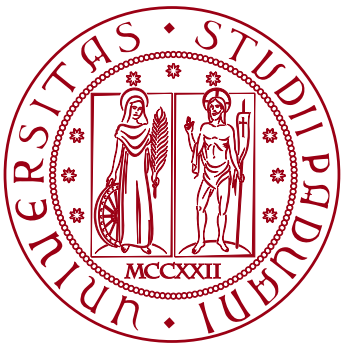

UNIVERSITÀ DEGLI STUDI DI PADOVA

Dipartimento di Fisica e Astronomia "Galileo Galilei"

Corso di Laurea in Fisica

Tesi di Laurea

Strain fluctuation in a non-isothermal solid

Relatrice

Dr.ssa Livia Conti

Correlatore

Dr. Gianmaria Falasco

Laureando

Giorgio Mentasti

Anno Accademico 2018/2019

Abstract

In this thesis we use nonequilibrium thermodynamics tools in order to investigate spontaneous vibration fluctuations of continuous, elastic, conductive and dissipative solids in and out of equilibrium states. In particular we want to advance with respect to previous theoretical models, based on global equilibrium thermodynamics, and to obtain the strain fluctuations of displacement under the assumption of local equilibrium. We develop explicit calculations for 1-dimensional solids under constant thermal gradients. Ultimate goal of the research which inspires this work, is the assessment of thermal noise of Advanced VIRGO, Advanced LIGO and next generation of gravitational wave interferometers under realistic nonequilibrium assumptions.

Ringrazio la mia Relatrice ed il mio Correlatore per il supporto che mi hanno sempre dimostrato durante il presente lavoro.

Contents

1 Introduction

1.1 Mechanical oscillator as a toy model

An oscillator consists in a physical system which responds (anti)linearly in the displacement to an external force that displaces it from its equilibrium position. This is equivalent to a wide range of systems and its mathematical model represents a first approximation to phenomena in different fields (as LC and RLC circuits in electronics, nuclear vibrations and so on). In mechanics it can represent vibrations of atoms in molecular boundaries, or base units of solid lattices around their equilibrium position in the potential field of the solid. Another relevant case where a system can be studied on the basis of mechanical oscillators is the continuous model of a finite solid.

At this point for a complete picture that takes also into account the effect of non harmonic potentials, i.e. more realistic model of the solid, explaining for instance not vanishing thermal expansion coefficients, one has to further consider that real solids are subjected to thermoelastic effects, and that these solids are conductive and dissipative. This implies to rewrite the differential equations for the motion, and it becomes necessary to introduce temperature as a new variable of the equations. The analytical solution of the coupled differential equations describing elasticity and thermal conduction can be hardly computed and, in the first approximation, the temperature field can be taken as constant in the system. This approximation, called (thermal) equilibrium hypothesis, is valid for lot of cases, where temperature disomogeneity is small and, under equilibrium hypothesis at a given temperature, the fluctuation-dissipation-theorem (FDT) can be proven; this theorem predicts a precise relation between the damping coefficient in the equation of motion and the displacement autocorrelation [4].

However, a global form of thermal equilibrium hypothesis shall not be valid in all systems where a thermal gradient is present. It has been shown that spontaneous thermal fluctuations depend on heat fluxes in a way that can not be predicted by a natural extension of equilibrium thermodynamics [8]. For instance at micro scales, the authors of [10] studied cantilevers subjected to a strong thermal gradient at their boundaries, imposed by heating their free tip with a laser and leaving the other extremity fixed at environment temperature. It has been shown that thermal fluctuations do not depend only on the mean temperature of the cantilever, but also on thermal fluxes and temperature gradients involved, in such a way that is not enough to simply extend global equilibrium theory in order to predict displacement fluctuations dependence on temperature.

Another relevant field where it would be important to estimate carefully the thermal noise is the VIRGO interferometer and other gravitational waves detectors. In this case, the laser power absorbed in the mirrors and substrates poses thermal gradient in the substrate themselves and in the fibres that support them: also in this case the current modelling for the thermal noise is based on equilibrium thermodynamics but it unclear if this approximation is valid. Indeed, in all these cases we introduced in the equations of motion of the system a dissipative term, that couples the differential equation for displacement (of cantilever's tip from its equilibrium position, for instance) with the one for temperature field of the solid. This work aims at addressing the issue of esteeming spontaneous vibration fluctuations when the hypothesis is broken.

1.2 Solid dynamics

An homogeneous solid can be schematized as a set of atoms bounded together by some forces, that can be easily assumed to be acting between pairs of atoms. These forces are considered repulsive for short distances between atoms, while they become attractive for higher values of

separation between them, strongly decreasing in modulus. It is computationally impossible to study the whole dynamics of the macroscopic system by considering the whole equations for the atoms involved. Indeed, we can schematize the solid as a set of some elements of matter, called mesoscopic particles, which are large enough to assume to be continuous distributions of atoms, but small enough to think that some thermodynamics proprieties, describing the microscopic degrees of freedom, are constant in their volume. We can further consider that the forces acting on atoms behave similarly on these subsets of the solid, and the first assumption is that this interaction is among contiguous mesoscopic particles. In the first approximation, the shape of this kind of forces is harmonic, and we take this hypothesis in our subsequent analysis; this is justified because we are considering only displacements small enough from equilibrium.

We can argue whether a perfect solid, where all the mesoscopic particles are bounded in a rigid scheme and whose dynamics are coupled each other with just harmonic forces, does correspond to a real solid. Indeed, at room temperatures and in general for any nonvanishing temperature T, the atoms constituting the solid have kinetic energy, and one in principle should take into account these contributions to the total energy of the system. So, it is computationally impossible and it is why we introduce temperature as a new mesoscopic variable of the system, that encodes the information about these microscopic degrees of freedom where energy can be stored. Since energy distribution between these microscopic degrees of freedom follows a statistical distribution, the introduction of temperature as a variable for our system implies that the equations we write to describe it need to include some stochastic terms.

