{\Gamma_1\Gamma_2(K^2 - L^2)^2}, \tag{4.97}$$

and

$$\overline{\Pi} \sim \left(\frac{f_{01}^2\Gamma_2 + f_{02}^2\Gamma_1}{\Gamma_1\Gamma_2}\right)\frac{\gamma^2}{\gamma^2 + \omega^2}, \tag{4.98}$$

respectively, implying that $\overline{\Pi}$ vanishes as ω^2 and $1/\omega^2$ for low and large periods, respectively.

Third, there is an intermediate frequency ω^* in which $\bar{\Pi}$ is maximum. Although ω^* can be evaluated exactly, it displays an unwieldy dependence on the control parameters. For this reason, we split the analysis in four parts, by inspecting its dependence on the interaction parameters K and L, the dissipation constant γ and the ratio between external forces f_{02}/f_{01}, as depicted in Fig. 4.1. Whenever ω^* increases by raising K,L and the ratio f_{02}/f_{01}, it decreases when γ is increased. Fourth, when the interaction between particles is "weak", $k << k^*$, $\overline{\Pi}$ reduces to the single forced harmonic oscillator expression:

$$\overline{\Pi} \sim \frac{\gamma^2\omega^2(f_{01}^2\Gamma_2 + f_{02}^2\Gamma_1)}{\Gamma_1\Gamma_2[\gamma^2\omega^2 + (K-\omega^2)^2]}, \tag{4.99}$$

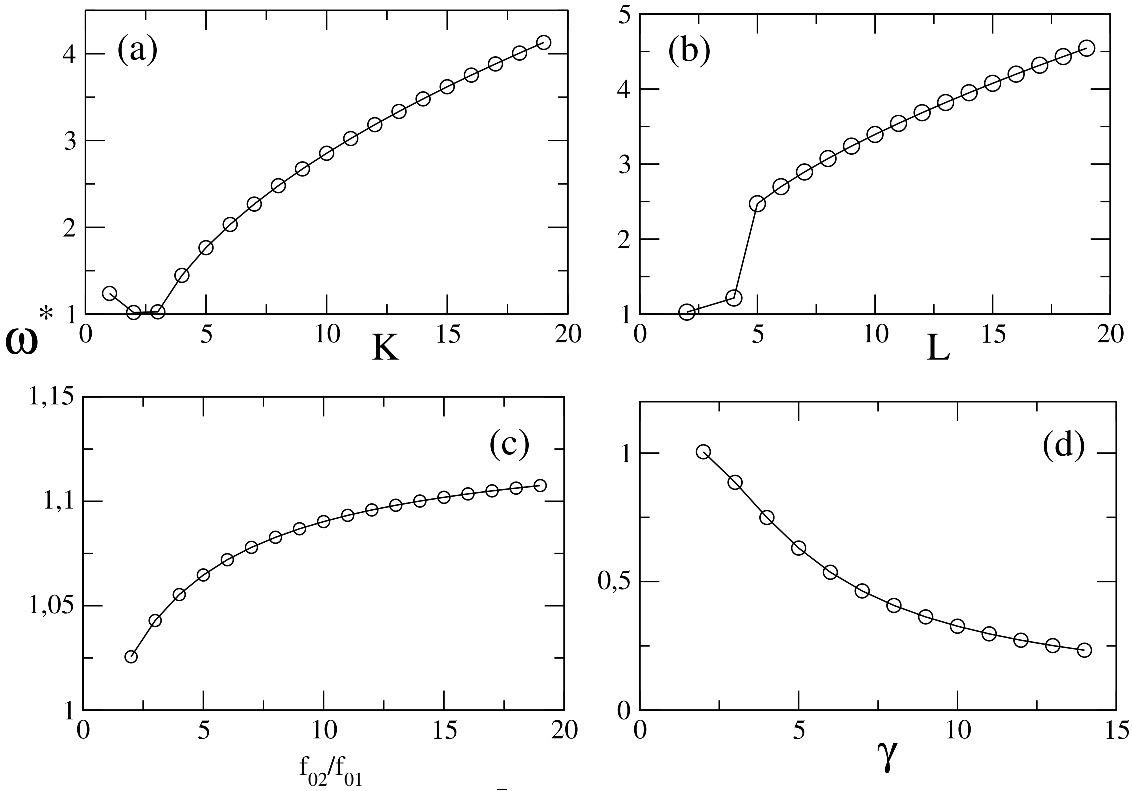

Figure 4.1: The frequency ω^* in which $\bar{\Pi}$ is maximum versus distinct control parameters for $\Gamma_1 = 1$ and $\Gamma_2 = 10$. In (a), (b), (c) and (d) we take $\gamma = 1, L = 2$ and $f_{02}/f_{01} = 2$, $\gamma = 1, K = 3$ and $f_{02}/f_{01} = 2$, $\gamma = 1$, $K = 3$ and $L = 2$ and $K = 3, L = 2$ and $f_{02}/f_{01} = 2$, respectively.

acquiring the simpler form

$$\overline{\Pi} \sim \frac{\gamma^2\omega^2 f_{01}^2}{\Gamma_1[\gamma^2\omega^2 + (K-\omega^2)^2]}, \tag{4.100}$$

as $\Gamma_1 = \Gamma_2$ and $f_{01} = f_{02}$. Fifth and last, in the strong coupling regime, $k >> k^*$ and $k/m >> \omega^2$ (or equivalently $L \approx K$ and $L >> \omega^2$), $\overline{\Pi}$ becomes

$$\overline{\Pi} \sim \Big(\frac{\gamma^2}{\gamma^2+\omega^2}\Big)\Big(\frac{1}{\Gamma_1}+\frac{1}{\Gamma_2}\Big)(f_{01}+f_{02})^2, \tag{4.101}$$

which is independent on strength oscillator parameters K and L.

4.3.2 Bilinear form and Onsager coefficients

In similarity to Chapter 2, the shapes of Eqs. (4.92) and (4.96) show that the entropy production components can be written as flux-times-force expressions $\Pi_T = \mathcal{J}_T f_T$ and

$$\overline{\Pi} = \mathcal{J}_1^f f_{01} + \mathcal{J}_2^f f_{02}, \tag{4.102}$$

respectively, where the forces $f_T = 1/\Gamma_1 - 1/\Gamma_2$ and $f_{0i(j)}$ have associated fluxes $\mathcal{J}_T$, $\mathcal{J}_1^f$ and $\mathcal{J}_2^f$ given by

$$\mathcal{J}_T = \frac{\Gamma_1\Gamma_2\gamma L^2}{2\,(L^2+K\gamma^2)}\Big(\frac{1}{\Gamma_1}-\frac{1}{\Gamma_2}\Big), \tag{4.103}$$

and

$$\mathcal{J}_1^f = L_{11}f_{01} + L_{12}f_{02}, \quad \text{and} \quad \mathcal{J}_2^f = L_{21}f_{01} + L_{22}f_{02}, \tag{4.104}$$

respectively. The bilinear form for $\overline{\Pi}$ provides to identify the terms L_{11} and L_{12} as the associated Onsager coefficients given by

$$L_{11} = \frac{\gamma^2\omega^2\left[\Gamma_2\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2\right)+L^2\Gamma_1\right]}{\Gamma_1\Gamma_2\left[\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right]\left[\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right]}, \tag{4.105}$$

and

$$L_{12} = \frac{L\left(K-\omega^2\right)\left(\Gamma_1+\Gamma_2\right)}{\Gamma_1\Gamma_2\left[\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right]\left[\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right]}, \tag{4.106}$$

respectively. Analogous expressions are hold valid for L_{21} and L_{22} by exchanging $1 \leftrightarrow 2$. Note that $L_{11} \geq 0$ and $L_{22} \geq 0$ (as expected). The non-negativity of the entropy production also requires that $4L_{11}L_{22} - (L_{12} + L_{21})^2 \geq 0$. To verify this, let us consider $\Gamma_2 = r\Gamma_1$ with r being an arbitrary (non negative) real number. Such above inequality is always satisfied, since the term

$$\frac{\left[\gamma^2\omega^2 + \left(K - \omega^2\right)^2 + L^2 r\right]\left[r\left(\gamma^2\omega^2 + \left(K - \omega^2\right)^2\right) + L^2\right]}{L^2(r+1)^2\left(K - \omega^2\right)^2},$$

is greater than 1/4 for all values of r,K,ω and γ.

4.3.3 Phase difference between harmonic forces

Here we extend the results from previous subsection but taking into account a phase difference between external forces $f_1^{ext}(t)$ and $f_2^{ext}(t)$. More specifically, $f_1^{ext}(t)$ has the same expression as previously, but $f_2^{ext}(t)$ now reads $f_2^{ext}(t) = f_{02}\cos(\omega t + \phi)$. By repeating aforedescribed procedures, we assume that $\langle v_i \rangle = w\left(C_{2i}\cos\omega t - C_{1i}\sin\omega t\right)$, whose coefficients C_{1i} and C_{2i} are decomposed in two parts: $C_{1i} = A_{1i} + B_{1i}(\phi)$, whose A_{1i} and A_{2i} are the same as Eqs. (7.1) and (7.2) and the dependence on the phase difference appears only in B_{1i} and B_{2i}, whose explicit coefficients are listed in Appendix 7.2. We then arrive at the following expression for the steady entropy production $\overline{\Pi}$

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left[\Gamma_1\left(C_{12}^2 + C_{22}^2\right) + \Gamma_2\left(C_{11}^2 + C_{21}^2\right)\right]}{\Gamma_1\Gamma_2}, \tag{4.107}$$

which is quite similar to Eq. (4.95). As in the lagless case, it has three terms with first and third terms being identical to Eq. (4.96) and the phase difference dependence appearing only in middle term reading

$$\left[\frac{2f_{01}f_{02}L\left[\gamma\omega(\Gamma_2 - \Gamma_1)\sin\phi + \left(K - \omega^2\right)\left(\Gamma_1 + \Gamma_2\right)\cos\phi\right]}{\Gamma_1\Gamma_2\left(\gamma^2\omega^2 + \left(K + L - \omega^2\right)^2\right)\left(\gamma^2\omega^2 + \left(-K + L + \omega^2\right)^2\right)}\right]. \tag{4.108}$$

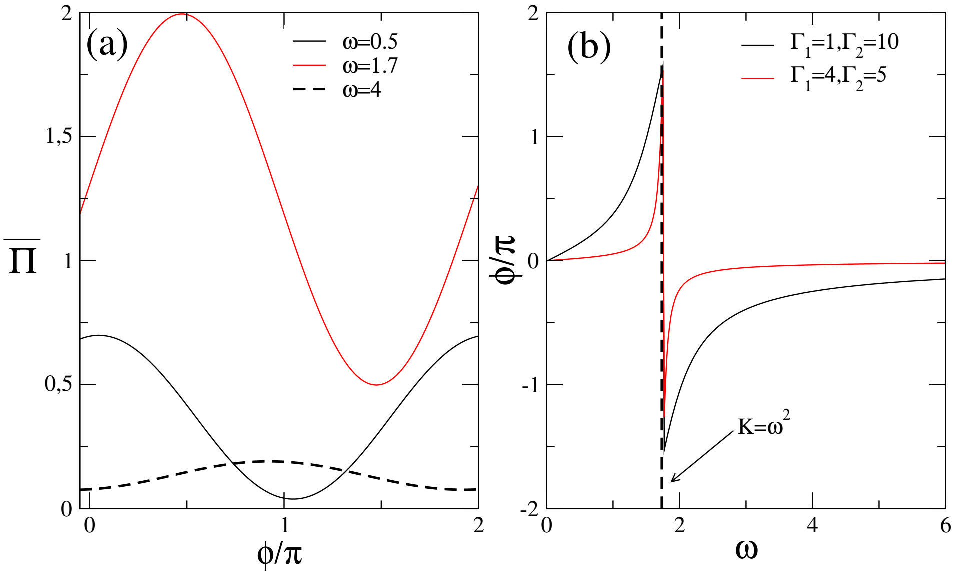

Figure 4.2: For distinct frequencies ω's, panel (a) depicts the average entropy production $\overline{\Pi}$ versus the phase difference ϕ for $\Gamma_1 = 1$, $\Gamma_2 = 10$, $K = 3$ and $\gamma = 1$. For $K = 3$ and $\gamma = 1$ and distinct sets of Γ_1 and Γ_2, panel (b) shows the positions ϕ of maximum/minimum of entropy production $\overline{\Pi}$ versus ω.

Note that the it reduces to the middle term from Eq. (4.96) when $\phi = 0$. The position of the maximum and minimum in $\overline{\Pi}$ fulfills the above relation

$$\phi = \tan^{-1}\left[\frac{\gamma\omega(\Gamma_2 - \Gamma_1)}{(K - \omega^2)\,(\Gamma_1 + \Gamma_2)}\right]. \tag{4.109}$$

Note that ϕ depends only on the signs of both $\Gamma_2 - \Gamma_1$ and $K - \omega^2$ and it is independent on L. In particular, in the regime of $\Gamma_2 >> \Gamma_1 (\Gamma_2 << \Gamma_1)$, ϕ is independent on Γ_i's, reading $\pm\gamma\omega/(K - \omega^2)$. Conversely, for fast and slow oscillations, it approaches to zero as $\gamma(\Gamma_1 - \Gamma_2)/K\omega(\Gamma_2 + \Gamma_1)$ and $\gamma\omega(\Gamma_2 - \Gamma_1)/K(\Gamma_2 + \Gamma_1)$, respectively. Fig. 4.2 plots $\overline{\Pi}$ versus ϕ for distinct set of values of ω and Γ_i's. Note that the maxima of mean entropy production yields at $\phi \sim 0(\pi)$ for small (large) values of ω and $\phi \to \pi/2$ when $\omega \to \sqrt{K}$. The dependence of extremes clearly follows theoretical predictions from Eq. (4.109) (see e.g. panels (a) and (b) in Fig. 4.2).

