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PAPER

Phase space trajectories generated under coupling between a dynamic system and a thermal reservoir

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Abstract

We analyze the phase space trajectories generated under coupling between a dynamic system and a thermal reservoir which generates a fluctuating as well as dissipative force field. We argue that the phase space trajectory of particles associated with intermediate equilibrium states under heat transfer possess a symmetric form, while the corresponding trajectory is asymmetric in energy transfer as work. The new perspective can help in developing a closed form expression of heat and work at microscopic dimensions with a few degrees of freedom. We also present a novel mathematical model of thermal reservoir as a dynamic system described using a transfer function comprising of a set of zeros. It addresses the theoretical weaknesses of current models of a thermal reservoir comprising of a collection of harmonic oscillators.

1. Introduction

Classical thermodynamics defines heat as a macroscopic physical quantity which is an outcome of statistical interactions of a number of constituent particles at the microscopic level, which are disordered. Thermodynamic work is considered to be an ordered form of energy which is defined in terms of variation of volume at a given pressure [1, 2]. A system's internal energy and temperature increase under adiabatic transfer of work and an isochoric transfer of heat [1, 2]. As the macroscopic physical variables like volume and temperature are connected to a given macrostate [3], a distinction between work and heat in microscopic systems with limited degrees of freedom need a more refined physical analysis and novel mathematical formulations. Currently, stochastic formulations are used to analyze work and heat in microscopic systems [4, 5]. For example, the stochastic trajectories linked with non-equilibrium states are used to define the Second law of thermodynamics [6, 7]. However, the key problem is that a number of experimental results have been interpreted from the perspective of apparent violation of the second law at small scale [8, 9]. Such experiments comprise of a thermal reservoir surrounding a cavity, fluid comprising of atoms, molecules or electrons and a physical mechanism of extraction of work actuated by a potential gradient. A noted example is experiments on validation of fluctuation theorem, in non-equilibrium microscopic systems, where a specific ratio is defined between production of positive and negative entropy [10]. In optical tweezer based experiments, a potential energy gradient is generated [11, 12] which applies finite values of force which can transfer work to the beads, resulting in entropy reduction. Levitation of a microparticle under a laser beam comprises of an interaction between conservative and dissipative force fields, where definition of heat and work need a novel theoretical framework, which will lead to novel insights on understanding entropy changes from a deterministic framework. Optical tweezer based potential gradient was also used in order to study the principle of Landauer on erasure of information under thermal transfer. The problem with the work was that an internal energy of the system $U(q, t)$ dependent on position q and time t was defined and heat transfer was expressed as, $Q = \int dt \dot{q} \partial U(q, t) / \partial q$. The fact is that, the expression of Q does not represent heat, but it expresses work where, an electron, moves with a velocity \dot{q} against a potential gradient [13]. A practical realization of the Maxwell demon was done by Koski *et al* where electron transfer across superconducting wires coupled by a

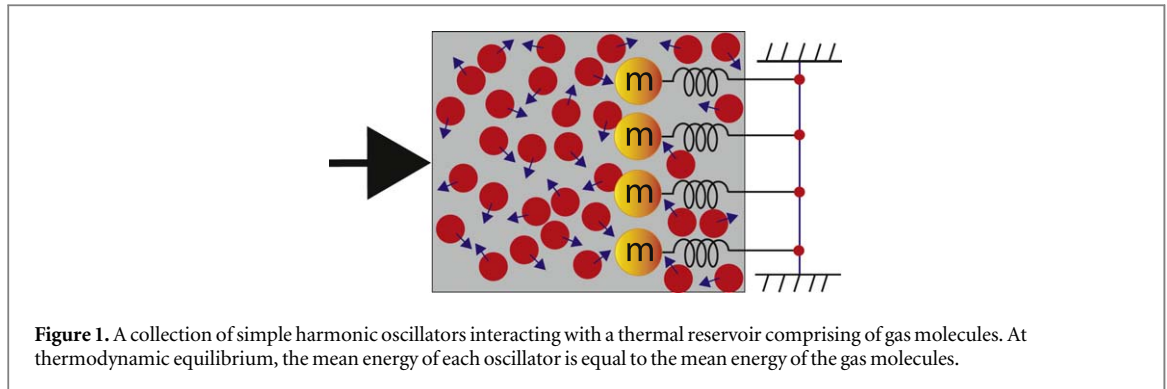


Figure 1. A collection of simple harmonic oscillators interacting with a thermal reservoir comprising of gas molecules. At thermodynamic equilibrium, the mean energy of each oscillator is equal to the mean energy of the gas molecules.

copper island was achieved through a single electron transistor [14]. For example, the authors assumed that transfer of electrons leads to generation of heat without explicitly defining the process of dissipation. In a related work by Mihai *et al*, which was based on Maxwell demon like set up, useful work was shown to be extracted from two beams falling on a photodiode linked with a capacitor [15]. In the experiments, photonic energy was transformed into the energy of electrons, which cannot be assumed to transformation of heat into work, unless the issue of dissipation is addressed. In a similar work, Strasberg *et al* assumed that current flow caused by electron tunneling between quantum dots or a ballistic transport in a system increases entropy [16]. The fact is that current flow increases entropy only if there are resistive losses in the system. However, there are instances where attempts to establish a distinction between work and heat has been done in mesoscopic experiments. For example, Jezouin *et al* [17], performed experiments on quantum of thermal conductance and the part of transport, which contributed to noise was considered as heat. They defined power dissipation under Joule heating under DC current transfer through ballistic channels in terms of momentum loss associated with noise generation. In all these experiments, a major issue is representation of time domain based dynamics in order to understand the nature of the system. A study of the evolution of particle's phase with time and frequency of the system could lead to a more refined understanding of the physics of the system.