From a physical point of view it means that we are introducing some thermodynamic parameters for the solid, such as heat conduction and damping. The meaning of these new parameters can be understood imagining that the mesoscopic particles live in a thermal bath (as brownian particles do in an homogeneous fluid for instance), with some generic temperature profile, depending on position in the volume of the solid, in such a way that each mesoscopic particle at position $\vec{r}$ lays in a locally uniform thermal bath at temperature $T(\vec{r})$. The ways this bath acts on the leading dynamics of this system are two. The first one is a damping effect on the mesoscopic particles, since they interact thermo-mechanically with the thermal bath in their motion, which means that the bath can absorb energy from the mesoscopic particles. The second is a stochastic force, due to random collisions of the (small but still discrete) particles which constitute the thermal bath with the mesoscopic particles of the solid. Since our solid is thermally conductive, we have also to treat the dynamics for the thermal bath, and in particular for its temperature field at local level: the main contribution to this dynamics is due to thermal conductivity, caused by variations of temperature at a local level due to the energy exchanged with the thermal bath by mesoscopic particles in friction with it.

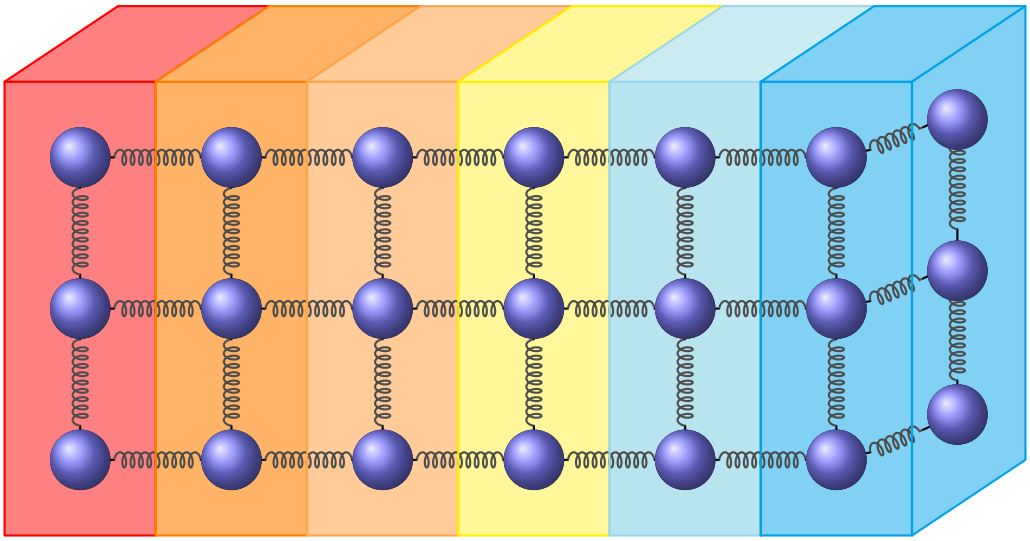

Figure 1: Sketch of the solid, where the mesoscopic particles live in a thermal bath with a position-dependent temperature field $T(\vec{r})$.

1.3 Purposes and steps of the work

The aim of this thesis is to solve the coupled stochastic differential equations for the local displacement and temperature field of an elastic, conductive and dissipative solid subject to heat fluxes, with an approach similar to what has been done for harmonic chains [9]. This steady state out of equilibrium problem is addressed under the assumption of local equilibrium, i.e. the assumption of a locally uniform thermal bath in equilibrium at temperature $T(\vec{r})$ for each point of the solid at the position $\vec{r}$. General solutions for the local displacement is obtained. Later we will introduce further assumptions in order to solve numerically a specific case of this problem, a 1-dimensional solid under under a constant temperature profile, showing how this new approach is consistent with previous models and is able to predict new physics.

In the next chapter we recall some fundamental concepts in the theory of elasticity and statistical mechanics building on the work of Landau [3], and the results of Langevin theory [2] for a mechanical oscillator as a didactic example. In particular we introduce the notion of stochastic Langevin force obtaining a form of fluctuation-dissipation theorem for the harmonic oscillator and, later, the definition of autocorrelation for displacement field. In chapter 3, we formulate the specific problem of a continuous, elastic, conductive and dissipative solid subject to heat fluxes, under the assumption of local equilibrium for the thermal bath. Then we write the differential equations for displacement field and temperature, and formally solve them in Fourier space. Further reasoned assumptions has been implemented in order to obtain a theoretical relationship, at a high level of generality, of the value of the frequency autocorrelation of the displacement field. In chapter 4, as an example, we focus on the specific case of an infinite solid with a temperature gradient only in one dimension, and compute the displacement fluctuations which a specific readout shall measure. The results of this specific problem are discussed and, in the conclusions, we suggest the approach for a future continuation of this research.

2 Theory of elasticity and FDT

2.1 Theory of elasticity

In elasticity theory a solid is conceived as a continuous distribution of matter; physically, it is divided in volumes, small with respect to the macroscopic dimension of the object (e.g. the length) but large enough to contain a large number of atomic constituents. Mathematically, these volumes are treated as infinitesimal and thus can be identified by vectors living in a 3-dimensional space. If r_i is the position of a specific point of the solid at mechanical equilibrium, and r'_i after a deformation, then the displacement field we are interested to study is

$$u_i = r'_i - r_i, \tag{2.1}$$
$$i = 1, 2, 3. \tag{2.2}$$

If one defines $dl = \sqrt{dx_i^2}$ the differential distance between two near points of the solid at equilibrium and $dl' = \sqrt{dx_i'^2}$ after a deformation, then

$$dl'^2 = dl^2 + 2u_{ik}dx_i dx_k, \tag{2.3}$$

with

$$u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} + \frac{\partial u_l}{\partial x_k}\frac{\partial u_l}{\partial x_i}\right), \tag{2.4}$$

which is called displacement tensor and is symmetric by construction. For our purpose we further assume that displacements involved are small, which implies a simpler writing of our displacement tensor, as

$$u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right). \tag{2.5}$$

Another important assumption at this point is to consider that, when a deformation occurs, the solid reacts in order to re establish equilibrium: these reaction forces are typically short ranged, so that only occur between neighbour points of the solid. The whole force acting on the solid along each direction is

$$\int F_i dV = \int \frac{\partial \sigma_{ik}}{\partial x_k} dV = \oint \sigma_{ik} dS_k. \tag{2.6}$$