4.4 More than two particles

In this section we present the main results for long chains of oscillators. In real systems, due to the lattice imperfections and impurities, the difference of temperature between particles placed at extremities is responsible for a transport of heat following Fourier's law. More concretely, it states that the heat current is proportional to the inverse of the length of the chain given by

$$\mathcal{J}_T = -\kappa \frac{dT}{dx}, \tag{4.110}$$

where κ is the heat conductivity. In the case of a finite difference of temperatures ΔT, it follows that $\mathcal{J}_T \sim 1/N$ and thereby the heat flux is proportional to the inverse of the system size. Obtaining Fourier's Law from microscopic models have attracted great interest in the last years [111, 112, 102, 103]. In principle, one could suppose that a linear chain of particles interacting through harmonic forces in contact with two temperature reservoirs placed at extremities would lead to a heat flux obeying Fourier's law. However this is not the case [113]. Among the distinct approaches aimed at obtaining a heat flux inversely proportional to the system chain, we mention the self-consistent protocol proposed by Bosterli et al. [104]. It consists of baths acting on all sites, but intermediate temperatures are chosen self-consistently in such a way that they do not exchange any heat with the system in the steady state, ensuring that heat flux is only due to particles placed at extremities. Here we take a similar approach by Bosterli et al., in which each intermediate temperature is chosen so that it equals to the variance $\langle v_i^2 \rangle_{cv}$, $\Gamma_i^* = 2\gamma \langle v_i^2 \rangle_{cv}$. Although it reduces to the original protocol when external forces are absent, here all self-consistent reservoirs are expected to produce entropy coming from external forces. Fig. 4.3 illustrates a linear chain in the presence of thermal and self-consistent baths.

In order to compare the distinct sources of dissipation, thermal and time oscillating forces, we will consider that particles placed at extremities are not subjected to external forces. Thereby, under the above choice of the intermediate Γ_i's, the

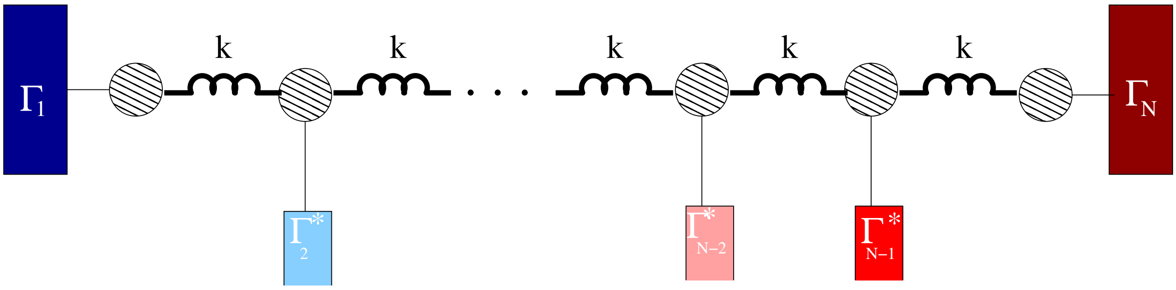

Figure 4.3: Schematic diagram consisting of an one-dimensional chain of N harmonic oscillators with individual and coupling interactions k^* and k, respectively. Γ_1 and Γ_N denote the cold and hot bath temperatures, respectively, whereas the self-consistent reservoirs are ranged from Γ_2^* to Γ_{N-1}^*. Each intermediate particle is also subject to an external force $f_i^{ext}(t)$. The usage of our protocol leads to intermediate temperatures changing linearly from Γ_1 to Γ_N, consistent to a flux of heat along the chain, symbolized by the color gradient from the red to the blue reservoirs.

flux of entropy becomes

$$\Phi(t) = \Phi_T + \Phi_f(t), \tag{4.111}$$

where Φ_T read

$$\Phi_T = \frac{2\gamma^2}{\Gamma_1}\left\langle v_1^2 \right\rangle_{cv} + \frac{2\gamma^2}{\Gamma_N}\left\langle v_N^2 \right\rangle_{cv} - 2\gamma, \tag{4.112}$$

and $\Phi_f(t)$ is a sum of individual contributions

$$\Phi_f(t) = 2\gamma^2\left(\frac{\langle v_1\rangle^2}{\Gamma_1} + \sum_{i=2}^{N-1}\frac{\langle v_i\rangle^2}{\Gamma_i^*} + \frac{\langle v_N\rangle^2}{\Gamma_N}\right). \tag{4.113}$$

Despite the absence of external forces for extreme particles, the averages $\langle v_1\rangle$ and $\langle v_N\rangle$ present oscillating behavior coming from couplings with neighboring particles (see e.g. Eqs. (4.36) and (4.37)).

In all cases, $\Pi_T = \Phi_T$ can be written as for the two particles case

$$\Pi_T = \mathcal{J}_T f_T, \tag{4.114}$$

where the thermodynamic force f_T and its associate flux $\mathcal{J}_T$ read $f_T = 1/\Gamma_1 - 1/\Gamma_N$ and $\mathcal{J}_T = \kappa(\Gamma_N - \Gamma_1)/N$, respectively. Thereby, the expression for Π_T becomes

$$\Pi_T = \frac{\kappa}{N}\frac{(\Gamma_N - \Gamma_1)^2}{\Gamma_1\Gamma_N}. \tag{4.115}$$

Since the thermal conduction coefficient κ is finite (it depends only on parameters

Γ_1,Γ_N,K and L), the entropy production Π_T decays as N^{-1} (see e.g. Fig. 4.5(b)).

4.4.1 Three particles case

Here we derive explicit results for a chain of $N = 3$ particles. In such case, Eq. (4.113) becomes

$$\Phi_f(t) = \frac{2\gamma^2}{\Gamma_1}\langle v_1\rangle^2 + \frac{2\gamma^2}{\Gamma_2^*}\langle v_2\rangle^2 + \frac{2\gamma^2}{\Gamma_3}\langle v_3\rangle^2, \tag{4.116}$$

and the entropy production Π_T due to thermal reservoirs has the shape of Eq. (4.114) with $\mathcal{J}_T$ given by

$$\mathcal{J}_T = \frac{\Gamma_1\Gamma_3\gamma L^2\left(2\gamma^2 K + L^2\right)}{2\left[L^2+\gamma^2\left(4K-2L\right)\right]\left[L^2+\gamma^2\left(K+L\right)\right]} f_T. \tag{4.117}$$

Once again, $\Pi_T \geq 0$, since $4K - 2L = 2(k + 2k^*)/m$. Using the motion equations we arrive at the following expression for $\overline{\Pi}$:

$$\overline{\Pi} = \frac{f_{02}^2\gamma^2\omega^2\left[\Gamma_1\Gamma_3\left(\gamma^2\omega^2+(K-\omega^2)^2\right)+L^2\Gamma_2^*(\Gamma_1+\Gamma_3)\right]}{\Gamma_1\Gamma_2^*\Gamma_3\left[\gamma^2\omega^2+(K+2L-\omega^2)^2\right]\left[\gamma^2\omega^2+(-K+L+\omega^2)^2\right]}, \tag{4.118}$$

which is strictly positive and vanishes when f_{02} and/or ω are equal to zero. Also, in the regime of slow and fast oscillations, $\overline{\Pi}$ exhibit similar dependencies on ω to the two particles case:

$$\overline{\Pi} \sim \left(\frac{K^2}{\Gamma_2^*} + \frac{L^2(\Gamma_1+\Gamma_3)}{\Gamma_1\Gamma_3}\right)\frac{\gamma^2\omega^2 f_{02}^2}{(K+2L)^2(-K+L)^2}, \tag{4.119}$$

for $\omega << 1$ and

$$\overline{\Pi} \sim \frac{\gamma^2 f_{02}^2}{\Gamma_2^*}\frac{1}{\omega^2}, \tag{4.120}$$

for $\omega >> 1$, respectively, implying that for such latter limit the entropy production is independent on extreme temperatures. For strong couplings between particles,

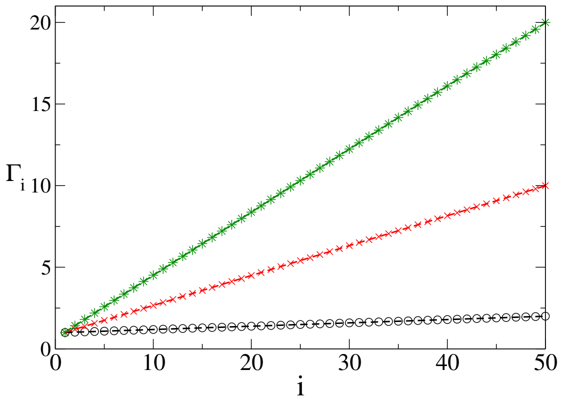

Figure 4.4: For a chain of $N = 50$ particles with $K = 2$,$L = 1$,$\gamma = 1$ and $\omega = 1$, the rescaled temperatures Γ_i's versus the position of the i-th site for three set of temperatures (Γ_1,Γ_N). The intermediate temperatures are calculated according to the prescription $\Gamma_i^* = 2\gamma \langle v_i^2 \rangle_{cv}$.

$L \approx K >> \omega^2$, $\overline{\Pi}$ approaches to

$$\overline{\Pi} \sim \frac{\gamma^2}{\gamma^2 + \omega^2}\left(\frac{1}{\Gamma_1} + \frac{1}{\Gamma_2^*} + \frac{1}{\Gamma_3}\right) f_{02}^2, \tag{4.121}$$

which is quite similar to Eq. (4.101) [for $N = 2$] and it is independent on the interaction strengths.

4.4.2 The limit of long particles chains

All results obtained for $N = 3$ particles can be straightforward extended for long chains. However, it becomes very cumbersome to obtain simplified expressions for $\overline{\Pi}$ in such cases. For this reason, we will restrict the next analysis for specific values of control parameters. Fig. 4.4 shows, for a chain of $N = 50$ particles and three sets of temperatures (Γ_1,Γ_N), the temperature profiles calculated from the self consistent protocol. In all cases, the set of intermediate temperatures changes linearly from Γ_1 to Γ_N, consistent to a flux of heat along the chain from the hot to the cold reservoirs.

Fig. 4.5(a) compares the individual entropy production contributions for distinct system sizes for $f_{02} = f_{03} = ... = f_{0N-1}$. Since external forces are equally presented in all intermediate particles, the entropy production associated to self consistent baths increases linearly with N. Also, panel (a) depicts the existence of two regimes. For small chains the thermal reservoir contribution Π_T dominates

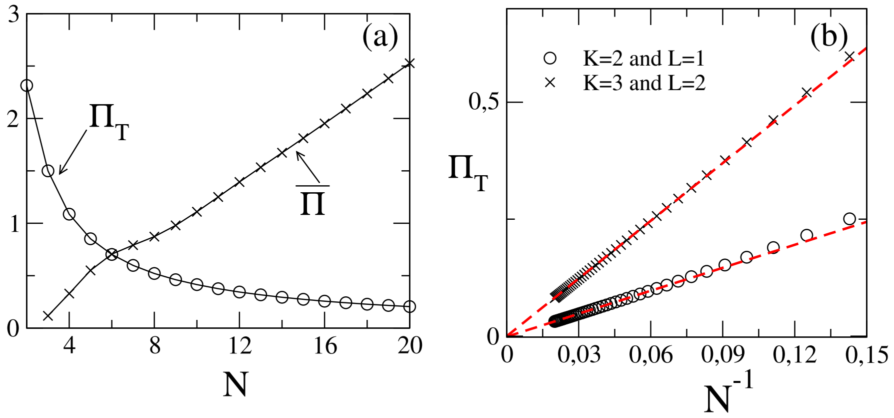

Figure 4.5: For $\Gamma_1 = 1$ and $\Gamma_N = 10$, panels (a) depicts the individual entropy production contributions from the thermal and self-consistent baths versus N for $K = 3, L = 2$ and $\omega = 1.5$. In (b) the behavior of entropy production from the thermal reservoirs Π_T vs N^{-1}.

over the self-consistent ones $\overline{\Pi}$, whereas $\overline{\Pi}$ wins over Π_T upon N is increased. In the limit $N \to \infty$ (see e.g panel (b)), only the contributions from self-consistent reservoirs prevail, in consonance with Fourier's law [Eq. (4.115)]. Finally, it is worth emphasizing two distinct linear behaviors of $\overline{\Pi}$. It arises from the particles closer to the thermal reservoirs providing more contribution for the entropy production for small chains than for large ones.

Chapter 5

Linear chains in the presence of oscillating temperature

The investigation of systems under oscillating temperature has been reported in several works [84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101], which provides a way of measuring the heat capacity experimentally. Here we intend to verify the nonequilibrium trademarks of a chain of two interacting particles under time oscillating temperatures. For simplicity, we consider external forces absent. The entropy production can also be evaluated straightforwardly from Eq. (4.21), but instead the temperature $\Gamma_i(t)$ of the each reservoir is now time dependent $\Gamma_i(t) = \Gamma_{0i} + F_{T_i}\cos(\omega t)$, with Γ_{0i} and F_{T_i} being the reference temperature and the strength of temperature driving, respectively.

In the first analysis, we shall reproduce the main results from Ref. [73], in which a single harmonic oscillator is subject to an oscillating temperture. Next, we describe our original contribution, in which a chain of two interacting particles is subject to periodic temperature drivings.

By reapeating the aforementioned procedures for the Fokker-Planck equation in the presence of oscillating temperature, the motion equations are given by

$$\frac{d\left\langle v^2\right\rangle}{dt} = -2K\left\langle xv\right\rangle - 2\gamma\left\langle v^2\right\rangle + k_B\Gamma, \tag{5.1}$$

$$\frac{d\left\langle x^2\right\rangle}{dt} = 2\left\langle xv\right\rangle, \tag{5.2}$$

and

$$\frac{d\left\langle xv\right\rangle}{dt}=\left\langle v^2\right\rangle-K\left\langle x^2\right\rangle-\gamma\left\langle xv\right\rangle. \tag{5.3}$$

Solving this set of equations and for $k_B=1$ we can find an expression for $\langle v^2\rangle$ as

$$\left\langle v^2\right\rangle=\frac{\Gamma_0}{2\gamma}+\frac{\Gamma_0}{2\gamma}\left(A_1\cos\omega t+A_2\sin\omega t\right), \tag{5.4}$$

where

$$A_1=\frac{4\omega^2\left(\omega^4-3K\omega^2+4K^2+\gamma^2\omega^2\right)}{\left(\gamma^2+\omega^2\right)\left(4\gamma^2\omega^2+\left(\omega^2-4K\right)^2\right)}, \tag{5.5}$$

and

$$A_2=\frac{2\gamma\omega\left(\omega^4-6K\omega^2+8K^2+\gamma^2\omega^2\right)}{\left(\gamma^2+\omega^2\right)\left(4\gamma^2\omega^2+\left(\omega^2-4K\right)^2\right)}. \tag{5.6}$$

We know from previous chapter that the entropy flux can be given by Equation (3.48) which for one particle is

$$\Phi=\frac{2\gamma^2}{\Gamma_i}\left\langle v^2\right\rangle-\gamma, \tag{5.7}$$

since the entropy production rates $\overline{\Pi}=\overline{\Phi}$ (In the steady state) and taking the average over a cycle like before, we find

$$\overline{\Pi}=\frac{\gamma\omega^2\left(\omega^4-8K\omega^2+16K^2+4K\gamma^2+\gamma^2\omega^2\right)}{\left(\gamma^2+\omega^2\right)\left(4\gamma^2\omega^2+\left(\omega^2-4K\right)^2\right)}\left(\frac{\Gamma_0}{\left(\Gamma_0-\Gamma_1\right)\left(\Gamma_0+\Gamma_1\right)}-1\right), \tag{5.8}$$

in accordance with the entropy production found in Ref. [73]. Note that it vanishes as $\omega\to0$ and becomes $\gamma^2\left(\frac{\Gamma_0}{(\Gamma_0-\Gamma_1)(\Gamma_0+\Gamma_1)}-1\right)$ when $\omega\to\infty$.