An additional issue is defining the nature of coupling between a thermal reservoir and a dynamic system which under fluctuations and dissipation which was initially explored by Einstein, who calculated that the root mean square value of particle's displacement in a thermal reservoir is proportional to the square root of time [18]. The phenomenon was reformulated using Newton's laws of motion by Langevin while considering the interaction force with a thermal reservoir as comprising of a slowly varying part which takes the system towards an equilibrium and a fluctuating force with a net value of zero [19, 20]. The ideas further evolved with the work by Uhlenbeck and Orstein who gave a Gaussian distribution model of velocity [21] and a probabilistic models by Fokker and Planck [22, 23]. The mathematical formalism has been an integral part of statistical thermodynamics over the past century, however, the exact physical mechanism of the origin of Brownian motion and irregular trajectories remains a topic of debate [24, 25]. Another key issue is lack of knowledge on mechanical aspect of Langevin equation and the thermal aspects of thermal reservoir [26], although, it was briefly touched by Feynman in his thermal ratchet model [27].

2. Asymmetric phase space trajectories in thermodynamic work

We consider a set of oscillators, each comprising of a spring-mass system, immersed in a thermal reservoir comprising of gas molecules at a temperatures T (figure 1). We assume that the molecules in the reservoir have instantaneous velocities $v_i(t)$ which have Maxwell distribution. The average kinetic energy per molecule is related to the Boltzmann energy by the relationship, $(1/2)mv_m^2 = (3/2)k_B T$, where, k_B is Boltzmann constant, m represents the mass of a molecule, v_m is its mean velocity. Each of the oscillators is being hit by gas molecules transferring the kinetic energy of the molecules to the oscillator's mass which is passed on to the compressive energy of the spring. Equating the maximum kinetic energy of the oscillator's mass to the compression energy of the spring, we get, $mv_{iM}^2/2 = kx_{iM}^2/2$, where, v_{iM} is the maximum value of mass and x_{iM} , is the maximum compression of the spring and k is the spring constant. It leads to the following expression,

$$x_{iM} = v_{iM} \sqrt{\frac{m}{k}} = \frac{v_{iM}}{\omega}, \quad (1)$$

where ω is frequency of oscillation of the mass. As angular frequency is the rate of change of phase, θ with respect to time, t , i.e. $\omega = d\theta/dt$, the above analysis appears to violate the second law of thermodynamics, as it would mean deriving finite amount of work from a single thermal reservoir operating at a single temperature. Hence, $\omega = d\theta/dt \neq 0$, only for an infinitesimally small period of time and $d\theta = \omega dt = 0$ at each of the equilibrium

states associated with heat transfer. It implies that any interaction between the thermal reservoir and the oscillator, which imparts a finite phase to the oscillator is cancelled out within a short time frame resulting in a net phase change of zero.

In a system comprising of N oscillators, where the displacement of the i th spring is $x_i(t)$, the energy stored can be correlated to the kinetic energy of the masses at equilibrium, which implies that $(1/2)\sum_i^N m(v_i^2) = (1/2)\sum_i^N k_i x_i(t)^2$. Taking the partial derivative with displacement, we get,

$$\sum_i^N m_i \mathbf{v}_i \nabla \cdot \mathbf{v}_i = \sum_i^N k_i x_i(t) \quad (2)$$

At equilibrium, the following relationship holds for all velocities \mathbf{v}_i ,

$$\sum_i^N \mathbf{v}_i \nabla \cdot \mathbf{v}_i = \sum_i^N \frac{\partial \mathbf{v}_i}{\partial t} = \sum_i^N \omega_i \mathbf{v}_i = \sum_i^N \omega_i \sum_i^N \mathbf{v}_i = 0 \quad (3)$$

Equation (3) represents the fact that a set of oscillators immersed in a thermal reservoir in a given equilibrium have phase symmetry or $\sum_i^N d\theta_i/dt = 0$. Thus, in the context of a set of oscillators interacting with a thermal reservoir under thermodynamic equilibrium, not only the vector sum of velocity components are zero, but also the sum of phase variations are zero. In other words, the trajectory of phase of a particle along the temporal dimension, which we can refer as the phase domain trajectory, can give an indication of the nature of interactions within a system. In the context of heat transfer to a set of oscillators, the intermediate equilibrium states have a zero change in phase, i.e. $\sum_i^N d\theta_i = 0$. Hence, it can be stated that heat transfer is associated with symmetry of the phase domain trajectories as the phase has temporal invariance.

When the gas molecules in the thermal reservoir are subjected to work under compression, equation (3) has a finite value and the set of oscillators can generate finite amount of work. It can be stated that generation of work is associated with generation of asymmetric phase domain trajectories as $\sum_i^N \theta_i \neq 0$.