Here we introduced the stress tensor σ_{ik}, which is symmetric. As mentioned in the introduction, we can imagine that the resulting macroscopic force resulting contributes to the behavior of thermodynamic variables of the system, since it can make work on it and contribute to the whole energy balance. For this reason we now assume that the system lays always in thermodynamic equilibrium states, such that we can define the entropy function S and a temperature T, so that its heat exchanged during a thermodynamic transformation for an entropy variation equal to dS is TdS. Under these hypothesis we can define the Helmholtz free energy of our solid as $F = \mathcal{E} - TS$, where $\mathcal{E}$ is the internal energy of the system. During a generic thermodynamic transformation we have:

$$dF = -SdT + \sigma_{ik} du_{ik}, \tag{2.7}$$

such that $\sigma_{ik} = \frac{\partial F}{\partial u_{ik}}$. At mechanical equilibrium $\sigma_{ik} = 0$, which implies that no terms linear in displacement are present in the Helmholtz free energy for an isotropic solid, and we can write F as a linear combination of its quadratic terms. One can further imagine, as for displacement, that the variation of temperature before and after the thermodynamic transformation due to deformations is small in comparison with the equilibrium temperature T_0 for every point of the temperature field $T = T(\vec{r})$, that we suppose can depend on the position in the solid. With this approximation we take into account only the linear terms in u_{ii} for the expansion of the new Helmholtz free energy temperature dependent part, and since $u_{ik} = (u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}) + \frac{1}{3}\delta_{ik}u_{ll}$, we can otherwise write

$$F = F_0(T_0) - K\alpha(T - T_0)u_{ll} + \frac{K}{2}u_{ll}^2 + \mu\left(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll}\right), \tag{2.8}$$

with F_0 the Helmholtz free energy for the solid at rest at a temperature T_0 and no displacement, $K = \lambda + \frac{2}{3}\mu$ the uniform compression modulus, defined by Lamè coefficients λ and μ and the thermal expansion coefficient α. We introduced also an equation for the temperature field we have: actually, a variation in the displacement field for the solid implies different thermal proprieties, in the general case of nonzero thermal expansion coefficient.

It is known that entropy is the temperature partial derivative of F, so that

$$S(T) = \frac{\partial F}{\partial T} = S_0(T) + K\alpha u_{ll}, \tag{2.9}$$

with S_0 the entropy for the solid at rest. We define the heat flux density divergence $\partial_i q_i = -T\frac{\partial S}{\partial t}$ in time, while we can consider valid the Fourier approximation for the heat flux density: $q_i = -a\partial_i T$, where we introduced the thermal diffusivity a, obtaining

$$T\frac{\partial S_0}{\partial t} + K\alpha T\frac{\partial u_{ii}}{\partial t} = a\partial_{ii}T. \tag{2.10}$$

This equation can be rewritten with specific heat capacity coefficients, since $C_p - C_v = K\alpha^2 T$:

$$C_v\frac{\partial T}{\partial t} + \frac{C_p - C_v}{\alpha}\frac{\partial u_{ii}}{\partial t} = a\partial_{ii}T. \tag{2.11}$$

2.2 Langevin theory and FDT for an harmonic damped oscillator

We first consider a simple model of an harmonic oscillator, which satisfies the ordinary differential equation

$$m\,\ddot{d} = -K\,d - \gamma\,\dot{d}. \tag{2.12}$$

Now, for time independent coefficients, we consider that there is also a stochastic noise force that enters in the dynamics, so that the equation becomes

$$m\,\ddot{d} = -K\,d - \gamma\,\dot{d} + F(t), \tag{2.13}$$

where $F(t)$ is called Langevin generalized force, and represents the stochastic forces that contribute at the evolution of displacement function $d(t)$, which we assume to have N possible realizations $\{F_1(t), ..., F_N(t)\}$. This force needs to satisfy these conditions:

1. We want $F(t)$ not to brake the time symmetry, since it is suppose to be stochastic, hence

$$\langle F(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} F_i(t) = 0. \tag{2.14}$$

2. We want to specify the time correlation of $F(t)$ as a certain function of time $\eta(t)$:

$$\langle F(t_1) F(t_2) \rangle = \frac{1}{N} \sum_{i=n}^{N} F_n(t_1) F_n(t_2) = A^2 \eta(t_1 - t_2). \tag{2.15}$$

Langevin approach consists in writing down an implicit solution for $d(t)$.

For this reason the first we first want to obtain the response function for the system without Langevin forces. We imagine now a deterministic external force $F_E(t)$ that contributes at the dynamics:

$$m\,\ddot{d}(t) = -K\,d - \gamma\,\dot{d} + F_E(t), \tag{2.16}$$

in Fourier space,

$$-m\,\omega^2\,d(\omega) = -K\,d(\omega) - i\,\omega\,\gamma\,d(\omega) + F_E(\omega). \tag{2.17}$$

Now we can thus define the response function $R(\omega)$ such that

$$d(\omega) = R(\omega) F_E(\omega), \tag{2.18}$$

$$R(\omega) = \frac{1}{K + i\,\omega\,\gamma - m\,\omega^2}. \tag{2.19}$$

In the next paragraph we will show that the imaginary part of $R(\omega)$ is related to the Fourier transform of the displacement autocorrelation $C_d(\omega, \omega' = -\omega) = \langle d(\omega) d(\omega' = -\omega) \rangle$. The next step, for this reason, is to compute the quantity $C_d(\omega, -\omega)$, assuming there is no deterministic external force F_E acting on the system. We assume now that Langevin forces are present, in such a way that in fact we consider the equation (2.13). In this case the formal solution of the differential equation is

$$d(\omega) = R(\omega) F(\omega), \tag{2.20}$$

with

$$R(\omega) = \frac{1}{K + i\,\omega\,\gamma - m\,\omega^2}. \tag{2.21}$$

We can thus compute the autocorrelation function

$$C_d(\omega, -\omega) = \langle d(\omega) d(-\omega) \rangle = \frac{A^2 \eta(\omega)}{\left(K + i\,\omega\,\gamma - m\,\omega^2\right)\left(K - i\,\omega\,\gamma - m\,\omega^2\right)}. \tag{2.22}$$

With $\eta(\omega) = \int e^{-i\omega t} dt \eta(t)$. We suppose now that this noise is

$$\eta(\omega) = \gamma, \tag{2.23}$$

where this hypothesis will be generalized and motivated in the next paragraph. We can find this autocorrelation to be, after an initial transient and considering Langevin forces are delta correlated,

$$C_d(\omega, -\omega) = \frac{\gamma A^2}{\left(K - m\,\omega^2\right)^2 + \gamma^2\,\omega^2}, \tag{2.24}$$