Now we can study a chain of two interacting particles under time oscillating temperatures which are given by

$$\Gamma_i(t)=\Gamma_{0i}+F_{T_i}\cos(\omega t), \tag{5.9}$$

with Γ_{0i} and F_{T_i} being the reference temperature and the strength of temperature driving, respectively. Although such problem is exactly solvable [see e.g. Fig. 5.1 (*b*)] and reduces to previous expression (Eq. (5.8)) when $\Gamma_{01}=\Gamma_{02}$ and $L=0$, the expression for $\overline{\Pi}$ is much more complex than previous cases and involves many terms related to distinct powers of interaction parameters K,L and driving frequency ω. For this reason, our analysis will be carried out close to equilibrium regime, in which a linear treatment can be performed. More specifically, we take both reference temperatures to be equal $\Gamma_{01} = \Gamma_{02} = \Gamma_0$ and the driving strengths are low $F_{T_i} << \Gamma_0$. In such case, the entropy production $\overline{\Pi}$ can also be written down in the bilinear form $\overline{\Pi} = \mathcal{J}_{T_1} F_{T_1} + \mathcal{J}_{T_2} F_{T_2}$, where the fluxes $\mathcal{J}_{T_1}$ and $\mathcal{J}_{T_2}$ read

$$\mathcal{J}_{T_1} = L_{T_1,T_1} F_{T_1} + L_{T_1,T_2} F_{T_2}, \tag{5.10}$$

and

$$\mathcal{J}_{T_2} = L_{T_2,T_1} F_{T_1} + L_{T_2,T_2} F_{T_2}, \tag{5.11}$$

respectively, where L_{T_i,T_j} are the associated Onsager coefficients given by

$$L_{T_1,T_1} = \frac{\gamma}{2\Gamma_0^2} \left(\frac{\sum_{\ell=0}^{9} B_\ell \; \omega^{2\ell}}{\sum_{\ell=0}^{9} G_\ell \; \omega^{2\ell}} \right), \tag{5.12}$$

and

$$L_{T_1,T_2} = \frac{-4\gamma^3 L^2}{\Gamma_0^2} \left(\frac{\sum_{\ell=0}^{6} A_\ell \; \omega^{2\ell}}{\sum_{\ell=0}^{9} G_\ell \; \omega^{2\ell}} \right), \tag{5.13}$$

respectively, where $L_{T_1,T_1} = L_{T_2,T_2}$ and $L_{T_1,T_2} = L_{T_2,T_1}$ and coefficients A_i's, B_i's and G_i's solely depend on the parameters γ and $L = 2K$ and are listed in the Appendix 7.3.

We pause again to make some few comments: First, in the limit of slow and fast frequencies, $\overline{\Pi}$ approaches to the following expressions

$$\overline{\Pi} \sim \frac{4\gamma^3 L^2 A_0}{\Gamma_0^2 G_0} (F_{T_1} - F_{T_2})^2, \tag{5.14}$$

and

$$\overline{\Pi} \sim \frac{\gamma}{2\Gamma_0^2} (F_{T_1}^2 + F_{T_2}^2), \tag{5.15}$$

respectively. They contrast with the oscillating forced case, since are independent on ω and different from zero in both extreme cases. Whenever it depends on L for low oscillations, the entropy production is independent on the coupling for fast

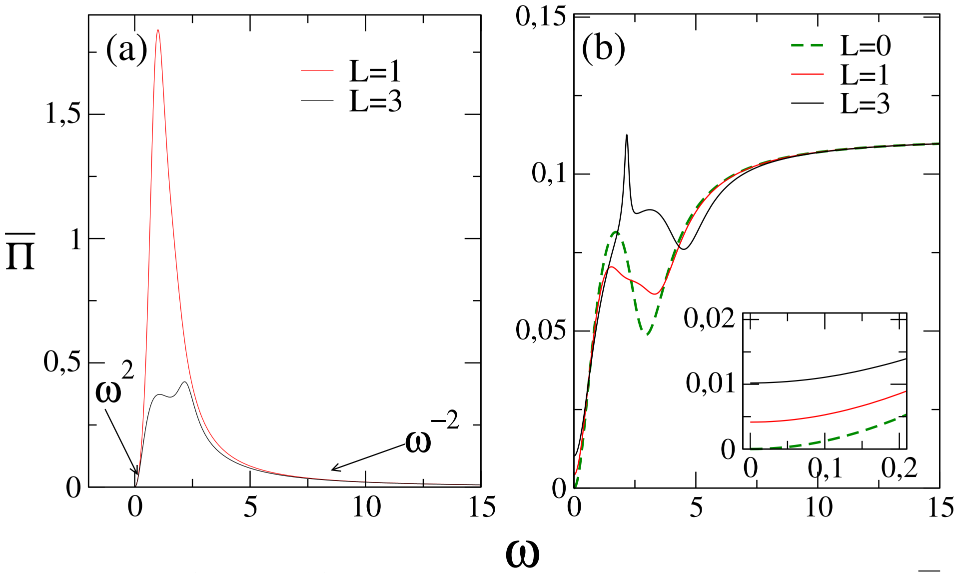

Figure 5.1: Panels (a) and (b) depict the steady entropy production rate $\overline{\Pi}$ versus frequency driving ω for time dependent oscillating forces and temperatures, respectively. In all cases we take $\gamma = 1$,$K = 2$,$\Gamma_1 = \Gamma_2 = 10$ and $f_{02} = 2f_{01} = 4$ [panel (a)] and $F_{T_2} = 2F_{T_1} = 4$ [panel (b)]. Inset: The steady $\overline{\Pi}$ for distinct L's for low ω.

oscillations. Finally, for strong interaction strength, $L >> 1$ and $L >> \omega^2$, $\overline{\Pi}$ reads

$$\overline{\Pi} \sim \frac{\gamma}{4\Gamma_0^2(\gamma^2+\omega^2)}\left[\gamma^2(F_{T_1}-F_{T_2})^2 + 2\omega^2(F_{T_1}^2+F_{T_2}^2)\right], \tag{5.16}$$

which is also independent on L. We close this section by comparing, in Fig. 5.1 (a) and (b) the steady entropy production behaviors versus the frequency driving ω for both oscillating temperature and forces (obtained from the exact solution). They exhibit meaningfully different dependence on ω, even for extreme ω. Whenever $\overline{\Pi}$ vanishes for $\omega << 1$ and $\omega >> 1$ in the case of time oscillating forces, it reaches constant values for temperature drivings, in accordance with asymptotic expressions Eqs. (5.14) and (5.15), respectively, obtained from the linear regime approximation.

Chapter 6

Conclusions

Nonequilibrium thermodynamics have attracted great deal of interest in the last years and a particular attention has been given to periodically driven systems. In this work, we analyzed, via stochastic thermodynamics, the properties of linear chains of Brownian particles. Our results constituted a further step in the previous studies [73, 63] in which periodic drivings have been considered for the underdamped harmonic oscillator. We derived exact expressions for the heat flux, entropy production and allied quantities. The analysis were splitted in two parts: regimes of short and long chains.

Several conclusions have been drawn from our work. In the former case the interaction between partícles is responsible for a bilinear form of the entropy production, whose Onsager coefficients are functions of interaction parameters and frequency drivings. They behave very differently depending on the kind of driving, e.g. when the driving is introduced in the temperature or forces. Reciprocal relations were also obtained.

Second, the limit of long chains was studied by means of a self-consistent protocol for choosing intermediate temperatures. In such a case, the entropy production is a sum of two terms: one coming from the real baths and the other from the self-consistent reservoirs. Whenever the former dominates for short chains, the latter contribution prevails for long ones. The contribution from the thermal reservoirs is responsible to heat flux according to Fourier's law.

There are serveral perspectives to be addressed. The inclusion of both temperature and external force drivings in harmonic chains should be interesting, in order to compare not only the structure of entropy production but also the Onsager coefficients. In this case, considerations about the efficiency can be performed. The oscillating force can be interpreted as a source of mechanical work, whereas the oscillating temperature as a source of heat. Also, the investigation of other kinds of drivings, such as the time discrete drivings should also be interesting in order to compare with sinusoidally time dependent ones. We intend to develop these topics in ongoing studies.

Chapter 7

Appendix

7.1 Obtaining the coefficients A_{ij} for $N = 2$ particles case with no phase difference

Here we show explicit expressions for the coefficients A_{ij}'s for the two particles case subject to oscillating forces. The index i stands for the i-th particle (i = 1,2).

$$A_{1i} = \frac{f_{0i}\left(K-\omega^2\right)\left[\gamma^2\omega^2+\left(K-\omega^2\right)^2-L^2\right]+f_{0j}L\left[-\omega^2\left(\gamma^2+2K\right)+K^2-L^2+\omega^4\right]}{\left[\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right]\left[\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right]}, \tag{7.1}$$

and

$$A_{2i} = \frac{\gamma\omega\left[f_{0i}\left(\gamma^2\omega^2+\left(K-\omega^2\right)^2+L^2\right)+2f_{0j}L\left(K-\omega^2\right)\right]}{\left(\gamma^2\omega^2+\left(K+L-\omega^2\right)^2\right)\left(\gamma^2\omega^2+\left(-K+L+\omega^2\right)^2\right)}. \tag{7.2}$$

Having the A_{ij}'s, the steady entropy production $\overline{\Pi}$ is straightforwardly evaluated.

7.2 Obtaining the coefficients B_{ij} for $N = 2$ particles case and phase difference

Here we show explicit expressions for the coefficients B_{ij}'s for the two particles subject to phase difference between oscillating forces.

$$B_{11} = \frac{f_{02}L\left((\cos\phi - 1)\left(-\omega^2\left(\gamma^2 + 2K\right) + K^2 - L^2 + \omega^4\right) + 2\gamma\omega\left(K - \omega^2\right)\sin\phi\right)}{\left(\gamma^2\omega^2 + \left(K + L - \omega^2\right)^2\right)\left(\gamma^2\omega^2 + \left(-K + L + \omega^2\right)^2\right)}, \tag{7.3}$$

$$B_{21} = \frac{f_{02}L\left(\sin\phi\left(\gamma^2\omega^2 - \left(K - \omega^2\right)^2 + L^2\right) + 2\gamma\omega\left(K - \omega^2\right)(\cos\phi - 1)\right)}{\left(\gamma^2\omega^2 + \left(K + L - \omega^2\right)^2\right)\left(\gamma^2\omega^2 + \left(-K + L + \omega^2\right)^2\right)}, \tag{7.4}$$

$$B_{12} = \frac{f_{02}\gamma\omega\sin\phi\left(\gamma^2\omega^2 + \left(K - \omega^2\right)^2 + L^2\right) + f_{02}\left(K - \omega^2\right)(\cos\phi - 1)\left(\gamma^2\omega^2 + \left(K - \omega^2\right)^2 - L^2\right)}{\left(\gamma^2\omega^2 + \left(K + L - \omega^2\right)^2\right)\left(\gamma^2\omega^2 + \left(-K + L + \omega^2\right)^2\right)}, \tag{7.5}$$

and

$$B_{22} = \frac{f_{02}\left(\omega^2 - K\right)\sin\phi\left(\gamma^2\omega^2 + \left(K - \omega^2\right)^2 - L^2\right) + f_{02}\gamma\omega(\cos\phi - 1)\left(\gamma^2\omega^2 + \left(K - \omega^2\right)^2 + L^2\right)}{\left(\gamma^2\omega^2 + \left(K + L - \omega^2\right)^2\right)\left(\gamma^2\omega^2 + \left(-K + L + \omega^2\right)^2\right)}, \tag{7.6}$$

respectively. Note that all of them vanishes as $\phi = 0$, restoring the expressions Eqs. (7.1) and (7.2), respectively.

7.3 Obtaining the coefficients A_i's, B_i's and G_i's for $N = 2$ particles case and oscillating temperature

Here we show explicit expressions for the coefficients A_i's, B_i's and G_i's for the two particles case and time oscillating temperatures.

$$A_0 = 2304L^5\left(2\gamma^2 + L\right),$$

$$A_1 = -128L^3\left(-7\gamma^4 + 58\gamma^2 L + 123L^2\right),$$

$$A_2 = 16L\left(8\gamma^6 - 50\gamma^4 L + 34\gamma^2 L^2 + 931L^3\right),$$

$$A_3 = 4\left(-11\gamma^6 + 78\gamma^4 L + 319\gamma^2 L^2 - 1606L^3\right),$$

$$A_4 = -3\left(17\gamma^4 + 82\gamma^2 L - 548L^2\right),$$

$$A_5 = 3\gamma^2 - 214L,$$

$$A_6 = +10,$$

$$B_0 = 36864\gamma^4 L^7 + 18432\gamma^2 L^8,$$

$$B_1 = 31744\gamma^6 L^5 + 112640\gamma^4 L^6 + 27648\gamma^2 L^7 + 36864L^8,$$

$$B_2 = 4608\gamma^8 L^3 + 18176\gamma^6 L^4 - 77056\gamma^4 L^5 + 203904\gamma^2 L^6 - 172032L^7,$$

$$B_3 = 128\gamma^{10} L + 608\gamma^8 L^2 - 6592\gamma^6 L^3 + 85920\gamma^4 L^4 - 230720\gamma^2 L^5 + 269824L^6,$$

$$B_4 = 16\gamma^{10} - 64\gamma^8 L + 4536\gamma^6 L^2 - 34864\gamma^4 L^3 + 125488\gamma^2 L^4 - 170496L^5,$$

$$B_5 = 56\gamma^8 - 792\gamma^6 L + 8112\gamma^4 L^2 - 34928\gamma^2 L^3 + 54288L^4,$$

$$B_6 = 73\gamma^6 - 928\gamma^4 L + 5120\gamma^2 L^2 - 9536L^3,$$

$$B_7 = 43\gamma^4 - 376\gamma^2 L + 936L^2,$$

$$B_8 = 11\gamma^2 - 48L,$$

$$B_9 = 1,$$

$$G_0 = 147456\gamma^6 L^6 + 147456\gamma^4 L^7 + 36864\gamma^2 L^8,$$

$$G_1 = 50176\gamma^8 L^4 - 94208\gamma^6 L^5 + 262144\gamma^4 L^6 - 24576\gamma^2 L^7 + 36864L^8,$$

$$G_2 = 3584\gamma^{10} L^2 - 23552\gamma^8 L^3 + 166400\gamma^6 L^4 - 323584\gamma^4 L^5 + 384512\gamma^2 L^6 - 172032L^7,$$

$$G_3 = 64\gamma^{12} - 768\gamma^{10} L + 14720\gamma^8 L^2 - 77312\gamma^6 L^3 + 262528\gamma^4 L^4 - 399872\gamma^2 L^5 + 269824L^6,$$

$$G_4 = 240\gamma^{10} - 2688\gamma^8 L + 24672\gamma^6 L^2 - 96960\gamma^4 L^3 + 200592\gamma^2 L^4 - 170496L^5,$$

$$G_5 = 348\gamma^8 - 3504\gamma^6 L + 20024\gamma^4 L^2 - 52736\gamma^2 L^3 + 54288L^4,$$

$$G_6 = 245\gamma^6 - 2064\gamma^4 L + 7424\gamma^2 L^2 - 9536L^3,$$

$$G_7 = 87\gamma^4 - 528\gamma^2 L + 936L^2,$$

$$G_8 = 15\gamma^2 - 48L,$$

$$G_9 = 1.$$

Bibliography

[1] J. S. Thomsen, Phys. Rev. **91**, 1263 (1953).