The symmetry in trajectory of particles at a given thermodynamic equilibrium is also reflected in the phase space diagram in the sense that the average momentum of a particle is zero as for every value of momentum of $+\mathbf{p}$, for a gas molecule moving in the $+\mathbf{q}$ direction, there is another molecule moving in the $-\mathbf{q}$, there is a negative value of \mathbf{p} leading to net zero momentum flux at all instants of time. Hence, $\nabla \cdot \mathbf{p}_i = 0$, where, $\mathbf{p}_i = 0$ is momentum of the i th particle. The vector sum of momentum and position change is zero, i.e.

$$\sum_{i=1}^N \mathbf{p}_i \sum_{i=1}^N \mathbf{q}_i = 0 \quad (4)$$

Under reversible isochoric heat transfer, the phase space volume spreads out along the dimension of momentum only while there is no change in the value of \mathbf{q}_i i.e. $\delta \mathbf{q}_i = 0$. Under energy transfer, the evolution of the trajectories in the given phase space are defined by,

$$\sum_{i=1}^N (\delta \mathbf{p}_i) \delta \mathbf{q}_i = \delta E \delta t \quad (5)$$

The possible evolution of phase space diagram under heat transfer, at a given equilibrium, is graphically illustrated in figure 2(a), where $\nabla \cdot \mathbf{v}_i = 0$. The expression of equation (5), expresses the fact that an input energy leads to an increase in a change in momentum, but the exact trajectory in the phase space diagram is lost under the constraints of the system.

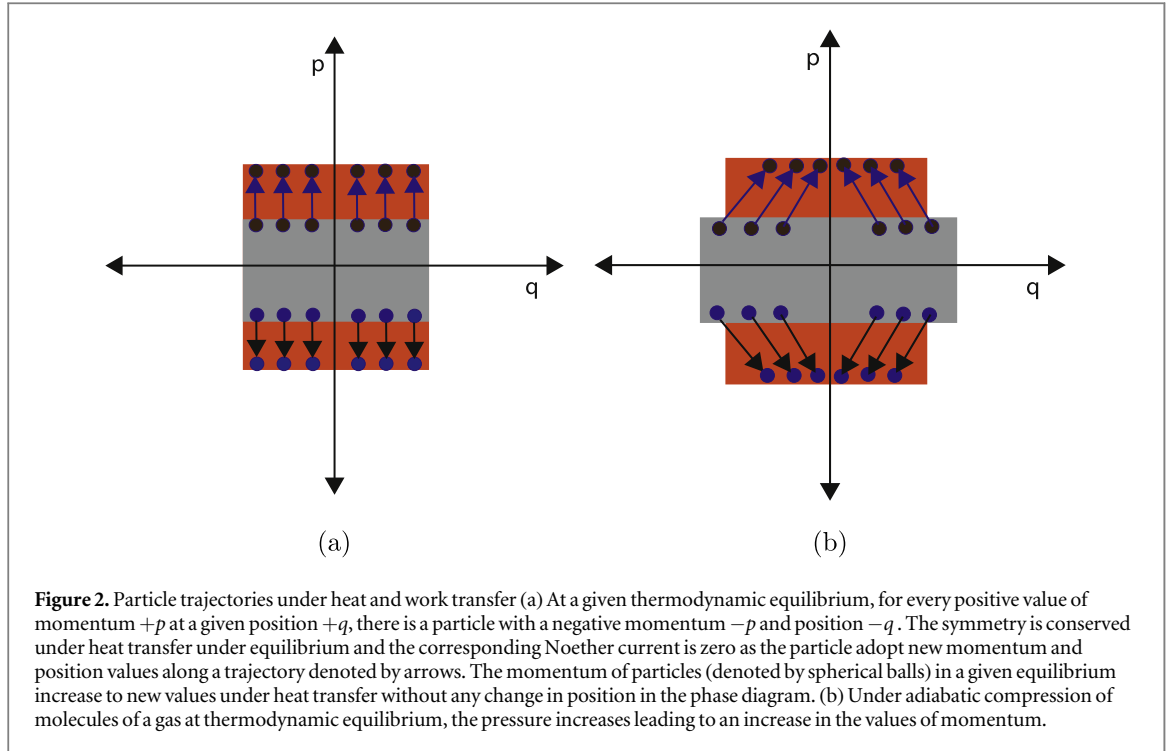
While considering the context of adiabatic work, changes in position as well as momentum of the particles appear in the phase space evolution as illustrated in figure 2(b) and $\nabla \cdot \mathbf{p}_i \neq 0$. Going back to the example of a set of oscillators illustrated in figure 1, transfer of adiabatic work leads to a finite amount of phase, i.e.

$$\theta = \int_0^T \omega dt \neq 0.$$

The analysis of phase trajectories in the context of adiabatic work implies that work is associated with generation of asymmetric phase trajectories which can lead to measurable values of frequencies of constituent elements in a dynamic system while such trajectories are absent under heat transfer. Here, the temporal changes in phases of particles are different from the asymmetric phase trajectories in a dynamic system under interaction with a conservative force field.

Thus, we can say that heat is associated with a system where the phase domain trajectories as well as phase space trajectories are symmetric while work has asymmetric phase domain trajectories as well as asymmetric phase space trajectories having a specific set of frequencies.

The analysis of work and heat based on particle trajectories in the phase space diagram offers novel insights into the nature of thermal reservoirs. A system, acting as a thermal reservoir must be able to annihilate the asymmetric trajectories of a particle in the phase space diagram. At the same time, it must not drive the particle any specific value of momentum or position, as it would mean transfer of finite work to the system.