This is a particular solution, of a general case treated in literature [7] where a similar approach is used.

$$\left\langle d^2 \right\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} C_d(\omega, -\omega) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\gamma\, A^2}{\left(K - m\,\omega^2\right)^2 + \gamma^2\,\omega^2} = \frac{A^2}{2\,m\,K\,\gamma}. \tag{2.25}$$

From equipartition theorem we know that mechanical energy is stored in the possible degrees of freedom in such a way that at equilibrium

$$\langle E \rangle = \frac{1}{2}\,k_B\,T, \tag{2.26}$$

with the Boltzmann constant k_B and the temperature associated at the bath where the harmonic oscillator lays. In our case $\langle E \rangle = \frac{1}{2}\,K \left\langle d^2 \right\rangle$ and, since our damping effect is considered negligible in comparison with the elastic force, we have

$$A^2 = 2\,\gamma\,m\,k_B\,T. \tag{2.27}$$

The direct proportionality of autocorrelation function from A^2, shows the link between the variance of the fluctuating force and the variance of the displacement field, which is, in our case, a particular result of fluctuation dissipation theorem.

2.3 Extension for time dependent constants

Physical constants involved in equations for the solid that we will write, can be function of time. For this reason, as an example, we can write the equation 2.12 in the following form:

$$m\ddot{d} = -Z * d, \tag{2.28}$$

with

$$Z(t) = K\,\delta(t) - \gamma\,\dot{\delta}(t), \tag{2.29}$$

since we have

$$Z * d \equiv \int_{-\infty}^{+\infty} ds\, d(s)\, \left(K\,\delta(t-s) - \gamma\,\partial\,\delta(t-s)\right) = K\,d(t) + \gamma\,\dot{d}(t). \tag{2.30}$$

If we have a generic function $Z(t)$ instead, it is useful to work in Fourier space, defining the Fourier transform of $Z(t)$:

$$Z(\omega) \equiv \int_{-\infty}^{\infty} dt Z(t) e^{i\omega t}. \tag{2.31}$$

For instance, using the explicit writing of $Z(t)$ of eq. (2.29), we have

$$Z(\omega) \equiv \int_{-\infty}^{\infty} dt Z(t) e^{i\omega t} = \int_{-\infty}^{\infty} dt \left(K\,\delta(t) - \gamma\,\dot{\delta}(t) \right) e^{i\omega t} = k + i\gamma\omega. \tag{2.32}$$

We can see that $\mathrm{Im}[Z(\omega)]$ encodes dissipation that occurs in our system: a similar approach will be developed in the next paragraph, where we will encode in Lamé coefficients of the solid an imaginary part to represent dissipative effects affecting the solid dynamics.

Before doing this, we can also compute the spectral density of displacement field for a generic writing of $Z(\omega)$. In this case equation (2.13) becomes in Fourier space

$$-m\,\omega^2\,d(\omega) = -Z\,d(\omega) + F(\omega), \tag{2.33}$$

which admits the solution

$$d(\omega) = \frac{1}{Z(\omega) - m\omega^2} F(\omega) \equiv R(\omega) F(\omega), \tag{2.34}$$

with R the response function of the displacement d. We can then compute its spectral density

$$C_d(\omega, \omega' = -\omega) \equiv \left\langle d(\omega) d(-\omega) \right\rangle = |R(\omega)|^2 A^2 \eta(\omega) = \frac{A^2 \eta(\omega)}{(\mathrm{Re}Z(\omega) - m\omega^2)^2 - (\mathrm{Im}Z(\omega))^2}. \tag{2.35}$$

If we now assume that the noise correlation function is

$$\eta(\omega) = \frac{\mathrm{Im}Z(\omega)}{\omega}, \tag{2.36}$$

the spectral density simplifies to

$$C_d(\omega, -\omega) = \frac{A^2}{\omega} \mathrm{Im}R(\omega). \tag{2.37}$$

Integrating for all frequencies $C_d(\omega, -\omega)$ we find the mean squared displacement

$$\left\langle d^2 \right\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} C_d(\omega, -\omega) = A^2 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\mathrm{Im}R(\omega)}{\omega}. \tag{2.38}$$

Closing the integral in the upper complex plane (see e.g.[1]), we realize, as in the previous paragraph, that $A^2 = 2\,m\,\gamma k_B T$ in order for the equipartition (2.26) to be satisfied.

3 General statements and spectral density

3.1 The macroscopic dynamical equation

We want apply now the theory of elasticity in order to write the differential equations for the displacement field $d_i(\vec{r}, t)$ and the temperature field $T(\vec{r}, t)$ of a linear, homogeneous and isotropic solid. The first equation of motion is Newton law built with the two contributions of the forces related to mechanical stress tensor and the thermal expansion terms, while the second formula is the continuity equation for temperature:

$$\begin{cases} \rho\,\ddot{d}_i = \mu * \partial_i(\partial_j d_j) + (\mu + \lambda) * \partial_{jj} d_i - \alpha(3\lambda + 2\mu) * \partial_i T, & \text{(3.1a)} \\ \dot{T} = a\,\partial_{jj} T - b * T\,\partial_j \dot{d}_j, & \text{(3.1b)} \end{cases}$$

with α the thermal expansion coefficient, a the thermal diffusivity, and $b = \frac{\alpha(3\lambda+2\mu)}{\rho C}$ (ρ is the density, and C the specific heat).

Unlike what was done in (2.13), now we take the Lamé coefficients λ and μ to be functions of time. In this case we encode disspative effects in the non-zero imaginary part of Lamé coefficients.

The shorthand notation $*$ is used as in the previous paragraph to denote convolutions of the type

$$\mu * \partial_i(\partial_j d_j) \equiv \int_{-\infty}^{\infty} dt' \mu(t-t')\, \partial_i(\partial_j d_j(t')). \tag{3.2}$$

Another important assumption we make on coefficients μ and λ is the causal hypothesis, meaning that, $\mu(t), \lambda(t) = 0$ if $t < 0$. A quasi-static approximation can be used in (3.1a), setting $\ddot{d}_i$ to zero, if the analysis is restricted to times longer than the ones associated to the propagation of sound waves, since in this approximation the inertia of the mesoscopic particle is negligible.