[2] M. J. Klein and P. H. E. Meijer, Phys. Rev. **96**, 250 (1954).

[3] M. J. Klein, Phys. Rev. **97**, 1446 (1955).

[4] T. L. Hill and O. Kedem, J. Theor. Biol. **10**, 399 (1966).

[5] D. A. McQuarrie, J. Appl. Prob. **4**, 413 (1967).

[6] J. Schnakenberg, Rev. Mod. Phys. **48**, 571 (1976).

[7] L. Jiu-Li, C. Van den Broeck, and G. Nicolis, Z. Phys. B **56**, 165 (1984).

[8] C. Y. Mou, J.-L. Luo, and G. Nicolis, J. Chem. Phys. **84**, 7011 (1986).

[9] D. T. Gillespie, Physica A **188**, 404 (1992).

[10] A. Pérez-Madrid, J. R. Rub´ı, and P. Mazur, Physica A **212**, 231 (1994).

[11] B. Gaveau and L. S. Schulman, Phys. Lett. A **229**, 347 (1997).

[12] K. Sekimoto, Prog. Theor. Phys. Suppl. **130**, 17 (1998).

[13] T. Tomé and M. J. de Oliveira, Braz. J. Phys. **27**, 525 (1997).

[14] P. Mazur, Physica A 274, 491 (1999).

[15] L. Crochik and T. Tomé, Phys. Rev. E **72**, 057103 (2005).

[16] R. K. P. Zia and B. Schmittmann, J. Phys. A: Math. Gen. **39**, L407 (2006).

[17] D. Andrieux and P. Gaspard, Phys. Rev. E **74**, 011906 (2006).

[18] T. Schmiedl and U. Seifert, J. Chem. Phys. **126**, 044101 (2007).

[19] R. J. Harris and G. M. Schutz, J. Stat. Mech. (2007) P07020.

[20] R. K. P. Zia and B. Schmittmann, J. Stat. Mech. (2007) P07012.

[21] U. Seifert, Eur. Phys. J. B **64**, 423 (2008).

[22] R. A. Blythe, Phys. Rev. Lett. **100**, 010601 (2008).

[23] B. Gaveau, M. Moreau, and L. S. Schulman, Phys. Rev. E **79**, 010102 (2009).

[24] B. Gaveau and L. S. Schulman, Phys. Rev. E **79**, 021112 (2009).

[25] M. Esposito, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. **102**, 130602 (2009).

[26] T. Tomé and M. J. de Oliveira, Phys. Rev. Lett. **108**, 020601 (2012).

[27] M. Esposito, Phys. Rev. E **85**, 041125 (2012).

[28] X.-J. Zhang, H. Qian, and M. Qian, Phys. Rep. **510**, 1 (2012).

[29] H. Ge, M. Qian, and H. Qian, Phys. Rep. **510**, 87 (2012).

[30] J. W. Gibbs, Elementary Principles in Statistical Mechanics (Scribner, New York, 1902).

[31] A. Einstein, Ann. Phys. **322**, 549 (1905).

[32] M. Smoluchowski, Ann. Phys. **326**, 756 (1906).

[33] P. Langevin, Comp. Rend. **146**, 530 (1908).

[34] A. D. Fokker, Ann. Phys. **348**, 810 (1914).

[35] M. Smoluchowski, Ann. Phys. **353**, 1103 (1915).

[36] M. Planck, Sitz. Knig. Preuss. Akad. Wiss. 324 (1917).

[37] L. S. Ornstein, KNAW, Proceedings, Amsterdam **21**, 96 (1919).

[38] H. A. Kramers, Physica **7**, 284 (1940).

[39] N. T. J. Bailey, TheMathematical Theory of Epidemics (Hafner, New York, 1957).

[40] M. S. Bartlett, Stochastic Population Models in Ecology and Epidemiology (Methuen, London, 1960).

[41] R. M. Nisbet and W. C. S. Gurney, Modelling Fluctuating Populations (Wiley, New York, 1982).

[42] T. L. Hill, Free Energy Transduction and Biochemical Cycle Kinetics (Springer, New York, 1989).

[43] P. Ao, Commun. Theor. Phys. 49, 1073 (2008).

[44] G. Lan, P. Sartori, S. Neumann, V. Sourjik, and Y. Tu, Nat. Phys. 8, 422 (2012).

[45] H. Berry, Phys. Rev. E 67, 031907 (2003).

[46] J. L. England, J. Chem. Phys. 139, 121923 (2013).

[47] R. J. Glauber, J. Math. Phys. 4, 294 (1963).

[48] T. E. Harris, Ann. Probab. 2, 969 (1974).

[49] T. M. Ligget, Interacting Particle Systems (Springer, New York, 1985).

[50] R. M. Ziff, E. Gulari, and Y. Barshad, Phys. Rev. Lett. 56, 2553 (1986).

[51] J. E. Satulovsky and T. Tom´e, Phys. Rev. E 49, 5073 (1994).

[52] M. J. de Oliveira, J. Stat. Phys. 66, 273 (1992).

[53] J. Marro and R. Dickman, Nonequilibrium Phase Transitions in Lattice Models (Cambridge University Press, Cambridge, UK, 1999).

[54] M. J. de Oliveira, Phys. Rev. E 67, 066101 (2003).

[55] I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, 2nd ed. (Wiley, New York, 1961).

[56] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).

[57] T. Tomé and M. J. de Oliveira, *Stochastic Dynamics and Irreversibility* (Springer, Cham, 2015).

[58] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).

[59] O.-P. Saira, Y. Yoon, T. Tanttu, M. Möttönen, D.V. Averin and J. P. Pekola, Phys. Rev. Lett. **109**, 180601 (2012).

[60] K. Proesmans and C. Van den Broeck, Europhys. Lett. **119**, 20001 (2017).

[61] Andre C. Barato and Udo Seifert Phys. Rev. Lett. **114**, 158101 (2015).

[62] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).

[63] T. Tomé and M. J. de Oliveira, Phys. Rev. E **91**, 042140 (2015).

[64] C. Van den Broeck and M. Esposito, Phys. A **418**, 6 (2015).

[65] K Proesmans, B Cleuren and C Van den Broeck, Phys. Rev. Lett. **116**, 220601 (2016).

[66] C. E. F. Noa, P. E. Harunari, M. J. de Oliveira and C. E. Fiore, Phys. Rev. E **100**, 012104 (2019).

[67] T. Herpich, J. Thingna and M. Esposito, Phys. Rev. X **8**, 031056 (2018).

[68] T. Herpich and M. Esposito, Phys. Rev. E **99**, 022135 (2019).

[69] M. Esposito and C. Van den Broeck, Phys. Rev. E **82**, 011143 (2010).

[70] S. Ray and A. C. Barato, Phys. Rev. E **96**, 052120 (2017).

[71] T. Tomé, Braz. J. Phys. **36**, 1285 (2006).

[72] T. Tomé and M. J. de Oliveira, Phys. Rev. E **82**, 021120 (2010).

[73] C. E. Fiore and M. J. de Oliveira, Phys. Rev. E **99**, 052131 (2019).

[74] C. Van den Broeck and M. Esposito, Phys. Rev. E **82**, 011144 (2010).

[75] A. Rosas, C. Van den Broeck and K. Lindenberg, Phys. Rev. E **94**, 052129 (2016).

[76] P. Pradhan and U. Seifert, Europhys. Lett. **89**, 37001 (2010).

[77] C. Kwon, J. D. Noh, and H. Park, Phys. Rev. E **83**, 061145 (2011).

[78] Y. Tang, R. Yuan, J. Chen, and P. Ao, Phys. Rev. E **91**, 042108 (2015).

[79] K. Proesmans and C. Van den Broeck, Chaos **27**, 104601 (2017).

[80] K. Brandner, K. Saito and Udo Seifert, Phys. Rev. X **5**, 031019 (2015).

[81] K. Proesmans, B. Cleuren and C. Van de Broeck, J. Stat. Mech **2016** 023202 (2016).

[82] K. Proesmans and C. E. Fiore, Phys. Rev. E **100**, 022141 (2019).

[83] B. Cleuren and K. Proesmans, Stochastic impedance, Physica A (2019) 122789, https://doi.org/10.1016/j.physa.2019.122789.

[84] G. W. H. Höhne, W. F. Hemminger, and H.-J. Flammersheim, *Differential Scanning Calorimetry* (Springer, Berlin, 2003).

[85] Y. Kraftmakher, *Modulation Calorimetry, Theory and Applications* (Springer, Berlin, 2004).

[86] L. P. Filippov, Int. J. Heat Mass Transfer. **9**, 681-691 (1966).

[87] P. F. Sullivan and G. Seidel, Phys. Rev. **173**, 679-685 (1968).

[88] H. Gobrecht, K. Hamann and G. Willers, J. Phys. E: Sci. Instrum. 4, 21 (1971).

[89] N. O. Birge and S. R. Nagel, Phys. Rev. Lett. **54**, 2674 (1985).

[90] P. S. Gill, S. R. Sauerbrunn and M. Reading, J. Therm. Anal. **40**, 931 (1993).

[91] J. E. K. Schawe, Thermochim. Acta **260**, 1 (1995).

[92] Y.-H. Jeong, Thermochim. Acta **304-305**, 67 (1997).

[93] J. E. K. Schawe, Thermochim. Acta **304-305**, 119 (1997).

[94] G. W. H. Höhne, Thermochim. Acta **304-305**, 121 (1997).

[95] S. L. Simon and G. B. McKenna, J. Chem. Phys. **107** 8678 (1997).

[96] K. J. Jones, I. Kinshott, M. Reading, A. A. Lacey, C. Nikolopoulos, and H. M. Pollock, Thermochim. Acta **304-305**, 187 (1997).

[97] H. Baur and B. Wunderlich, J. Therm. Anal. **54**, 437 (1998).

[98] P. Claudy and J. M. Vignon, J. Therm. Anal. Calorim. **60**, 333 (2000).

[99] J.-L. Garden, Thermochim. Acta **452**, 85 (2007).

[100] J.-L. Garden and J. Richard, Thermochim. Acta **462**, 57 (2007).

[101] J.-L. Garden, J. Richard and Y. Saruyama, J. Therm. Anal. Calorim. **94**, 585 (2008).

[102] G. T. Landi and M. J. de Oliveira, Phys. Rev. E **87**, 052126 (2013).

[103] M. J. de Oliveira, J. Phys. A **50**, 335001 (2017).

[104] M. Bolsterli, M. Rich, and W. M. Visscher, Phys. Rev. A **1**, 1086 (1970).

[105] R. E. Spinney and I. J. Ford, Phys. Rev. E **85**, 051113 (2012).

[106] F. Zhang, L. Xu, K. Zhang, E. Wang and J. Wang, J. Chem. Phys. **137**, 065102(2012).

[107] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).

[108] M. Santillan and H. Qian, Physica A **392**, 123 (2013).

[109] D. Luposchainsky and H. Hinrichsen, J. Stat. Phys. **153**, 828 (2013).

[110] W. Wu and J. Wang, J. Chem. Phys. **141**, 105104 (2014).

[111] S. Lepri, R. Livi and A. Politi Phys. Rep. **377** 1 (2003).

[112] A. Dhar, Adv. Phys. **57**, 457 (2008).

[113] Z. Rieder, J. L. Lebowitz and E. Lieb, J. Math. Phys. **8**, 1073 (1967).

PHYSICAL REVIEW E **101**, 012132 (2020)

Entropy production and heat transport in harmonic chains under time-dependent periodic drivings

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Using stochastic thermodynamics, the properties of interacting linear chains subject to periodic drivings are investigated. The systems are described by Fokker-Planck-Kramers equation and exact solutions are obtained as functions of the modulation frequency and strength constants. Analysis will be carried out for short and long chains. In the former case, explicit expressions are derived for a chain of two particles, in which the entropy production is written down as a bilinear function of thermodynamic forces and fluxes, whose associated Onsager coefficients are evaluated for distinct kinds of periodic drivings. The limit of long chains is analyzed by means of a protocol in which the intermediate temperatures are self-consistently chosen and the entropy production is decomposed as a sum of two individual contributions, one coming from real baths (placed at extremities of lattice) and other from self-consistent baths. Whenever the former dominates for short chains, the latter contribution prevails for long ones. The thermal reservoirs lead to a heat flux according to Fourier's law.

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I. INTRODUCTION

The description of thermodynamic quantities at the mesoscopic level gives rise to the stochastic thermodynamics [1–3], in which fluctuations in the thermodynamic fluxes become important. This theory not only allows to reproduce the fundamental concepts of thermodynamics of equilibrium systems but can also be extended for the more general case of nonequilibrium ones. In particular, it shows that stochastic fluxes satisfy general relations such as the Jarzynski equality [4,5] or/and it predicts the existence of general bounds among thermodynamic fluxes [6,7].