3. Inadequacies in current models on Thermal reservoir

An emergent challenge in the current context is associated with the nature of phase domain trajectories when a set of particles interact with a thermal reservoir under Brownian motion. The discussion so far on asymmetric phase domain trajectories in work and symmetric phase trajectories in heat transfer gives some insights on the nature of a thermal reservoir. The fluctuations of a simple harmonic oscillator under interaction with a thermal reservoir, which is described using Langevin equation [19, 20], where the interaction force $F(t)$ contains a slowly varying part tending to restore the charge centre to equilibrium and a rapidly fluctuating force whose average value vanishes is expressed by,

$$F(t) = m \frac{d^2 y}{dt^2} = -\alpha \dot{y} + -ky + \xi(t) \quad (6)$$

Here, y is the displacement of the mass, $\xi(t)$ is the fluctuating force representing interaction with the thermal reservoir, has the property $\langle \xi(0)\xi(t) \rangle = 2\alpha k_B T \delta(t)$, $\delta(t)$ is the Kronecker delta function and α is the drag coefficient given by, $\alpha = (1/2k_B T) \int_{-\infty}^{\infty} F(0)F(t)dt$. Taking the Laplace transform of equation (6) and separating the terms, we can get the expression for displacement away from its mean position as,

$$x(s) = \frac{\xi(s)}{m(\omega_n^2 + 2\zeta_n \omega_n s + s^2)} \quad (7)$$

Here, $s = \omega\sqrt{-1}$, where ω is the angular frequency of fluctuating field arising out of thermal interactions, ω_n is resonant frequency of the oscillator and $\zeta_m = \alpha/(2m\omega_m)$ is the mechanical damping coefficient. As the random fluctuating function representing interaction with the thermal reservoir has the property $\langle \xi(0)\xi(t) \rangle = 2\alpha k_B T \delta(t)$, the spectral density can be written as its Fourier Transform,

$$S_{\mathfrak{R}}(\omega) = \int_{-\infty}^{\infty} dt e^{-j\omega t} \langle \xi(t_1)\xi(t_2) \rangle = \xi(\omega_1)\xi(\omega_1) = 2\alpha k_B T \quad (8)$$

The spectral density is proportional to $x|\omega|^2$, hence, we can write,

$$S_{\mathfrak{R}}(\omega) = \frac{2\alpha k_B T}{m^2(\omega_n^2 + 2\zeta\omega_n s + s^2)^2} \quad (9)$$

Thus, the spectral density, of net displacement can be written as,

$$y(\omega) = \frac{\sqrt{2\alpha k_B T}}{m(\omega_n^2 + 2\zeta\omega_n s + s^2)} \quad (10)$$

Substituting, $\alpha = 2\zeta m\omega_n$ in the numerator of equation (10), we get $2\sqrt{\zeta\omega_n k_B T m}$. Its time domain representation is written as,

$$y(t) = 2\sqrt{\frac{\zeta k_B T}{m\omega_n(1-\zeta^2)}} e^{-\zeta\omega_n t} \sin(\omega_n \sqrt{1-\zeta^2} t) \quad (11)$$

The time and frequency domain representations of the response are illustrated in figures 4(a) and (b) respectively. Equation (11) illustrates the annihilation of the spatial trajectory of dynamic system under interaction with a thermal reservoir. This aspect is well known in the existing scientific literature, however the graphs underscores that interaction with a thermal reservoir leads to annihilation of spatial trajectories of an oscillator, hence, a mathematical model of a thermal reservoir must incorporate this critical physical aspect.

According to the oscillator model on thermal reservoir by Ford, Kac and Mazur, a thermal reservoir can be modeled using a system of coupled harmonic oscillators and coupling of a particle to the reservoir will generate Brownian motion [28]. The work was further refined by Zwanzig, where he defines the Hamiltonian of a thermal reservoir as [29],

$$H_B = \sum_j \left(\frac{p_j^2}{2} + \frac{1}{2} \omega_j^2 \left(q_j - \frac{\gamma_j}{\omega_j^2} x \right)^2 \right) \quad (12)$$

where p_j is conjugate momentum and q_j is a set of coordinates, x is displacement, ω_j is the frequency of the j th oscillator, γ_j indicates the strength of coupling of the system to the j th oscillator. The Hamiltonian of a system S of mass m , momentum p immersed in a potential well $U(x)$ can be expressed as, $H_S = p^2/2m + U(x)$ [30]. The equations of motion of the system comprising the particle and the thermal reservoir with a Hamiltonian $H_S + H_B$, is expressed as [29],

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -U'(x) + \sum_j \gamma_j \left(q_j - \frac{\gamma_j}{\omega_j^2} x \right) \quad (13)$$

$$\frac{dq_j}{dt} = p_j, \quad \frac{dp_j}{dt} = -\omega_j^2 q_j + \gamma_j x \quad (14)$$

The dynamics of thermal reservoir oscillators is expressed as [29],

$$q_j(t) = q_j(0) \cos \omega_j t + p_j(0) \frac{\sin \omega_j t}{\omega_j} + \gamma_j \int_0^t d\tau x(\tau) \frac{\sin \omega_j(t-\tau)}{\omega_j} \quad (15)$$

where $x(\tau)$ is the position of the particle of system S at time τ . Integrating it by parts and using the expression dp/dt , we get,

$$\frac{dp}{dt} = -U'(x(t)) - \int_0^t d\tau K(\tau) \frac{p(t-\tau)}{m} + F_p(t) \quad (16)$$

where the memory function is, $K(t) = \sum_j \frac{\gamma_j^2}{\omega_j^2} \cos \omega_j t$ and the noise is [29]

$$F_p(t) = \sum_j \gamma_j p_j(0) \frac{\sin \omega_j t}{\omega_j} + \sum_j \gamma_j \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x \right) \cos \omega_j t \quad (17)$$