3.2 Dynamics with Langevin forces contribution

Equations (3.1) provides the basis for describing the deterministic evolution of a solid at mesoscopic level. In order to encode the stochastic forces mentioned before, and so thermal fluctuations, we introduce stochastic terms to the stress tensor and the heat flux in (3.1). They represent the random exchange of momentum and energy, respectively between the mesoscopic continuous degrees of freedom and the microscopic ones. As a consequence, each field can be decomposed into a mean value and a fluctuating part, namely, $\langle d_i \rangle + \delta d_i$ and $\langle T \rangle + \delta T$. We focus on bulk fluctuations, meaning that formally the distances involved between the boundaries of the system tends to infinity. The averages $\langle d_i \rangle$ and $\langle T \rangle$ are the steady-state solutions of (3.1),

$$0 = \mu * \partial_i(\partial_j \left\langle d_j \right\rangle) + (\mu + \lambda) * \partial_{jj}\langle d_i \rangle - \alpha(3\lambda + 2\mu) * \partial_i \langle T \rangle, \tag{3.3a}$$

$$\partial_{jj}\langle T \rangle = 0. \tag{3.3b}$$

On the other hand, the fluctuations are obtained by linearizing (3.1) around $\langle d_i \rangle$ and $\langle T \rangle$, and adding the aforementioned stochastic forcing,

$$\rho\, \delta\ddot{d}_i = \mu * \partial_i(\partial_j\, \delta d_j) + (\mu + \lambda) * \partial_{jj}\, \delta d_i - \alpha(3\lambda + 2\mu) * \partial_i\, \delta T + \partial_j \tau_j, \tag{3.4a}$$

$$\delta\dot{T} = a\, \partial_{jj}\, \delta T - b * T_0\, \partial_j\, \delta\dot{d}_j + \partial_j Q_j, \tag{3.4b}$$

where T_0 represents the zero order term of the Taylor expansion for $T(\vec{r})$ (which will be $T_0 = \bar{T}$ in the next paragraph). In (3.4b) we have dropped non-linear terms and time derivatives of $\langle d_i \rangle$ (time derivatives of any mean value are zero in the stationary state). The generalized Langevin forces we added τ_{ij} and Q_i have by definition zero mean. We write down them as a divergence since they conserve momentum and energy, respectively.

The assumption that the solid is locally in equilibrium at mesoscopic level ensures that these forces are Gaussian distributed with two-point correlation functions (in frequency space) given by the local fluctuation-dissipation relation. Now we follow treatment of Ortiz-De Zarate work [6] (adapting the analysis for solids instead of fluids equations), if one assumes that the heat fluxes involved in a solid consist in a part related to the bulk dynamics of the system and another fluctuating contribution due to Langevin generalized forces, respectively τ_{im} and f_i. Hence,

$$\left\langle \tau_{im}(\vec{r},\omega)\tau_{jn}(\vec{r}',\omega')\right\rangle = -\frac{2k_B\left\langle T(\vec{r})\right\rangle}{\omega}\Big(\mathrm{Im}\mu(\omega)\delta_{im}\delta_{jn} + \mathrm{Im}(\mu+\lambda)(\omega)\delta_{ij}\delta_{mn}\Big)\delta(\vec{r}-\vec{r}')\delta(\omega+\omega'),$$
$$\left\langle Q_i(\vec{r},\omega)Q_j(\vec{r}',\omega')\right\rangle = 2k_B\left\langle T(\vec{r})\right\rangle^2 a\,\delta_{ij}\delta(\vec{r}-\vec{r}')\delta(\omega+\omega'), \tag{3.5}$$

where k_B is Boltzmann constant. We see that the autocorrelations of the random forces is determined by the dissipative part of the equation of motion; moreover, the random forces are defined to be independent from each other. Correlations between δd_i and δT are brought in by the thermal expansivity of the solid.

To compute the statistics of the fluctuating fields and obtain a general form for the spectral density we take the space-time Fourier transform of (3.4), writing (for instance for $Q_i(\vec{r},t)$)

$$Q_i(\vec{k},\omega) \equiv \mathscr{F}[Q_i(\vec{r},t)](\vec{k},\omega) \equiv \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d^3r\, e^{-i\vec{k}\cdot\vec{r}}\int_{-\infty}^{\infty} dt Q_i(\vec{r},t)e^{-i\omega t}. \tag{3.6}$$

In this case we have

$$\begin{cases} -\rho\,\omega^2\,\delta d_i = -k_i k_j\,\mu\,\delta d_j - k^2(\mu+\lambda)\delta d_i + i\,k_i\,\alpha(3\lambda+2\mu)\delta T - i\,k_j\,\tau_{ij}, & \text{(3.7a)}\\ -i\,\omega\,\delta T = -a\,k^2\delta T + k_j\,\omega\,b\,\bar{T}\,\delta d_j - i\,k_j\,Q_j, & \text{(3.7b)}\end{cases}$$

and we plug δT obtained by (3.7b),

$$\delta T(\vec{k},\omega) = \frac{ik_jQ_j - k_j\omega b\bar{T}\delta d_j}{i\omega - ak^2}, \tag{3.8}$$

into (3.7a). The fluctuations of the displacement field are thus given by

$$R_{ij}^{-1}\delta d_j(\vec{k},\omega) = k_j\left(-\frac{\alpha(3\lambda+2\mu)}{i\omega-ak^2}k_iQ_j - i\tau_{ij}\right) \equiv k_j\left(k_i\alpha\,\phi\,Q_j - i\tau_{ij}\right), \tag{3.9}$$

where we defined for compactness the auxiliary function

$$\phi(k,\omega) \equiv -\frac{(3\lambda+2\mu)}{i\omega-ak^2}, \tag{3.10}$$

and the inverse response matrix

$$R_{ij}^{-1}(\vec{k},\omega) = \left(k^2(\mu+\lambda)-\rho\omega^2\right)\delta_{ij} + \left(\mu - i\omega b\bar{T}\alpha\phi(k,\omega)\right)k_ik_j \equiv \delta_{ij}g(k,\omega) + k_ik_jh(k,\omega). \tag{3.11}$$