Entropy production has played a fundamental role in nonequilibrium statistical physics not only for typifying the irreversibility [8–10], but also for tackling general considerations about efficiency of heat engines [11], the analysis of (irreversible) phase transition portraits [12–14], thermodynamic uncertainties relations [6,7], and others. A fundamental relation for the entropy production comes from simple entropic arguments in which the system is coupled to a thermal reservoir. Its time entropy variation dS/dt is the difference of two terms

$$\frac{dS}{dt} = \Pi(t) - \Phi(t), \tag{1}$$

where $\Pi(t)$ is the entropy production rate and $\Phi(t)$ is the entropy flux rate from/to the system to/from the environment. Since the environment works as a subsystem in equilibrium, $\Pi(t)$ corresponds to the entropy produced inside the system. Equation (1) implies that all entropy spontaneously produced (by the system) has to be delivered to the environment in the steady state regime. When the system is in thermal equilibrium, it follows that $\Pi_s = \Phi_s = 0$, whereas $\Pi_s = \Phi_s > 0$ out of the equilibrium regime. Thereby entropy production discerns equilibrium and nonequilibrium systems, since it is continuously produced in the latter case. In such case, the steady entropy production rate can alternatively be evaluated through the calculation of the steady entropy flux Φ_s.

The thermodynamic properties of Markovian systems have been extensively studied in the framework of master [8–10,15,16] and Fokker-Planck equations [17–25]. A special recent attention has been devoted to periodically driven systems [26–29]. In part because their thermodynamic properties can be experimentally accessible [26,30–47]. In addition, some of their remarkable features, such as a general description in the linear regime (Onsager coefficients and general reciprocal relations can be achieved), the existence of uncertainties constraints leading to existence of bounds among macroscopic averages and other features have been put under a firmer basis. In other cases, the probability distribution of work for systems described by Langevin equations with time dependent drivings has also been analyzed [24]. However, the more general case of interacting particles subject to time periodic drivings has not been studied thoroughly. In particular, the question of how the inclusion of interaction changes the nonequilibrium trademarks as well as the entropy production properties has not been addressed before.

In this paper, we fill this gap by investigating the thermodynamic properties of interacting chains of Brownian particles subject to (time dependent) periodic forces and temperature drivings. Exact expressions for the thermodynamic quantities, including the dissipated heat, entropy production, heat flux and others are obtained. The limits of short and long particle chains are thoroughly investigated. For the latter case, intermediate temperatures are self-consistently chosen through a protocol taking into account an inner entropy production source. This is meaningfully different from the original approach by Bosterli *et al.* [48], in which no heat flux is exchanged among the particles and self-consistent baths. Thus, our approach provides us not only to analyze the role of two distinct sources of dissipation, but also establishing which contribution dominates in the limits of short and long chains. Two main findings can be drawn: For the case of two interacting particles, the entropy production is derived as a bilinear function of fluxes and forces for both drivings in forces and temperatures, whose associated Onsager coefficients depend on the interaction parameters and frequency driving. Remarkably, the effect of a phase difference (a lag) between external forces is investigated and the condition for maximum/minimum entropy production is found to depend only on the temperature reservoirs and frequency driving, irrespective of the interaction strength between particles. The entropy production of long particle chains can be split in two terms: one coming from the thermal reservoirs and the other from the self-consistent ones.

This paper is organized as follows. In Sec. II we describe the theoretical background and the exact solution for time dependent drivings is evaluated in Sec. III. In Secs. IV and V, the two and several particles cases are analyzed, respectively. Conclusions are discussed in Sec. VI.

II. FOKKER-PLANCK-KRAMERS EQUATION

We consider a set of N interacting particles with equal masses m, in which the ith particle evolves in time according to the following set of coupled Langevin equations:

$$\frac{dv_i}{dt} = f_i^* - \gamma v_i + \mathcal{F}_i(t), \tag{2}$$

and

$$\frac{dx_i}{dt} = v_i, \tag{3}$$

with x_i denoting its position with velocity $v_i = dx_i/dt$, respectively, whereas γ is the dissipation constant. Here, f_i^* stands for the force acting to the ith particle, which is assumed to be decomposed as the sum of a time dependent term $f_i^{\text{ext}}(t)$ plus a term f_i depending only on the positions. Thus, f_i can be written as the derivative of the potential energy V, $f_i = -\partial V/\partial x_i$. The stochastic force $\mathcal{F}_i(t)$ accounts for the interaction between particle i and the environment and satisfies the properties

$$\langle \mathcal{F}_i(t) \rangle = 0, \tag{4}$$

and

$$\langle \mathcal{F}_i(t)\mathcal{F}_j(t') \rangle = 2\gamma T_i \delta_{ij}\delta(t-t'), \tag{5}$$

respectively, where $T_i > 0$ is distinct for each particle. Let $P(x, v, t) \equiv P(x_1, \dots, x_N, v_1, \dots, v_N, t)$ be the joint probability distribution at time t, where x and v denote the collection of particle positions x_i and velocities v_i, respectively. Its time evolution is described by the Fokker-Planck-Kramers (FPK) equation [3,9,18]

$$\frac{\partial P}{\partial t} = -\sum_i \left(v_i \frac{\partial P}{\partial x_i} + \left[f_i + f_i^{\text{ext}}(t)\right] \frac{\partial P}{\partial v_i} + \frac{\partial J_i}{\partial v_i} \right), \tag{6}$$

where

$$J_i = -\gamma v_i P - \frac{\gamma k_B T_i}{m} \frac{\partial P}{\partial v_i}. \tag{7}$$

If the temperatures of all particles T_i are the same and the external forces are null, the probability distribution approaches for large times the Gibbs equilibrium distribution,

$$P^e(x, v) = \frac{1}{Z} e^{-E/k_B T}, \tag{8}$$

where $E = mv^2/2 + V$ is the energy of the system. This result shows that the FPK Eq. (6) indeed describes the contact of a system with a heat reservoir at a temperature T. On the other hand, this will not be the case of the system in contact with distinct reservoirs and/or when it is subject to time oscillating forces or temperatures. In such case, the system dissipates heat and continuously produce entropy.

From the FK equation, the time variation of the energy $U = \langle E \rangle$ reads

$$\frac{dU}{dt} = -\sum_{i=1}^N \left(\Phi_q^{(i)} + \Phi_w^{(i)} \right), \tag{9}$$

where the heat flux $\Phi_q^{(i)}$ from the system to the environment (thermal bath) is expressed as [9,18]

$$\Phi_q^{(i)} = \gamma \left(m\langle v_i^2 \rangle - k_B T_i \right), \tag{10}$$

whose first and second terms can be understood as the heating power and the power of heat losses, respectively. The term $\Phi_w^{(i)}$ can be interpreted as the work per unity of time given by

$$\Phi_w^{(i)} = -m\langle v_i \rangle f_i^{\text{ext}}(t). \tag{11}$$

In the absence of external forces all heat flux comes from/goes to the thermal bath.

The entropy S of the system is determined from the Gibbs expression

$$S = -k_B \int P \ln P dx dv. \tag{12}$$

From the FPK equation, one finds that its time derivative has the form of Eq. (1), where the first is identified as the rate of entropy production given by [9,18]

$$\Pi = \frac{mk_B}{\gamma} \sum_{i=1}^N \frac{1}{T_i} \int \frac{J_i^2}{P} dx dv. \tag{13}$$

Note that $\Pi \geqslant 0$ (as expected). Conversely, the second term corresponds to the flux of entropy given by

$$\Phi = -\sum_{i=1}^N \frac{mk_B}{T_i} \int v_i J_i dx dv, \tag{14}$$

or even rewritten as

$$\Phi = k_B \sum_{i=1}^N \frac{\Phi_q^{(i)}}{T_i}. \tag{15}$$

As mentioned previously, Eq. (15) can be alternatively used for evaluated the steady production of entropy, since it depends only on averages $\langle v_i^2 \rangle$ and on the temperatures T_i.

III. EXACT SOLUTION FOR TIME DEPENDENT EXTERNAL FORCES

For simplifying matters, from now on we shall adopt $k_B = 1$. Except in Sec. IV B, all analyses will be restricted to the case of a chain of N particles interacting to its nearest neighbors by means of harmonic forces and also subject to individual and external forces. The expression for the force of ith particle f_i^* then reads

$$f_i^* = -\frac{k}{m}(x_i - x_{i+1}) - \frac{k^*}{m}x_i + f_i^{\text{ext}}(t), \tag{16}$$

$$f_i^* = -\frac{k}{m}(x_i - x_{i-1}) - \frac{k^*}{m}x_i + f_i^{\text{ext}}(t), \tag{17}$$

for particles placed at extremities, $i = 1$ and N, respectively, and

$$f_i^* = -\frac{k}{m}(2x_i - x_{i-1} - x_{i+1}) - \frac{k^*}{m}x_i + f_i^{\text{ext}}(t), \tag{18}$$

for the intermediate ones. Quantities k^* and k are spring constants characterizing individual harmonic forces and the coupling between neighboring particles, respectively. Above expressions can be conveniently rewritten as

$$f_i^* = -Kx_i + Lx_{i+1} + f_i^{\text{ext}}(t), \tag{19}$$

$$f_i^* = -Kx_i + Lx_{i-1} + f_i^{\text{ext}}(t), \tag{20}$$

and, for $i = 1$ and $i = N$, respectively, and

$$f_i^* = -(K+L)x_i + L(x_{i+1} + x_{i-1}) + f_i^{\text{ext}}(t), \tag{21}$$

respectively, where $L = k/m$ and $K = (k + k^*)/m$ for $i \neq 1$ and $i \neq N$.

The time evolution of a generic average of type $\langle g\rangle = \int g(x, v)P(x, v, t)dxdv$ is obtained through the expression

$$\frac{d}{dt}\langle g\rangle = \int g(x, v)\frac{\partial P}{\partial t}dxdv, \tag{22}$$

and by inserting Eq. (6) into Eq. (22) and performing appropriate partial integrations, an explicit equation for the time evolution of $\langle g\rangle$ is evaluated in terms of correlations associated to the positions and velocities. Due to the time dependence on the external forces, the evaluation of averages like $\langle g\rangle$ becomes cumbersome. However, the calculations become quite simpler by rewriting the motion equations in terms of their associate covariances. For instance, let us take for example a generic average $\langle g\rangle = \langle v_i^l x_j^m\rangle$ (with $l \geqslant 1$ and $m \geqslant 1$) with covariance given by $\langle v_i^l x_j^m\rangle_{cv} \equiv \langle v_i^l x_j^m\rangle - \langle v_i^l\rangle\langle x_j^m\rangle$. Unlike the time evolution of $\langle v_i^l x_j^m\rangle$, the time equation for $d\langle v_i^l x_j^m\rangle_{cv}/dt = d\langle v_i^l x_j^m\rangle/dt - \langle x_j^m\rangle d\langle v_i^l\rangle/dt - \langle v_i^l\rangle d\langle x_j^m\rangle/dt$ does not depend explicitly on t. Since the equations for all covariances are linear and time independent, the exact solution is possible for all system sizes N. Finally, having the covariances $\langle v_i^2\rangle_{cv}$ and the averages $\langle v_i\rangle$, the entropy flux can be directly evaluated from the usage of Eqs. (10) and (15).

Below we derive explicit expressions for distinct covariances between the i-th and $i+1$-th particles for a generic chain of N sites:

$$\frac{d}{dt}\langle x_i^2\rangle_{cv} = 2\langle v_i x_i\rangle_{cv}, \tag{23}$$

$$\frac{d}{dt}\langle x_i x_{i+1}\rangle_{cv} = \langle v_i x_{i+1}\rangle_{cv} + \langle v_i x_{i+1}\rangle_{cv}, \tag{24}$$

$$\frac{d}{dt}\langle x_i v_i\rangle_{cv} = \langle v_i^2\rangle_{cv} - K\langle x_i^2\rangle_{cv} + L\langle x_i x_{i+1}\rangle_{cv} - \gamma\langle x_i v_i\rangle_{cv}, \tag{25}$$

$$\begin{aligned}\frac{d}{dt}\langle x_i v_{i+1}\rangle_{cv} = {} & \langle v_i v_{i+1}\rangle_{cv} - K\langle x_i x_{i+1}\rangle_{cv} + L\langle x_i^2\rangle_{cv} \\ & - \gamma\langle x_i v_{i+1}\rangle_{cv},\end{aligned} \tag{26}$$

$$\frac{d}{dt}\langle v_i^2\rangle_{cv} = -2K\langle v_i x_i\rangle_{cv} + 2L\langle x_{i+1} v_i\rangle_{cv} - 2\gamma\langle v_i^2\rangle_{cv} + \Gamma_i, \tag{27}$$

$$\begin{aligned}\frac{d}{dt}\langle v_i v_{i+1}\rangle_{cv} = {} & -K\langle x_i v_{i+1}\rangle_{cv} + L\langle x_{i+1} v_{i+1}\rangle_{cv} \\ & - K\langle x_{i+1} v_i\rangle_{cv} + L\langle x_i v_i\rangle_{cv} - 2\gamma\langle v_i v_{i+1}\rangle_{cv}.\end{aligned} \tag{28}$$

Here, we introduced the rescaled temperature Γ_i defined by $\Gamma_i = 2\gamma T_i/m$ and, thereby for fixed Γ_i's, the achievement of $\langle v_i^2\rangle_{cv}$'s reduces to systems of linear equations.

The time evolution of single averages $\langle v_i\rangle$ and $\langle x_i\rangle$ are also required for obtaining $\langle v_i^2\rangle$, whose expressions read

$$\begin{aligned}\frac{d}{dt}\langle v_i\rangle = {} & -(K+L)\langle x_i\rangle + L(\langle x_{i+1}\rangle + \langle x_{i-1}\rangle) \\ & - \gamma\langle v_i\rangle + f_i^{\text{ext}}(t),\end{aligned} \tag{29}$$

for $i \neq 1, N$ and

$$\frac{d}{dt}\langle v_i\rangle = -K\langle x_i\rangle + L\langle x_{i+1}\rangle - \gamma\langle v_i\rangle + f_i^{\text{ext}}(t), \tag{30}$$

$$\frac{d}{dt}\langle v_i\rangle = -K\langle x_i\rangle + L\langle x_{i-1}\rangle - \gamma\langle v_i\rangle + f_i^{\text{ext}}(t), \tag{31}$$

for $i = 1$ and N, respectively and from Eq. (3), the time evolution of $\langle x_i\rangle$ reads

$$\frac{d}{dt}\langle x_i\rangle = \langle v_i\rangle. \tag{32}$$

Although the previous procedure does not depend on the shape of external forces, from now on we will restrict our analysis to harmonic external forces given by $f_i^{\text{ext}}(t) = f_{0i}\cos(\omega t + \phi)$ with ω and ϕ being its frequency and phase difference (lag), respectively. By assuming that each $\langle x_i\rangle$ has solution of type $\langle x_i\rangle = A_{0i} + A_{1i}\cos\omega t + A_{2i}\sin\omega t$, $\langle v_i\rangle$ becomes $\langle v_i\rangle = \omega[A_{2i}\cos(\omega t) - A_{1i}\sin(\omega t)]$. By inserting above solutions in Eqs. (29) [or Eqs. (30), (31)] and (32), the coefficients A_{1i} and A_{2i} are obtained. It is worth mentioning that coefficients vary with the number of particles and their expressions for two particles are listed in Appendix A.