The initial conditions of the thermal reservoir are derived from the distribution $f_{eq}(p, q) \propto e^{-H_B/k_B T}$. The thermal reservoir is in thermal equilibrium with a constrained coordinate system $x(0)$. The average of q and p are [29],

$$\left\langle q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right\rangle = 0, \quad \langle p_j(0) \rangle = 0 \quad (18)$$

The second moments are expressed as [29],

$$\left\langle \left(q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0) \right)^2 \right\rangle = \frac{k_B T}{\omega_j^2}, \quad \langle p_j(0)^2 \rangle = k_B T \quad (19)$$

which leads to the express of fluctuation-dissipation theorem [1],

$$\langle F_p(t) F_p(t') \rangle = k_B T K(t-t') \quad (20)$$

Another related model of heat bath by Ford, Lewis, and O'connell developed for quantum systems, considers a heat bath as a set of oscillators [31]. The Hamiltonian of an oscillator of momentum p , a force constant k , a displacement, x , immersed in a heat bath is expressed as [31],

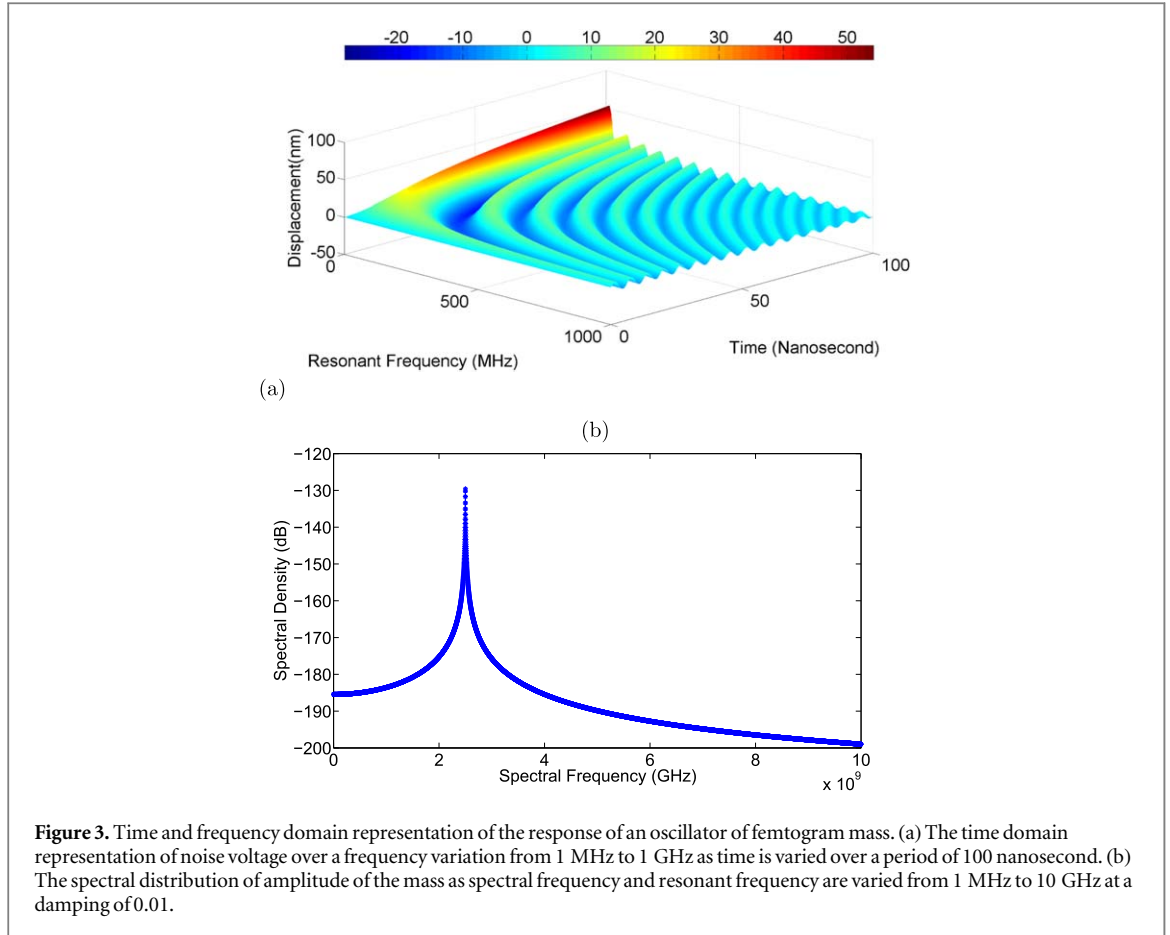


Figure 3. Time and frequency domain representation of the response of an oscillator of femtogram mass. (a) The time domain representation of noise voltage over a frequency variation from 1 MHz to 1 GHz as time is varied over a period of 100 nanosecond. (b) The spectral distribution of amplitude of the mass as spectral frequency and resonant frequency are varied from 1 MHz to 10 GHz at a damping of 0.01.

$$\frac{p^2}{2} + k\frac{x^2}{2} + \sum_j \left[\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2(q_j - x)^2 \right] \quad (21)$$