This 3x3 matrix can be inverted, obtaining

$$R_{ij}(\vec{k},\omega) = \frac{1}{g}\left(\delta_{ij} - \frac{h}{(g+hk^2)}k_ik_j\right). \tag{3.12}$$

We can now calculate the two-point correlations $C_{ij}(\vec{k},\vec{k}',\omega,\omega')$ (which are called power spectral densities for $\omega' = -\omega$) of the displacement field in Fourier space, averaging over the noise

$$C_{ij} \equiv \left\langle \delta d_i \delta d_j^{*\prime}\right\rangle = R_{im}R'_{jn}k_pk'_s\left[\alpha^2k_mk'_n\phi\phi'\left\langle Q_pQ'_s\right\rangle - \left\langle \tau_{mp}\tau'_{ns}\right\rangle\right], \tag{3.13}$$

where $R'_{jn} = R_{jn}(\vec{k}', \omega')$ and $\phi' = \phi(\vec{k}', \omega')$. We can identify two terms of these correlations: one is due to temperature Langevin forces, while the other represents the noise contribution from Langevin forces introduced for displacement field. The first term has quadratic dependence on α at limit $\alpha \to 0$, since the response matrix R has a finite value at this limit. That means this noise is negligible for small values of α.

Than making use of (3.5) in the mode-frequency representation

$$\begin{aligned}
\Big\langle \tau_{im}(\vec{k}, \omega)\tau'_{jn}(\vec{k}', \omega') \Big\rangle &= -\frac{2k_{\mathrm{B}}\Big\langle T(\vec{k} - \vec{k}') \Big\rangle}{\omega}\Big(\mathrm{Im}\mu(\omega)\delta_{im}\delta_{jn} + \mathrm{Im}(\mu + \lambda)(\omega)\delta_{ij}\delta_{mn}\Big)\delta(\omega - \omega'), \\
\Big\langle Q_i(\vec{k}, \omega)Q'_j(\vec{k}', \omega') \Big\rangle &= 2k_{\mathrm{B}}\Big\langle T(\vec{k} - \vec{k}') \Big\rangle^2 a\delta_{ij}.\delta(\omega - \omega')
\end{aligned} \tag{3.14}$$

Now, assuming that

$$\big\langle T(\vec{r}) \big\rangle = \bar{T} + cf(x), \tag{3.15}$$

which means that our temperature bath depends only on position on x axis, we can obtain the Fourier transform for the quantities

$$\begin{aligned}
&\Big\langle T(\vec{k} - \vec{k}') \Big\rangle = \big\langle \mathscr{F}[\bar{T} + cx](k - k') \big\rangle = \bar{T}\delta(\vec{k} - \vec{k}') + \mathscr{F}[cf(x)](\vec{k} - \vec{k}'), \\
&\Big\langle (T(\vec{k} - \vec{k}'))^2 \Big\rangle = \Big\langle \mathscr{F}[(\bar{T} + cf(x))^2](k) \Big\rangle = \bar{T}^2\delta(\vec{k} - \vec{k}') + 2\bar{T}\mathscr{F}(cf(x))(\vec{k} - \vec{k}') + \\
&+ \mathscr{F}(c^2f^2(x))(\vec{k} - \vec{k}').
\end{aligned} \tag{3.16}$$

We define now the new terms of these quantities, corresponding to the spatial dependent part of the Fourier transform of $\langle T \rangle$ and $\langle T \rangle^2$ given by

$$\langle T \rangle_{NE}(\vec{k} - \vec{k}') = \mathscr{F}[cf(x)](\vec{k} - \vec{k}'), \tag{3.17}$$

$$\langle T \rangle^2_{NE}(\vec{k} - \vec{k}') = 2\bar{T}\mathscr{F}(cf(x))(\vec{k} - \vec{k}') + \mathscr{F}(c^2f^2(x))(\vec{k} - \vec{k}'). \tag{3.18}$$

and the terms proportional to $\delta(\vec{k} - \vec{k}')$ produce instead the equilibrium part of C_{ij}. The additional non-equilibrium corrections are thus encoded in the spectral density $S_d^{NE}(\vec{k}, \vec{k}', \omega) = C_{ii}^{NE}(\vec{k}, \vec{k}', \omega, \omega' = -\omega)$

$$\begin{aligned}
S_d^{NE}(\vec{k}, \vec{k}', \omega) &= -2k_{\mathrm{B}}R_{im}(\vec{k}, \omega)R_{in}(-\vec{k}', -\omega)k_pk'_s\delta(\vec{k}_\perp - \vec{k}'_\perp)\cdot \\
&\quad \cdot \Bigg[\frac{1}{\omega}\Big(\mathrm{Im}\mu(\omega)\delta_{pm}\delta_{sn} + \mathrm{Im}(\mu + \lambda)(\omega)\delta_{ps}\delta_{mn}\Big)\langle T \rangle_{NE}(\vec{k} - \vec{k}') \\
&\quad + a\,\alpha^2\,k_mk'_n\phi(k, \omega)\phi(-k', -\omega)\langle T \rangle^2_{NE}(\vec{k} - \vec{k}')\delta_{ps}\Bigg]
\end{aligned} \tag{3.19}$$

$$\equiv N_1(\vec{k}, -\vec{k}', \omega)\langle T \rangle_{NE}(\vec{k} - \vec{k}') + N_2(\vec{k}, -\vec{k}', \omega)\langle T \rangle^2_{NE}(\vec{k} - \vec{k}'). \tag{3.20}$$

Here we can see that there are two new contributions to the PSD, due to considering non equilibrium effects. $N_1\langle T \rangle_{NE}$ is related to damping effect, since it encodes information about imaginary part of Lamé coefficients, and it is linearly dependent on c. Instead, the $N_2\langle T \rangle_{NE}$ term has both a linear and quadratic dependence on the c parameter, which means that can predict second order effects due to a non globally uniform thermal bath. We notice also the quadratic dependence of this contribution on α, which means that at limit $\alpha \to 0$ the term is negligible.