IV. TWO PARTICLES CASE

A. Oscillating forces

In the first application we analyze a chain of two interacting particles subject to harmonic forces without phase difference (lagless case, $\phi = 0$). From the solution of linear set of equations described in Sec. III, we obtain the following expressions for the covariances:

$$\langle v_1^2 \rangle_{cv} = \frac{\Gamma_1 + \Gamma_2}{4\gamma} + \frac{K\gamma(\Gamma_1 - \Gamma_2)}{4(L^2 + K\gamma^2)}, \tag{33}$$

and

$$\langle v_2^2 \rangle_{cv} = \frac{\Gamma_1 + \Gamma_2}{4\gamma} - \frac{K\gamma(\Gamma_1 - \Gamma_2)}{4(L^2 + K\gamma^2)}. \tag{34}$$

Taking into account that $\langle v_i^2 \rangle = \langle v_i^2 \rangle_{cv} + \langle v_i \rangle^2$ (for $i = 1$ and 2), we see that the entropy flux can be split in two parts,

$$\Phi(t) = \Phi_T + \Phi_f(t), \tag{35}$$

where Φ_T and $\Phi_f(t)$ read

$$\Phi_T = \frac{2\gamma^2}{\Gamma_1}\langle v_1^2 \rangle_{cv} + \frac{2\gamma^2}{\Gamma_2}\langle v_2^2 \rangle_{cv} - 2\gamma, \tag{36}$$

and

$$\Phi_f(t) = \frac{2\gamma^2}{\Gamma_1}\langle v_1 \rangle^2 + \frac{2\gamma^2}{\Gamma_2}\langle v_2 \rangle^2, \tag{37}$$

respectively. The former term can be identified as the entropy flux coming from the thermal reservoirs, whereas the latter is associated to the entropy flux coming from the oscillating forces.

The above expressions can be simplified, acquiring the following form:

$$\Phi_T = \frac{\gamma L^2}{2(L^2 + K\gamma^2)} \frac{(\Gamma_1 - \Gamma_1)^2}{\Gamma_1 \Gamma_2}, \tag{38}$$

and

$$\Phi_f(t) = 2\gamma^2\omega^2 \sum_i \left(\frac{(A_{2i}\cos\omega t - A_{1i}\sin\omega t)^2}{\Gamma_i} \right), \tag{39}$$

respectively, whose coefficients A_{1i} and A_{2i} are shown in Appendix A. Since we are interested in the steady state regime, we shall appeal to Eq. (1), referring to the first and second terms as the entropy production rates $\Pi_T \equiv \Phi_T$ and $\overline{\Pi} \equiv \frac{\omega}{2\pi}\int_0^{2\pi/\omega} \Phi_f(t)dt$, respectively. Once again, $\Pi_T \equiv \Phi_T$ solely depends on the difference of temperatures and are similar to the case with no external forces [18], whereas $\bar{\Pi}$ is related to the time dependent forces averaged over a oscillation period and it is given by

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left[\Gamma_1\left(A_{12}^2 + A_{22}^2\right) + \Gamma_2\left(A_{11}^2 + A_{21}^2\right)\right]}{\Gamma_1\Gamma_2}. \tag{40}$$

By substituting the expressions for A_{1i}'s and A_{2i}'s we finally arrive at the following expression:

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left\{f_{01}^2[\Gamma_2(\gamma^2\omega^2 + (K - \omega^2)^2) + L^2\Gamma_1] + 2f_{01}f_{02}L(K - \omega^2)(\Gamma_1 + \Gamma_2) + f_{02}^2[\Gamma_1(\gamma^2\omega^2 + (K - \omega^2)^2) + L^2\Gamma_2]\right\}}{\Gamma_1\Gamma_2[\gamma^2\omega^2 + (K + L - \omega^2)^2][\gamma^2\omega^2 + (-K + L + \omega^2)^2]}. \tag{41}$$

This is the one of main results of the paper, and we pause to make a few comments: First, from Eq. (40) it follows that $\overline{\Pi}$ is always greater than 0, vanishing when $f_{01} = f_{02} = 0$ and/or $\omega = 0$. Second, in the limit of slow or fast oscillations, $\omega \ll 1$ or $\omega \gg 1$, $\overline{\Pi}$ behaves as

$$\overline{\Pi} \sim \frac{\gamma^2[\Gamma_1(f_{01}K + f_{02}L)^2 + \Gamma_2(f_{01}L + f_{02}K)^2]\omega^2}{\Gamma_1\Gamma_2(K^2 - L^2)^2}, \tag{42}$$

and

$$\overline{\Pi} \sim \left(\frac{f_{01}^2\Gamma_2 + f_{02}^2\Gamma_1}{\Gamma_1\Gamma_2} \right) \frac{\gamma^2}{\gamma^2 + \omega^2}, \tag{43}$$

respectively, implying that $\overline{\Pi}$ vanishes as ω^2 and $1/\omega^2$ for low and large frequencies, respectively.

Third, there is an intermediate frequency ω^* in which $\bar{\Pi}$ is maximum. Although ω^* can be evaluated exactly, it displays an unwieldy dependence on the control parameters. For this reason, we split the analysis in four parts, by inspecting its dependence on the interaction parameters K and L, the dissipation constant γ and the ratio between external forces f_{02}/f_{01}, as depicted in Fig. 1. Whenever ω^* increases by raising K, L and the ratio f_{02}/f_{01}, it decreases when γ is increased. Fourth, when the interaction between particles is "weak", $k \ll k^*$, $\overline{\Pi}$ reduces to the single forced harmonic oscillator expression

$$\overline{\Pi} \sim \frac{\gamma^2\omega^2\left(f_{01}^2\Gamma_2 + f_{02}^2\Gamma_1\right)}{\Gamma_1\Gamma_2[\gamma^2\omega^2 + (K - \omega)^2]}, \tag{44}$$

acquiring the simpler form

$$\overline{\Pi} \sim \frac{\gamma^2\omega^2 f_{01}^2}{\Gamma_1[\gamma^2\omega^2 + (K - \omega)^2]}, \tag{45}$$

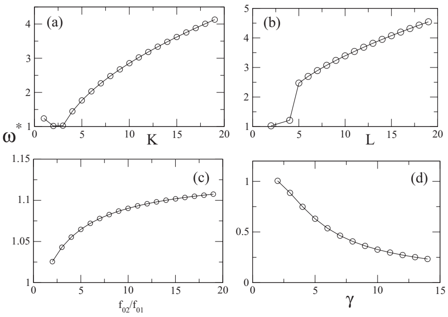

FIG. 1. The frequency ω^* in which $\bar{\Pi}$ is maximum versus distinct control parameters for $\Gamma_1 = 1$ and $\Gamma_2 = 10$. In (a), (b), (c), and (d) we take $\gamma = 1, L = 2$ and $f_{02}/f_{01} = 2$, $\gamma = 1, K = 3$ and $f_{02}/f_{01} = 2$, $\gamma = 1$, $K = 3$ and $L = 2$ and $K = 3, L = 2$ and $f_{02}/f_{01} = 2$, respectively.

as $\Gamma_1 = \Gamma_2$ and $f_{01} = f_{02}$. Fifth and last, in the strong coupling regime, $k \gg k^*$ and $k/m \gg \omega^2$ (or equivalently $L \approx K$ and $L \gg \omega^2$), $\overline{\Pi}$ becomes

$$\overline{\Pi} \sim \left(\frac{\gamma^2}{\gamma^2+\omega^2}\right)\left(\frac{1}{\Gamma_1}+\frac{1}{\Gamma_2}\right)(f_{01}+f_{02})^2, \tag{46}$$

which is independent on strength oscillator parameters K and L.

1. Bilinear form and Onsager coefficients

The shapes of Eqs. (38) and (41) show that the entropy production components can be written as flux-times-force expressions $\Pi_T = \mathcal{J}_T f_T$ and

$$\overline{\Pi} = \mathcal{J}_1^f f_{01} + \mathcal{J}_2^f f_{02}, \tag{47}$$

respectively, where the forces $f_T = 1/\Gamma_1 - 1/\Gamma_2$ and $f_{0i(j)}$ have associated fluxes $\mathcal{J}_T$, $\mathcal{J}_1^f$, and $\mathcal{J}_2^f$ given by

$$\mathcal{J}_T = \frac{\Gamma_1\Gamma_2\gamma L^2}{2(L^2+K\gamma^2)}\left(\frac{1}{\Gamma_1}-\frac{1}{\Gamma_2}\right), \tag{48}$$

and

$$\mathcal{J}_1^f = L_{11}f_{01} + L_{12}f_{02} \quad \text{and} \quad \mathcal{J}_2^f = L_{21}f_{01} + L_{22}f_{02}, \tag{49}$$

respectively. The bilinear form for $\overline{\Pi}$ provides to identify the terms L_{11} and L_{12} as the associated Onsager coefficients given by

$$L_{11} = \frac{\gamma^2\omega^2[\Gamma_2(\gamma^2\omega^2+(K-\omega^2)^2)+L^2\Gamma_1]}{\Gamma_1\Gamma_2[\gamma^2\omega^2+(K+L-\omega^2)^2][\gamma^2\omega^2+(-K+L+\omega^2)^2]}, \tag{50}$$

and

$$L_{12} = \frac{L(K-\omega^2)(\Gamma_1+\Gamma_2)}{\Gamma_1\Gamma_2[\gamma^2\omega^2+(K+L-\omega^2)^2][\gamma^2\omega^2+(-K+L+\omega^2)^2]}, \tag{51}$$

respectively. Analogous expressions are held valid for L_{21} and L_{22} by exchanging 1 ↔ 2. Note that $L_{11} \geqslant 0$ and $L_{22} \geqslant 0$ (as expected). The non-negativity of the entropy production also requires that $4L_{11}L_{22} - (L_{12}+L_{21})^2 \geqslant 0$. To verify this, let us consider $\Gamma_2 = r\Gamma_1$ with r being an arbitrary (non-negative) real number. Such above inequality is always satisfied, since the term

$$\frac{[\gamma^2\omega^2+(K-\omega^2)^2+L^2r][r(\gamma^2\omega^2+(K-\omega^2)^2)+L^2]}{L^2(r+1)^2(K-\omega^2)^2},$$

is greater than $1/4$ for all values of r, K, ω, and γ.

2. Phase difference between harmonic forces

Here, we extend the results from the previous subsection but taking into account a phase difference between external forces $f_1^{\text{ext}}(t)$ and $f_2^{\text{ext}}(t)$. More specifically, $f_1^{\text{ext}}(t)$ has the same expression as previously, but $f_2^{\text{ext}}(t)$ now reads $f_2^{\text{ext}}(t) = f_{02}\cos(\omega t + \phi)$. By repeating afore-described procedures, we assume that $\langle v_i \rangle = w(C_{2i}\cos\omega t - C_{1i}\sin\omega t)$, whose coefficients C_{1i} and C_{2i} are decomposed in two parts: $C_{1i} = A_{1i} + B_{1i}(\phi)$, whose A_{1i} and A_{2i} are the same as Eqs. (A1) and (A2) and the dependence on the phase difference appears only in B_{1i} and B_{2i}, whose explicit coefficients are listed in Appendix B. We then arrive at the following expression for the steady entropy production $\overline{\Pi}$:

$$\overline{\Pi} = \frac{\gamma^2\omega^2\left[\Gamma_1\left(C_{12}^2+C_{22}^2\right)+\Gamma_2\left(C_{11}^2+C_{21}^2\right)\right]}{\Gamma_1\Gamma_2}, \tag{52}$$

which is quite similar to Eq. (40). As in the lagless case, it has three terms with first and third terms being identical to Eq. (41) and the phase difference dependence appearing only in middle term reading

$$\left[\frac{2f_{01}f_{02}L[\gamma\omega(\Gamma_2-\Gamma_1)\sin\phi+(K-\omega^2)(\Gamma_1+\Gamma_2)\cos\phi]}{\Gamma_1\Gamma_2(\gamma^2\omega^2+(K+L-\omega^2)^2)(\gamma^2\omega^2+(-K+L+\omega^2)^2)}\right]. \tag{53}$$

Note that the it reduces to the middle term from Eq. (41) when $\phi = 0$. The position of the maximum and minimum in $\overline{\Pi}$ fulfills the above relation

$$\phi = \tan^{-1}\left[\frac{\gamma\omega(\Gamma_2-\Gamma_1)}{(K-\omega^2)(\Gamma_1+\Gamma_2)}\right]. \tag{54}$$

Note that ϕ depends only on the signs of both $\Gamma_2 - \Gamma_1$ and $K - \omega^2$ and it is independent on L. In particular, in the regime of $\Gamma_2 \gg \Gamma_1 (\Gamma_2 \ll \Gamma_1)$, ϕ is independent on Γ_i's, reading $\pm\gamma\omega/(K-\omega^2)$. Conversely, for fast and slow oscillations, it approaches to zero as $\gamma(\Gamma_1-\Gamma_2)/K\omega(\Gamma_2+\Gamma_1)$ and $\gamma\omega(\Gamma_2-\Gamma_1)/K(\Gamma_2+\Gamma_1)$, respectively. Figure 2 plots $\overline{\Pi}$ versus ϕ for distinct set of values of ω and Γ_i's. Note that the maxima of mean entropy production yields at $\phi \sim 0(\pi)$ for small (large) values of ω and $\phi \to \pi/2$ when $\omega \to \sqrt{K}$. The dependence of extremes clearly follows theoretical predictions from Eq. (54) (see, e.g., panels (a) and (b) in Fig. 2).

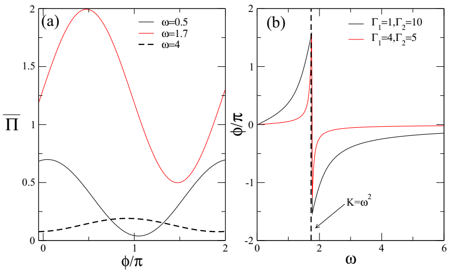

FIG. 2. For distinct frequencies ω's, (a) depicts the average entropy production $\overline{\Pi}$ versus the phase difference ϕ for $\Gamma_1 = 1$, $\Gamma_2 = 10$, $K = 3$, and $\gamma = 1$. For $K = 3$ and $\gamma = 1$ and distinct sets of Γ_1 and Γ_2, (b) shows the positions ϕ of maximum/minimum of entropy production $\overline{\Pi}$ versus ω.