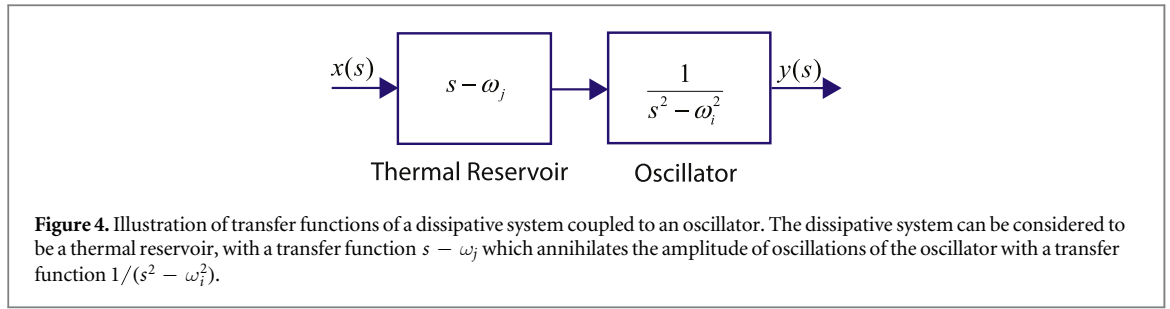
where, p_j is the momentum of the particle, m_j is mass, q_j is displacement associated with the mass of the j th oscillator. In equation (21), $q_j - x$ is displacement due to coupling between heat bath and the external oscillator. The model is inspired by related work by Ullersma, which considers a heat bath as comprising of a number of small oscillators of different resonant frequencies [32].

If we assume heat bath to be comprised of a number of simple harmonic oscillators of progressively increasing frequencies, the input on a dynamic system coupled to it can be expressed as, $\sum_1^N y_n \sin \omega_n t$, where, n is an integer, which varies from 1 to N . The output amplitude of an oscillator of a resonant frequency ω_k , which is brought in contact with one the heat bath, can be expressed by the following equation,

$$\frac{d^2y}{dt^2} + 2\zeta\omega_k\frac{dy}{dt} + \omega_k^2y = \sum_1^n y_n \sin \omega_n t \quad (22)$$

It is likely that the oscillator would be excited at its resonant mode, when, $\omega_k = \omega_n$ and it can generate a significant amount of work under such conditions. Thus, the overall impact of such a heat bath would be to impart a finite work to the oscillator. The impact of thermal fluctuations on an oscillator is an exponentially decaying response with time as illustrated in figure 3(b). However, when the a system is acted on by a plurality of oscillators, decay at one specific frequency will be compensated by excitation at some other frequency with an enhanced response around its resonant modes. Thus, the fundamental problem with the model of thermal reservoir comprising of a plurality of oscillators is that the frequency domain response of the system has finite amplitude and frequency which can be associated with finite amount of work. It implies that finite amount of work can be derived from a thermal reservoir by an oscillator due to finite amount of coupling. This is counter intuitive as the primary role of a thermal reservoir is to annihilate the energy of an oscillator under steady state condition. The ideal model of thermal reservoir should be such that the asymmetric phase trajectories of the particles are lost.

The exact nature by which the Boltzmann energy of a thermal reservoir gets coupled to a dynamic system and exerts a fluctuating force is not known. The Langevin equation based approach, which condenses the role of a thermal reservoir in a fluctuating function, also implies that the time domain representation of a thermal reservoir can be denoted by a Dirac Delta function at a time t , whose frequency domain representation is a unity



function comprising of a plurality of resonant modes or poles. It can be represented mathematically as,

$$\frac{d^2y}{dt^2} + 2\zeta\omega_k \frac{dy}{dt} + \omega_k^2 y = \delta(t) \quad (23)$$

Its time domain response is an exponentially decaying sinusoidal function.

$$y(t) = \frac{1}{\omega_n \sqrt{1 - \zeta^2}} e^{-\zeta\omega_n t} \sin(\omega_n \sqrt{1 - \zeta^2} t) \quad (24)$$

Here, we assume that $0 < \zeta < 1$. Such a model also does not truly represent a heat baths as, it implies that by coupling a number of oscillators of varying resonance frequencies and phases, in a thermal reservoir, a finite amount of work can be extracted at a given time, which appears to violate the second law of thermodynamics. Hence a new model of thermal reservoir is needed which describes its dissipative effect on a dynamic system.

4. Towards a new model of thermal reservoir

The primary physical characteristic of a thermal reservoir is that an oscillator connected to it loses its energy leading to annihilation of its phase change and amplitude. The dynamic equation of a mass with displacement, $x(t)$, unity mass, in a medium with coefficient of viscosity, α , is written as, $d^2x(t)/dt^2 - \alpha dx(t)/dt = 0$. The related equation for an oscillator with a unity mass, a resonant frequency, ω_i and displacement, $y(t)$, is, $d^2y(t)/dt^2 - \omega_i^2 y(t) = 0$. The differential equation for the two coupled systems, where the oscillator's amplitude interacts with the viscous system and eventually loses all its energy, is,

$$\frac{d^2y(t)}{dt^2} - \omega_i^2 y(t) = \frac{d^2x(t)}{dt^2} - \alpha_j \frac{x(t)}{dt} \quad (25)$$

Taking the Laplace Transform of equation (25) and separating the terms related to displacements, we get,

$$\frac{y(s)}{x(s)} = \frac{(s^2 - s\omega_j)}{(s^2 - \omega_i^2)} = \frac{s(s - \omega_j)}{(s - \omega_i)(s + \omega_i)} \quad (26)$$

where, $s = \omega\sqrt{-1}$, denotes the angular frequency of external excitation and $\omega_j = \alpha/m$. The analysis indicates that interaction between a system having a resonant frequency with a dissipative system can be modeled using a transfer function, having a pole at ω_j and zeros at $\pm\omega_i$. The dissipative system, which represents a thermal reservoir has got two poles and the oscillator has got two zeros as illustrated in figure 4. Its time domain representation, which represents the associated Green's function of the system, is expressed as,

$$\delta(t) + \frac{\omega_i - \omega_j}{\sqrt{\omega_i}} \left(\frac{e^{\sqrt{\omega_i}t} - e^{-\sqrt{\omega_i}t}}{2} \right) \quad (27)$$