4 A specific problem: 1-d linear shaped temperature

4.1 Boundary conditions

The next step is to consider a paradigmatic situation, simple enough to allow for analytical treatment but yet sufficiently general to display some relevant non-equilibrium features. Namely, we take a solid with a temperature difference along the x axis only, given by

$$\left\langle T(\vec{r})\right\rangle|_{x=\pm\ell} = T_{\pm}, \tag{4.1}$$

and isothermal at the other boundaries. We also assume for simplicity stress-free boundary conditions for displacement. Equation (3.3b) with the boundary condition (4.1) can be readily solved,

$$\left\langle T(\vec{r})\right\rangle = \bar{T} + cx, \tag{4.2}$$

where $c = (T_+ - T_-)/\ell$ is the constant gradient and $\bar{T} = (T_+ + T_-)/2$ is the average temperature. Since the PSD in (3.13) depends on the aforementioned correlations $\left\langle \tau_{im}(\vec{k},\omega)\tau^*_{jn}(\vec{k}',\omega')\right\rangle$ and $\left\langle Q_i(\vec{k},\omega)Q^*_j(\vec{k}',\omega')\right\rangle$, we can write, for the temperature profile:

$$\begin{aligned}
\left\langle T(\vec{k}-\vec{k}')\right\rangle &= \left\langle \mathscr{F}[\bar{T}+cx](k-k')\right\rangle = \bar{T}\delta(k-k') + \mathscr{F}[cx](k-k'),\\
\left\langle (T(\vec{k}-\vec{k}'))^2\right\rangle &= \left\langle \mathscr{F}[(\bar{T}+cx)^2](k)\right\rangle = \bar{T}^2\delta(k-k') + 2\bar{T}\mathscr{F}(cx)(k) + \mathscr{F}(c^2x^2)(k),
\end{aligned} \tag{4.3}$$

where we have, similarly to what we did in the previous paragraph,

$$\langle T\rangle_{NE}(\vec{k}-\vec{k}') = -i\,c\,\partial_{k'_x}\,\delta(k_x-k'_x)\delta(\vec{k}_\perp-\vec{k}'_\perp), \tag{4.4}$$

$$\langle T\rangle^2_{NE}(\vec{k}-\vec{k}') = -\left[c^2\partial^2_{k'_x}\delta(k_x-k'_x) + 2\,i\,\bar{T}\,c\,\partial_{k'_x}\,\delta(k_x-k'_x)\right]\delta(\vec{k}_\perp-\vec{k}'_\perp), \tag{4.5}$$

and where $\delta(\vec{k}_\perp-\vec{k}'_\perp) \equiv \delta(k_y-k'_y)\delta(k_z-k'_z)$

4.2 A case study

Now we further implement our last hypothesis that allow us to compute the calculation of the spectral density of a specific system. We suppose the thermal bath of the solid to just depend on one of the three cartesian cohordinates, that means that our equations can be simplified in order to consider just a 1-D problem. This strong approximation implies a rewriting of the spectral density $S_d(\vec{k},\vec{k}',\omega)$ as a function of only scalar parameters k,k' which represents the spatial modes on the direction considered $S_d(k,k',\omega)$. We also imagine we have a readout function on one of the two boundaries of the solid, in the same direction of the temperature profile, which is gaussian-shaped:

$$f(r) = \frac{e^{-(r/x_0)^2}}{\pi x_0^2}, \tag{4.6}$$

and its Fourier transform is

$$f(k) = \frac{e^{-(kx_0)^2/4}}{\sqrt{\pi}x_0}, \tag{4.7}$$

with the parameter $x_0 < L$

Following an approach similar to what Yu Levin did [5], we consider the observable read out

$$x(t) = \int dr f(r) d(r,t), \tag{4.8}$$

where $d(r,t)$ represents the displacement of our solid in its length direction, along which we measure the observable with the read out function $f(r)$.

In fact, since it is difficult to work in position and time space, we consider another observable: the frequency auto correlation of read out

$$\langle x(\omega)x(-\omega)\rangle = \int dk \int dk' \hat{f}(k)\hat{f}(k')S(k,k',\omega), \tag{4.9}$$

which is the Fourier transform at $\omega' = -\omega$ of time correlation of read out $\langle x(t)x(t')\rangle$

4.3 Fluctuations at equilibrium

At this point we can obtain for the equilibrium part of the spectral density

$$\begin{aligned}\langle x(\omega)x(-\omega)\rangle &= \int dk \int dk' \hat{f}(k)\hat{f}(k')S_d^{EQ}(k,k',\omega) = \frac{1}{\pi x_0^2}\int dk e^{-k^2x_0^2/4}\int dk' e^{-k'^2x_0^2/4}S_d^{EQ} \\ &= \frac{1}{\pi x_0^2}\int dk e^{-k^2x_0^2/4}\int dk' e^{-k'^2x_0^2/4} RR'kk'\left[\frac{2k_B\bar{T}}{\omega}\mathrm{Im}(2\mu+\lambda)(\omega) + \alpha^2 kk'\phi\phi' 2k_B\bar{T}^2 a\right]\delta(k-k'),\end{aligned} \tag{4.10}$$

where $S_d^{EQ}(k,k',\omega)$ is composed by the contributions of eq. (4.3) that do not depend on temperature shape correction, but only on mean temperature values:

$$S_d^{EQ}(k,k',\omega) = RR'kk'\left[\frac{2k_B\bar{T}}{\omega}\Big(\mathrm{Im}\mu(\omega) + \mathrm{Im}(\mu+\lambda)(\omega)\Big) + \alpha^2 kk'\phi\phi' 2k_B\bar{T}^2 a\right]\delta(k-k'). \tag{4.11}$$

So we obtain the following expression for our spectral density

$$\begin{aligned}\langle x(\omega)x(-\omega)\rangle &= \frac{1}{\pi x_0^2}\int dk e^{-k^2x_0^2/4} Rk \int dk' e^{-k'^2x_0^2/4} R'k'\left[\frac{2k_B\bar{T}}{\omega}\Big(\mathrm{Im}\mu(\omega) + \mathrm{Im}(\mu+\lambda)(\omega)\Big) + \right. \\ &\quad \left. + \alpha^2 kk'\phi\phi' 2k_B\bar{T}^2 a\right]\delta(k-k') \\ &= \frac{2k_B\bar{T}\Big(\mathrm{Im}\mu(\omega) + \mathrm{Im}(\mu+\lambda)(\omega)\Big)}{\pi x_0^2\omega}\int dk e^{-k^2x_0^2/2} R^2k^2 + \\ &\quad + \alpha^2\frac{2k_B\bar{T}^2 a}{\pi x_0^2}\int dk e^{-k^2x_0^2/4} R^2\phi^2 k^4.\end{aligned} \tag{4.12}$$

We notice the quadratic dependence on thermal expansion coefficient α of one term of PSD at equilibrium.