B. Oscillating temperatures

The investigation of systems under oscillating temperature has been reported in several works [30–47], which provides a way of measuring the heat capacity experimentally. Here, we intend to verify the nonequilibrium trademarks of a chain of two interacting particles under time oscillating temperatures. For simplicity, we consider external forces absent. The entropy production can also be evaluated straightforwardly from Eq. (15), but instead the temperature $\Gamma_i(t)$ of the each reservoir is now time dependent $\Gamma_i(t) = \Gamma_{0i} + F_{T_i}\cos(\omega t)$ with Γ_{0i} and F_{T_i} being the reference temperature and the strength of temperature driving, respectively.

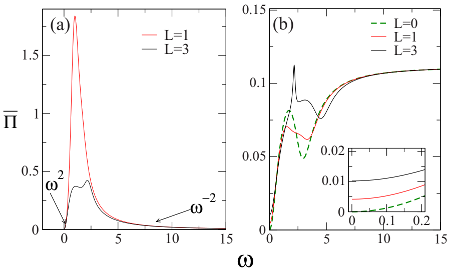

FIG. 3. (a) and (b) depict the steady entropy production rate $\overline{\Pi}$ versus frequency driving ω for time dependent oscillating forces and temperatures, respectively. In all cases we take $\gamma = 1$, $K = 2$, $\Gamma_1 = \Gamma_2 = 10$, and $f_{02} = 2f_{01} = 4$ [(a)] and $F_{T_2} = 2F_{T_1} = 4$ [(b)]. Inset: The steady $\overline{\Pi}$ for distinct L's for low ω.

Although such a problem is exactly solvable [see, e.g., Fig. 3(b)] and reduces to the findings from Ref. [19] when $\Gamma_{01} = \Gamma_{02}$ and $L = 0$, the expression for $\overline{\Pi}$ is much more complex than previous cases and involves many terms related to distinct powers of interaction parameters K, L and driving frequency ω. For this reason, our analysis will be carried out close to equilibrium regime, in which a linear treatment can be performed. More specifically, we take both reference temperatures to be equal $\Gamma_{01} = \Gamma_{02} = \Gamma_0$ and the driving strengths are sufficiently low $F_{T_i} \ll \Gamma_0$. In such case, the entropy production $\overline{\Pi}$ can also be written down in the bilinear form $\overline{\Pi} = \mathcal{J}_{T_1}F_{T_1} + \mathcal{J}_{T_2}F_{T_2}$, where the fluxes $\mathcal{J}_{T_1}$ and $\mathcal{J}_{T_2}$ read

$$\mathcal{J}_{T_1} = L_{T_1,T_1}F_{T_1} + L_{T_1,T_2}F_{T_2}, \tag{55}$$

and

$$\mathcal{J}_{T_2} = L_{T_2,T_1}F_{T_1} + L_{T_2,T_2}F_{T_2}, \tag{56}$$

respectively, where L_{T_i,T_j} are the associated Onsager coefficients given by

$$L_{T_1,T_1} = \frac{\gamma}{2\Gamma_0^2}\left(\frac{\sum_{\ell=0}^{9} B_\ell\, \omega^{2\ell}}{\sum_{\ell=0}^{9} G_\ell\, \omega^{2\ell}}\right), \tag{57}$$

and

$$L_{T_1,T_2} = \frac{-4\gamma^3 L^2}{\Gamma_0^2}\left(\frac{\sum_{\ell=0}^{6} A_\ell\, \omega^{2\ell}}{\sum_{\ell=0}^{9} G_\ell\, \omega^{2\ell}}\right), \tag{58}$$

respectively, where $L_{T_1,T_1} = L_{T_2,T_2}$ and $L_{T_1,T_2} = L_{T_2,T_1}$ and coefficients A_i's, B_i's, and G_i's solely depend on the parameters γ and $L = 2K$ and are listed in Appendix C.

We pause again to make some few comments: First, in the limit of slow and fast frequencies, $\overline{\Pi}$ approaches to the following expressions:

$$\overline{\Pi} \sim \frac{4\gamma^3 L^2 A_0}{\Gamma_0^2 G_0}\left(F_{T_1} - F_{T_2}\right)^2, \tag{59}$$

and

$$\overline{\Pi} \sim \frac{\gamma}{2\Gamma_0^2}\left(F_{T_1}^2 + F_{T_2}^2\right), \tag{60}$$

respectively. They contrast with the oscillating forced case, since are independent on ω and different from zero in both extreme cases. Whenever it depends on L for low oscillations, the entropy production is independent on the coupling for fast oscillations. Finally, for strong interaction strength, $L \gg 1$ and $L \gg \omega^2$, $\overline{\Pi}$ reads

$$\overline{\Pi} \sim \frac{\gamma}{4\Gamma_0^2(\gamma^2 + \omega^2)}\left[\gamma^2\left(F_{T_1} - F_{T_2}\right)^2 + 2\omega^2\left(F_{T_1}^2 + F_{T_2}^2\right)\right], \tag{61}$$

which is also independent on L. We close this section by comparing, in Fig. 3(a) and 3(b) the steady entropy production behaviors versus the frequency driving ω for both oscillating temperature and forces (obtained from the exact solution). They exhibit meaningfully different dependence on ω, even for extreme ω. Whenever $\overline{\Pi}$ vanishes for $\omega \ll 1$ and $\omega \gg 1$ in the case of time oscillating forces, it reaches constant values for temperature drivings, in accordance with asymptotic expressions Eqs. (59) and (60), respectively, obtained from the linear regime approximation.

V. MORE THAN TWO PARTICLES

In this section we present the main results for long chains of oscillators. In real systems, due to the lattice imperfections and impurities, the difference of temperature between particles placed at extremities is responsible for a transport of heat following Fourier's law. More concretely, it states that the heat

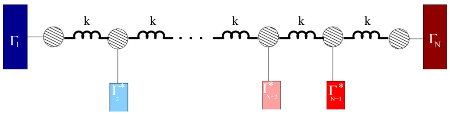

FIG. 4. Schematic diagram consisting of a one-dimensional chain of N harmonic oscillators with individual and coupling interactions k^* and k, respectively. Γ_1 and Γ_N denote the cold and hot bath temperatures, respectively, whereas the self-consistent reservoirs range from Γ_2^* to Γ_{N-1}^*. Each intermediate particle is also subject to an external force $f_i^{\rm ext}(t)$. The usage of our protocol leads to intermediate temperatures changing linearly from Γ_1 to Γ_N, consistent to a flux of heat along the chain, symbolized by the color gradient from the red to the blue reservoirs.

current is proportional to the inverse of the length of the chain given by

$$\mathcal{J}_T = -\kappa \frac{dT}{dx}, \tag{62}$$

where κ is the heat conductivity. In the case of a finite difference of temperatures ΔT, it follows that $\mathcal{J}_T \sim 1/N$ and thereby the heat flux is proportional to the inverse of the system size. Obtaining Fourier's law from microscopic models have attracted great interest in the last years [49–52]. In principle, one could suppose that a linear chain of particles interacting through harmonic forces in contact with two temperature reservoirs placed at extremities would lead to a heat flux obeying Fourier's law. However, this is not the case [53]. Among the distinct approaches aimed at obtaining a heat flux inversely proportional to the system chain, we mention the self-consistent protocol proposed by Bosterli *et al.* [48]. It consists of baths acting on all sites, but intermediate temperatures are chosen self-consistently in such a way that they do not exchange any heat with the system in the steady state, ensuring that heat flux is only due to particles placed at extremities. Here, we take a similar approach by Bosterli *et al.*, in which each intermediate temperature is chosen so that it equals to the variance $\langle v_i^2\rangle_{cv}$, $\Gamma_i^* = 2\gamma\langle v_i^2\rangle_{cv}$. Although it reduces to the original protocol when external forces are absent, here all self-consistent reservoirs are expected to produce entropy coming from external forces. Figure 4 illustrates a linear chain in the presence of thermal and self-consistent baths.

In order to compare the distinct sources of dissipation, thermal and time oscillating forces, we will consider that particles placed at extremities are not subjected to external forces. Thereby, under the above choice of the intermediate Γ_i's, the flux of entropy becomes

$$\Phi(t) = \Phi_T + \Phi_f(t), \tag{63}$$

where Φ_T read

$$\Phi_T = \frac{2\gamma^2}{\Gamma_1}\left\langle v_1^2\right\rangle_{cv} + \frac{2\gamma^2}{\Gamma_N}\left\langle v_N^2\right\rangle_{cv} - 2\gamma, \tag{64}$$

and $\Phi_f(t)$ is a sum of individual contributions

$$\Phi_f(t) = 2\gamma^2\left(\frac{\langle v_1\rangle^2}{\Gamma_1} + \sum_{i=2}^{N-1}\frac{\langle v_i\rangle^2}{\Gamma_i^*} + \frac{\langle v_N\rangle^2}{\Gamma_N}\right). \tag{65}$$

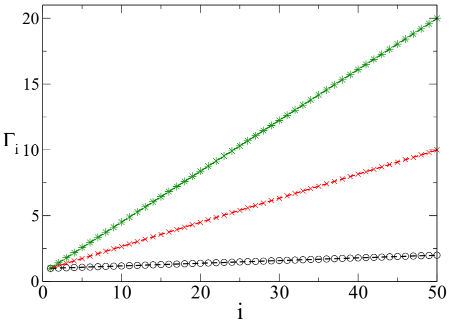

FIG. 5. For a chain of $N = 50$ particles with $K = 2, L = 1, \gamma = 1$, and $\omega = 1$, the rescaled temperatures Γ_i's versus the position of the ith site for three set of temperatures (Γ_1, Γ_N). The intermediate temperatures are calculated according to the prescription $\Gamma_i^* = 2\gamma\langle v_i^2\rangle_{cv}$.

Despite the absence of external forces for extreme particles, the averages $\langle v_1\rangle$ and $\langle v_N\rangle$ present oscillating behavior coming from couplings with neighboring particles [see, e.g., Eqs. (30) and (31)].

In all cases, $\Pi_T = \Phi_T$ can be written as for the two particles case

$$\Pi_T = \mathcal{J}_T f_T, \tag{66}$$

where the thermodynamic force f_T and its associate flux $\mathcal{J}_T$ read $f_T = 1/\Gamma_1 - 1/\Gamma_N$ and $\mathcal{J}_T = \kappa(\Gamma_N - \Gamma_1)/N$, respectively. Thereby, the expression for Π_T becomes

$$\Pi_T = \frac{\kappa}{N}\frac{(\Gamma_N - \Gamma_1)^2}{\Gamma_1\Gamma_N}. \tag{67}$$

Since the thermal conduction coefficient κ is finite (it depends only on parameters Γ_1, Γ_N, K and L), the entropy production Π_T decays as N^{-1} [see, e.g., Fig. 6(b)].

A. Three particles

Here, we derive explicit results for a chain of $N = 3$ particles. In such case, Eq. (65) becomes

$$\Phi_f(t) = \frac{2\gamma^2}{\Gamma_1}\langle v_1\rangle^2 + \frac{2\gamma^2}{\Gamma_2^*}\langle v_2\rangle^2 + \frac{2\gamma^2}{\Gamma_3}\langle v_3\rangle^2, \tag{68}$$

and the entropy production Π_T due to thermal reservoirs has the shape of Eq. (66) with $\mathcal{J}_T$ given by

$$\mathcal{J}_T = \frac{\Gamma_1\Gamma_3\gamma L^2(2\gamma^2K + L^2)}{2[L^2 + \gamma^2(4K - 2L)][L^2 + \gamma^2(K + L)]} f_T. \tag{69}$$

Once again, $\Pi_T \geqslant 0$, since $4K - 2L = 2(k + 2k^*)/m$. Using the motion equations we arrive at the following expression for $\overline{\Pi}$:

$$\overline{\Pi} = \frac{f_{02}^2\gamma^2\omega^2[\Gamma_1\Gamma_3(\gamma^2\omega^2 + (K-\omega^2)^2) + L^2\Gamma_2^*(\Gamma_1+\Gamma_3)]}{\Gamma_1\Gamma_2^*\Gamma_3[\gamma^2\omega^2 + (K+2L-\omega^2)^2][\gamma^2\omega^2 + (-K+L+\omega^2)^2]}, \tag{70}$$

which is strictly positive and vanishes when f_{02} and/or ω are equal to zero. Also, in the regime of slow and fast oscillations, $\overline{\Pi}$ exhibit similar dependencies on ω to the two particles case

$$\overline{\Pi} \sim \left(\frac{K^2}{\Gamma_2^*} + \frac{L^2(\Gamma_1+\Gamma_3)}{\Gamma_1\Gamma_3}\right)\frac{\gamma^2\omega^2 f_{02}^2}{(K+2L)^2(-K+L)^2}, \tag{71}$$

for $\omega \ll 1$ and

$$\overline{\Pi} \sim \frac{\gamma^2 f_{02}^2}{\Gamma_2^*}\frac{1}{\omega^2}, \tag{72}$$

for $\omega \gg 1$, respectively, implying that for such latter limit the entropy production is independent on extreme temperatures. For strong couplings between particles, $L \approx K \gg \omega^2$, $\overline{\Pi}$ approaches to

$$\overline{\Pi} \sim \frac{\gamma^2}{\gamma^2+\omega^2}\left(\frac{1}{\Gamma_1} + \frac{1}{\Gamma_2^*} + \frac{1}{\Gamma_3}\right)f_{02}^2, \tag{73}$$

which is quite similar to Eq. (46) [for $N = 2$] and it is independent on the interaction strengths.

B. The limit of long particle chains

All results obtained for $N = 3$ particles can be straightforwardly extended for long chains. However, it becomes very cumbersome to obtain simplified expressions for $\overline{\Pi}$ in such cases. For this reason, we will restrict the next analysis for specific values of control parameters. Figure 5 shows, for a chain of $N = 50$ particles and three sets of temperatures (Γ_1, Γ_N), the temperature profiles calculated from the self-consistent protocol. In all cases, the set of intermediate temperatures changes linearly from Γ_1 to Γ_N, consistent to a flux of heat along the chain from the hot to the cold reservoirs.