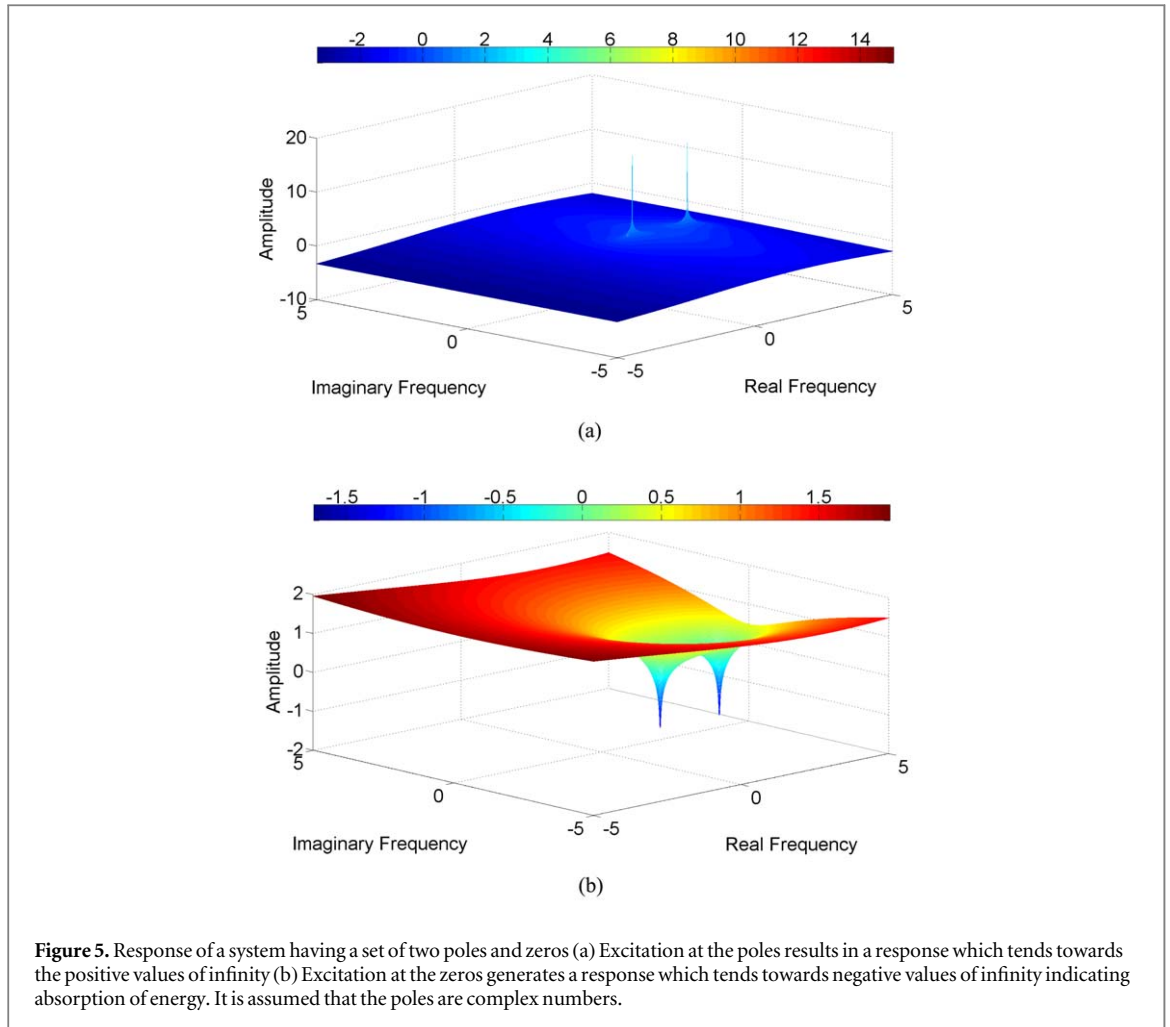
If the oscillator interacts with M such systems, each having one pole, it loses energy under each interaction and its overall response can be written as,

$$y(s) = \frac{\prod_{j=1}^M (s - \omega_j)}{(\omega_i^2 + s^2)} \quad (28)$$

Thus, the transfer function of a thermal reservoir can be denoted as,

$$T(s) = \prod_{j=1}^M (s - \omega_j) \quad (29)$$

As the oscillator interacts with the thermal reservoir, its spatial trajectory is annihilated. In order to address the above issues, we present a novel model of thermal reservoir comprising of a combination of poles and zeros, which gives a more accurate representation of a thermal reservoir.



The theoretical construct of an appropriate Green's function for a thermal reservoir is much more complicated in comparison to a typical dynamic system. For example, for a dynamic system, having a set of resonant frequencies can be represented by a transfer function having a set of poles at ω_k and ω_l [33] and can be written as,

$$H(s) = \frac{1}{(s - \omega_k)(s - \omega_l)} \quad (30)$$

Its time domain representation is denoted by,

$$h(t) = \frac{e^{\omega_k t} - e^{\omega_l t}}{\omega_k - \omega_l} \quad (31)$$

Equation (31), basically represents the Green's function for the system. The response of the system is the highest at its resonant frequencies. A graphical illustration of the impulse response of a system comprising two poles and two zeros is shown in figure 5, where figure 4(a) shows two peaks corresponding to the excitation at resonant frequencies. Similarly, figure 4(b), illustrates the response where the system is excited at its zeros.