4.4 Fluctuations out of equilibrium

For the non equilibrium part of the spectral density instead we have

$$\langle x(\omega)x(\omega'=-\omega)\rangle = \int dk \int dk' \hat{f}(k)\hat{f}(k')S^{NE}(k,k',\omega) = \frac{1}{\pi x_0^2}\int dk e^{-k^2x_0^2/4}\int dk' e^{-k'^2x_0^2/4}S_d^{NE}(k,k',\omega). \tag{4.13}$$

Using explicit writing of (4.4) and (3.19), where we don't write $\delta(\vec{k}_\perp - \vec{k}'_\perp)$, because of 1-d approximation, we can partial integrate this last expression. It consists in 3 integrals. The first one is produced by (4.4) term: it is an odd function on a symmetrical domain and vanishes. The second is produced by second term in (4.5) and vanishes for the same reasons. We have now to integrate the last term:

$$\langle x(\omega)x(-\omega)\rangle = \alpha^2\frac{2k_Bc^2a}{\pi x_0^2}\int_0^\infty e^{-k^2x_0^2/4}k^2\phi(k,\omega)R(k,\omega)\frac{\mathrm{d}}{\mathrm{d}k}[e^{-k^2x_0^2/4}k^2\phi(k,-\omega)R(k,-\omega)]. \tag{4.14}$$

Separating real part of the argument of the integral, we find that imaginary part vanishes, while real part is an even function in k. Analytic integration is found to be impossible, while we can see how imaginary part of Lamé coefficients doesn't affect the result and that the dependency of thermal gradient c is proportional to c^2 because of symmetries of our particular choice of thermal bath.

In this case we have to consider that, since our problem does not represent a physical system (we forgot about information from the other dimensions of the solid), we do not see first order effect in thermal bath temperature gradient c. In fact, we see that these effects are encoded in the two terms of S_d^{NE} that vanish because of symmetries.

4.5 Low thermal expansion coefficient limit

At this limit we find that non equilibrium part of the spectral density vanishes. For the same reason the second term of equilibrium part of the spectral density is equal to 0, that implies the following expression for the whole spectral density of the system:

$$\langle x(\omega)x(-\omega)\rangle = \frac{2k_B\bar{T}\Big(\mathrm{Im}\mu(\omega)+\mathrm{Im}(\mu+\lambda)(\omega)\Big)}{\pi x_0^2\omega}\int dk e^{-k^2x_0^2/2}R^2k^2. \tag{4.15}$$

Also this result, as the one aforementioned, is essentially due to strong symmetries imposed by strong hypothesis of our problem.

5 Conclusions

In this thesis work we learned how to define a mathematical model for an elastic, damped and thermally conductive solid, writing down the differential equations for temperature and displacement field, that are meaningful quantities to describe its dynamics. We further understood how to describe the contribution of internal degrees of freedom at the whole balance of the energy thanks to Langevine theory. In total generality we saw that, assuming FDT to be valid only at mesoscopic level, the power spectral density one can observe is different from the global-temperature case. In particular we studied a particular exemple where we could easily perform direct calculations and see the new contribution at the PSD of the system due to a nonzero thermal gradient imposed at the boundaries. Since our case preserve strong symmetries, we found that some relevant terms for the PSD in our case can vanish.

The next step of this research topic will be to implement this approach for some nontrivial cases. In particular it could be interesting to try to analytically obtain the PSD of a system that shares similar features with VIRGO experiment mirrors, where it will be necessary to model correctly the geometry of the problem and the boundary conditions for both temperature and displacement fields. At the end we showed the limit for the thermal expansion coefficient $\alpha \to 0$, which will be interesting for next generation interferometers, since it is known that it exist a temperature point where thermal expansion coefficient for material which mirrors are made of respect this limit.

References

[1] V Balakrishnan. "Fluctuation-dissipation theorems from the generalised Langevin equation". In: *Pramana* 12 (Apr. 1979), pp. 301–315. DOI: 10.1007/BF02894699.

[2] L. E. Reichl. *A modern course in statistical physics*. London: Arnold, 1980. URL: https://cds.cern.ch/record/101976.

[3] L.D. Landau, E.M. Lifshitz, and J.B. Sykes. *Theory of Elasticity*. Course of theoretical physics. Pergamon Press, 1989. ISBN: 9780029462232. URL: https://books.google.it/books?id=YjDiQwAACAAJ.

[4] Peter R. Saulson. "Thermal noise in mechanical experiments". In: *Phys. Rev.* D42 (1990), pp. 2437–2445. DOI: 10.1103/PhysRevD.42.2437.

[5] Yu Levin. "Internal thermal noise in the LIGO test masses: A direct approach". In: *Phys. Rev. D* 57 (Jan. 1998). DOI: 10.1103/PhysRevD.57.659.

[6] J.M.O. de Zárate and J.V. Sengers. *Hydrodynamic Fluctuations in Fluids and Fluid Mixtures*. Elsevier, 2006. ISBN: 9780444515155. URL: https://books.google.it/books?id=D56ckmEdRukC.

[7] J. T. Waldron William Coffey Yu. P. Kalmykov. *The Langevin Equation With Applications in Physics, Chemistry and Electrical Engineering*. World Scientific Publishing Co. Pte. Ltd., 2012.

[8] Livia Conti et al. "Effects of breaking vibrational energy equipartition on measurements of temperature in macroscopic oscillators subject to heat flux". In: *Journal of Statistical Mechanics Theory and Experiment* 2013 (May 2013). DOI: 10.1088/1742-5468/2013/12/P12003.

[9] Gianmaria Falasco et al. "Energy repartition for a harmonic chain with local reservoirs". In: *Physical review. E, Statistical physics, plasmas, fluids, and related interdisciplinary topics* 92 (May 2015). DOI: 10.1103/PhysRevE.92.022129.

[10] Mickael Geitner et al. "Low thermal fluctuations in a system heated out of equilibrium". In: *Physical Review E* 95 (Dec. 2016). DOI: 10.1103/PhysRevE.95.032138.