Figure 6(a) compares the individual entropy production contributions for distinct system sizes for $f_{02} = f_{03} = \cdots = f_{0N-1}$. Since external forces are equally presented in all intermediate particles, the entropy production associated to self-consistent baths increases linearly with N. Also, panel (a) depicts the existence of two regimes. For small chains the thermal reservoir contribution Π_T dominates over the self-consistent ones $\overline{\Pi}$, whereas $\overline{\Pi}$ wins over Π_T upon N is increased. In the limit $N \to \infty$ [see e.g., panel (b)], only the contributions from self-consistent reservoirs prevail, in consonance with Fourier's law [Eq. (67)]. Finally, it is worth emphasizing two distinct linear behaviors of $\overline{\Pi}$. It arises from the particles closer to the thermal reservoirs providing more contribution for the entropy production for small chains than for large ones.

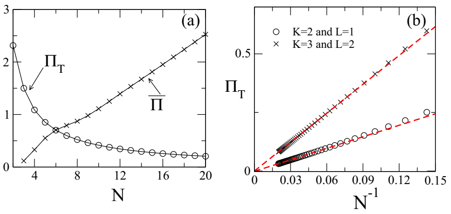

FIG. 6. For $\Gamma_1 = 1$ and $\Gamma_N = 10$, (a) depicts the individual entropy production contributions from the thermal and self-consistent baths versus N for $K = 3$, $L = 2$, and $\omega = 1.5$. In (b) the behavior of entropy production from the thermal reservoirs Π_T vs N^{-1}.

VI. CONCLUSIONS

The nonequilibrium properties of linear chains of Brownian particles were analyzed via stochastic thermodynamics. Expressions for the heat flux, entropy production, and allied quantities were exactly obtained. The regimes of short and long chains were detailed inspected. In the former case the entropy production was derived as bilinear functions of fluxes and forces, from which the associated Onsager coefficients depend on interaction couplings and frequency drivings. Reciprocal relations were also obtained. The limit of long chains was studied by means of a self-consistent protocol for choosing intermediate temperatures. The entropy production is a sum of two terms: one coming from the real baths and the other from the self-consistent reservoirs. Whenever the former dominates for short chains, the latter contribution prevails for long ones. The contribution from the thermal reservoirs is responsible to heat flux according to Fourier's law.

As a final comment, it is worth to discuss future extensions of the present study. The inclusion of both temperature and external force drivings in harmonic chains should be interesting, in order to compare not only the structure of entropy production but also the Onsager coefficients. Also, the investigation of other kinds of drivings, such as the time discrete drivings should also be interesting in order to compare with sinusoidally time dependent ones.

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APPENDIX A: OBTAINING THE COEFFICIENTS A_{ij} FOR $N = 2$ PARTICLES CASE WITH NO PHASE DIFFERENCE

Here, we show explicit expressions for the coefficients A_{ij}'s for the two particles case subject to oscillating forces.

The index i stands for the ith particle ($i = 1, 2$):

$$A_{1i} = \frac{f_{0i}(K-\omega^2)[\gamma^2\omega^2 + (K-\omega^2)^2 - L^2] + f_{0j}L[-\omega^2(\gamma^2+2K) + K^2 - L^2 + \omega^4]}{[\gamma^2\omega^2 + (K+L-\omega^2)^2][\gamma^2\omega^2 + (-K+L+\omega^2)^2]} \tag{A1}$$

and

$$A_{2i} = \frac{\gamma\omega[f_{0i}(\gamma^2\omega^2 + (K-\omega^2)^2 + L^2) + 2f_{0j}L(K-\omega^2)]}{(\gamma^2\omega^2 + (K+L-\omega^2)^2)(\gamma^2\omega^2 + (-K+L+\omega^2)^2)}. \tag{A2}$$

Having the A_{ij}'s, the steady entropy production $\overline{\Pi}$ is straightforwardly evaluated.

APPENDIX B: OBTAINING THE COEFFICIENTS B_{ij} FOR $N = 2$ PARTICLES CASE AND PHASE DIFFERENCE

Here, we show explicit expressions for the coefficients B_{ij}'s for the two particles subject to phase difference between oscillating forces:

$$B_{11} = \frac{f_{02}L((\cos\phi - 1)(-\omega^2(\gamma^2+2K) + K^2 - L^2 + \omega^4) + 2\gamma\omega(K-\omega^2)\sin\phi)}{(\gamma^2\omega^2 + (K+L-\omega^2)^2)(\gamma^2\omega^2 + (-K+L+\omega^2)^2)}, \tag{B1}$$

$$B_{21} = \frac{f_{02}L(\sin\phi(\gamma^2\omega^2 - (K-\omega^2)^2 + L^2) + 2\gamma\omega(K-\omega^2)(\cos\phi - 1))}{(\gamma^2\omega^2 + (K+L-\omega^2)^2)(\gamma^2\omega^2 + (-K+L+\omega^2)^2)}, \tag{B2}$$

$$B_{12} = \frac{f_{02}\gamma\omega\sin\phi(\gamma^2\omega^2 + (K-\omega^2)^2 + L^2) + f_{02}(K-\omega^2)(\cos\phi - 1)(\gamma^2\omega^2 + (K-\omega^2)^2 - L^2)}{(\gamma^2\omega^2 + (K+L-\omega^2)^2)(\gamma^2\omega^2 + (-K+L+\omega^2)^2)}, \tag{B3}$$

and

$$B_{22} = \frac{f_{02}(\omega^2 - K)\sin\phi(\gamma^2\omega^2 + (K-\omega^2)^2 - L^2) + f_{02}\gamma\omega(\cos\phi - 1)(\gamma^2\omega^2 + (K-\omega^2)^2 + L^2)}{(\gamma^2\omega^2 + (K+L-\omega^2)^2)(\gamma^2\omega^2 + (-K+L+\omega^2)^2)}, \tag{B4}$$

respectively. Note that all of them vanish as $\phi = 0$, restoring the expressions (A1) and (A2), respectively.

APPENDIX C: OBTAINING THE COEFFICIENTS A_i's, B_i's, AND G_i's FOR $N = 2$ PARTICLES CASE AND OSCILLATING TEMPERATURE

Here, we show explicit expressions for the coefficients A_i's, B_i's, and G_i's for the two particles case and time oscillating temperatures:

$$A_0 = 2304L^5(2\gamma^2 + L),$$

$$A_1 = -128L^3(-7\gamma^4 + 58\gamma^2L + 123L^2),$$

$$A_2 = 16L(8\gamma^6 - 50\gamma^4L + 34\gamma^2L^2 + 931L^3),$$

$$A_3 = 4(-11\gamma^6 + 78\gamma^4L + 319\gamma^2L^2 - 1606L^3),$$

$$A_4 = -3(17\gamma^4 + 82\gamma^2L - 548L^2),$$

$$A_5 = 3\gamma^2 - 214L,$$

$$A_6 = +10,$$

$$B_0 = 36864\gamma^4L^7 + 18432\gamma^2L^8,$$

$$B_1 = 31744\gamma^6L^5 + 112640\gamma^4L^6 + 27648\gamma^2L^7 + 36864L^8,$$

$$B_2 = 4608\gamma^8L^3 + 18176\gamma^6L^4 - 77056\gamma^4L^5 + 203904\gamma^2L^6 - 172032L^7,$$

$$B_3 = 128\gamma^{10}L + 608\gamma^8L^2 - 6592\gamma^6L^3 + 85920\gamma^4L^4 - 230720\gamma^2L^5 + 269824L^6,$$

$$B_4 = 16\gamma^{10} - 64\gamma^8L + 4536\gamma^6L^2 - 34864\gamma^4L^3 + 125488\gamma^2L^4 - 170496L^5,$$

$$B_5 = 56\gamma^8 - 792\gamma^6L + 8112\gamma^4L^2 - 34928\gamma^2L^3 + 54288L^4,$$

$$B_6 = 73\gamma^6 - 928\gamma^4L + 5120\gamma^2L^2 - 9536L^3,$$

$$B_7 = 43\gamma^4 - 376\gamma^2L + 936L^2,$$

$$B_8 = 11\gamma^2 - 48L,$$

$$B_9 = 1,$$

$$G_0 = 147456\gamma^6L^6 + 147456\gamma^4L^7 + 36864\gamma^2L^8,$$

$$G_1 = 50176\gamma^8L^4 - 94208\gamma^6L^5 + 262144\gamma^4L^6 - 24576\gamma^2L^7 + 36864L^8,$$

$$G_2 = 3584\gamma^{10}L^2 - 23552\gamma^8L^3 + 166400\gamma^6L^4 - 323584\gamma^4L^5 + 384512\gamma^2L^6 - 172032L^7,$$

$$G_3 = 64\gamma^{12} - 768\gamma^{10}L + 14720\gamma^8L^2 - 77312\gamma^6L^3 + 262528\gamma^4L^4 - 399872\gamma^2L^5 + 269824L^6,$$

$$G_4 = 240\gamma^{10} - 2688\gamma^8L + 24672\gamma^6L^2 - 96960\gamma^4L^3 + 200592\gamma^2L^4 - 170496L^5,$$

$$G_5 = 348\gamma^8 - 3504\gamma^6L + 20024\gamma^4L^2 - 52736\gamma^2L^3 + 54288L^4,$$

$$G_6 = 245\gamma^6 - 2064\gamma^4L + 7424\gamma^2L^2 - 9536L^3,$$

$$G_7 = 87\gamma^4 - 528\gamma^2L + 936L^2,$$

$$G_8 = 15\gamma^2 - 48L,$$

$$G_9 = 1.$$

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[1] I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, 2nd ed. (Wiley, New York, 1961).

[2] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).

[3] T. Tomé and M. J. de Oliveira, *Stochastic Dynamics and Irreversibility* (Springer, Cham, 2015).

[4] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997).

[5] O.-P. Saira, Y. Yoon, T. Tanttu, M. Möttönen, D. V. Averin, and J. P. Pekola, Phys. Rev. Lett. **109**, 180601 (2012).

[6] K. Proesmans and C. Van den Broeck, Europhys. Lett. **119**, 20001 (2017).

[7] A. C. Barato and U. Seifert, Phys. Rev. Lett. **114**, 158101 (2015).

[8] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).

[9] T. Tomé and M. J. de Oliveira, Phys. Rev. E **91**, 042140 (2015).

[10] C. Van den Broeck and M. Esposito, Physica A **418**, 6 (2015).

[11] K. Proesmans, B. Cleuren, and C. Van den Broeck, Phys. Rev. Lett. **116**, 220601 (2016).

[12] C. E. Fernandez Noa, P. E. Harunari, M. J. de Oliveira, and C. E. Fiore, Phys. Rev. E **100**, 012104 (2019).

[13] T. Herpich, J. Thingna, and M. Esposito, Phys. Rev. X **8**, 031056 (2018).

[14] T. Herpich and M. Esposito, Phys. Rev. E **99**, 022135 (2019).

[15] M. Esposito and C. Van den Broeck, Phys. Rev. E **82**, 011143 (2010).

[16] S. Ray and A. C. Barato, Phys. Rev. E **96**, 052120 (2017).

[17] T. Tomé, Braz. J. Phys. **36**, 1285 (2006).

[18] T. Tomé and M. J. de Oliveira, Phys. Rev. E **82**, 021120 (2010).

[19] C. E. Fiore and M. J. de Oliveira, Phys. Rev. E **99**, 052131 (2019).

[20] C. Van den Broeck and M. Esposito, Phys. Rev. E **82**, 011144 (2010).

[21] A. Rosas, C. Van den Broeck, and K. Lindenberg, Phys. Rev. E **94**, 052129 (2016).

[22] P. Pradhan and U. Seifert, Europhys. Lett. **89**, 37001 (2010).

[23] C. Kwon, J. D. Noh, and H. Park, Phys. Rev. E **83**, 061145 (2011).

[24] Y. Tang, R. Yuan, J. Chen, and P. Ao, Phys. Rev. E **91**, 042108 (2015).

[25] K. Proesmans and C. Van den Broeck, Chaos **27**, 104601 (2017).

[26] K. Brandner, K. Saito, and U. Seifert, Phys. Rev. X **5**, 031019 (2015).

[27] K. Proesmans, B. Cleuren, and C. Van den Broeck, J. Stat. Mech.: Theory Exp. (2016) 023202.

[28] K. Proesmans and C. E. Fiore, Phys. Rev. E **100**, 022141 (2019).

[29] B. Cleuren and K. Proesmans, Physica **A**, 122789 (2019).

[30] G. W. H. Höhne, W. F. Hemminger, and H.-J. Flammersheim, *Differential Scanning Calorimetry* (Springer, Berlin, 2003).

[31] Y. Kraftmakher, *Modulation Calorimetry, Theory and Applications* (Springer, Berlin, 2004).

[32] L. P. Filippov, Int. J. Heat Mass Transfer. **9**, 681 (1966).

[33] P. F. Sullivan and G. Seidel, Phys. Rev. **173**, 679 (1968).

[34] H. Gobrecht, K. Hamann, and G. Willers, J. Phys. E: Sci. Instrum. **4**, 21 (1971).

[35] N. O. Birge and S. R. Nagel, Phys. Rev. Lett. **54**, 2674 (1985).

[36] P. S. Gill, S. R. Sauerbrunn, and M. Reading, J. Therm. Anal. **40**, 931 (1993).

[37] J. E. K. Schawe, Thermochim. Acta **260**, 1 (1995).

[38] Y.-H. Jeong, Thermochim. Acta **304–305**, 67 (1997).

[39] J. E. K. Schawe, Thermochim. Acta **304–305**, 111 (1997).

[40] G. W. H. Höhne, Thermochim. Acta **304–305**, 121 (1997).

[41] S. L. Simon and G. B. McKenna, J. Chem. Phys. **107**, 8678 (1997).

[42] K. J. Jones, I. Kinshott, M. Reading, A. A. Lacey, C. Nikolopoulos, and H. M. Pollock, Thermochim. Acta **304–305**, 187 (1997).

[43] H. Baur and B. Wunderlich, J. Therm. Anal. **54**, 437 (1998).

[44] P. Claudy and J. M. Vignon, J. Therm. Anal. Calorim. **60**, 333 (2000).

[45] J.-L. Garden, Thermochim. Acta **452**, 85 (2007).

[46] J.-L. Garden and J. Richard, Thermochim. Acta **461**, 57 (2007).

[47] J.-L. Garden, J. Richard, and Y. Saruyama, J. Therm. Anal. Calorim. **94**, 585 (2008).

[48] M. Bolsterli, M. Rich, and W. M. Visscher, Phys. Rev. A **1**, 1086 (1970).

[49] G. T. Landi and M. J. de Oliveira, Phys. Rev. E **87**, 052126 (2013).

[50] M. J. de Oliveira, J. Phys. A **50**, 335001 (2017).

[51] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).

[52] A. Dhar, Adv. Phys. **57**, 457 (2008).

[53] Z. Rieder, J. L. Lebowitz, and E. Lieb, J. Math. Phys. **8**, 1073 (1967).