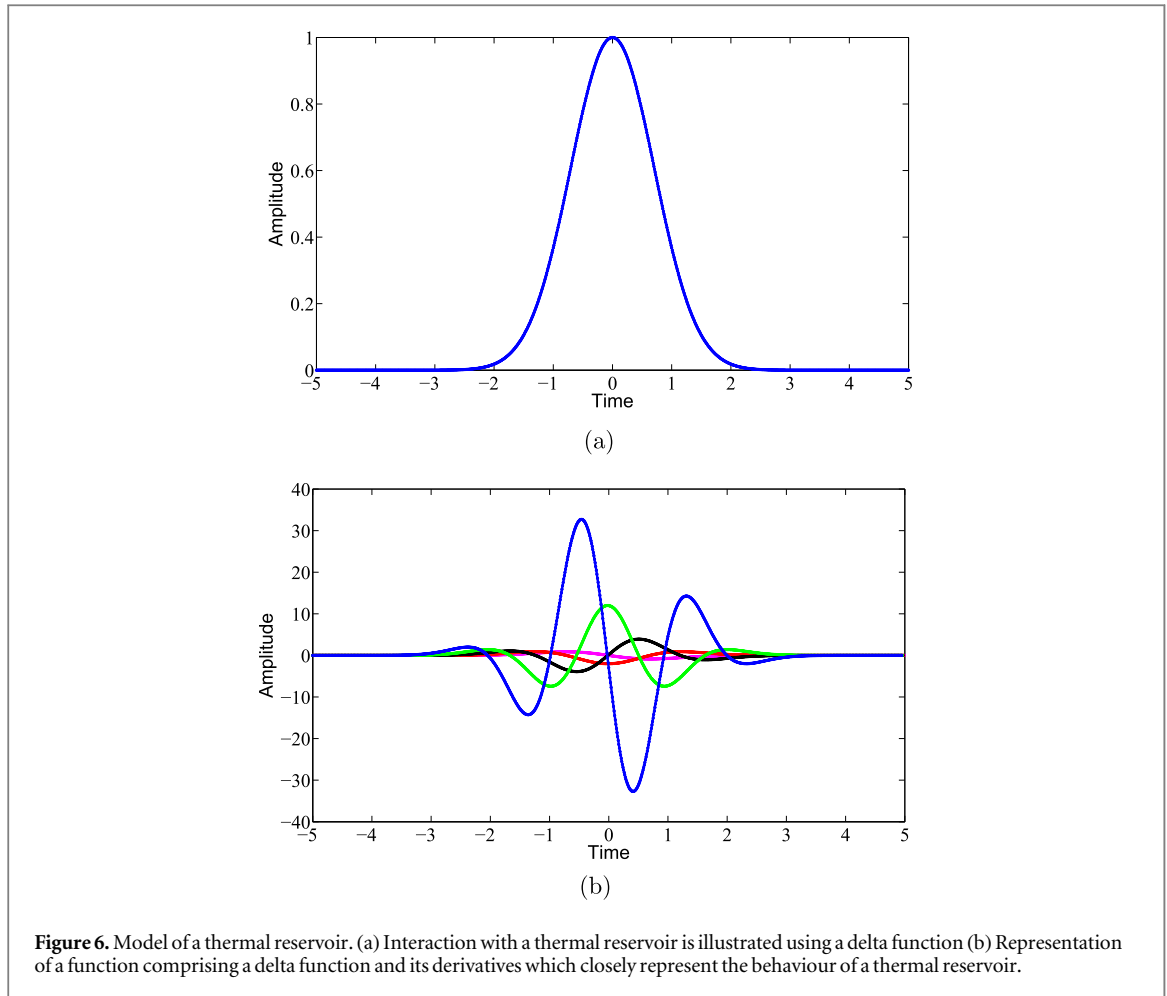
The transfer function of a given thermal reservoir with a zero at ω_k , is expressed as, $(s - \omega_k)$ and the time domain representation is, $\omega_k \delta(t) + \delta'(t)$. If the system has two zeros at ω_k and ω_l , the corresponding transfer function is expressed as,

$$H(s) = (s - \omega_k)(s - \omega_l) \quad (32)$$

Its time domain representation is denoted by,

$$h(t) = \omega_k \omega_l \delta(t) + \omega_k \delta'(t) + \omega_l \delta'(t) + \delta''(t) \quad (33)$$

For higher number of zeros, the expression becomes more complicated but has a series comprising of delta functions and its derivatives along with the set of frequencies as coefficients. For example, if the system has three zeros at ω_k , ω_l and ω_m , its transfer function is, $h(s) = (s - \omega_k)(s - \omega_l)(s - \omega_m)$ and the corresponding impulse response or the Green's function is,



$$h(t) = \delta(t)(\omega_k\omega_l + \omega_k\omega_m + \omega_l\omega_m) + \delta'''(t) - \delta''(t) * (\omega_k + \omega_l + \omega_m) - \omega_k\omega_l\omega_m\delta(t) \quad (34)$$

The analysis indicates that if the number of poles are M , the impulse response will have the following form

$$a_1\delta(t) + a_2\delta'(t) + a_3\delta''(t) + \dots a_n\delta^n(t) \quad (35)$$

where, $a_1, a_2, a_3, \dots, a_n$ are coefficients which represent the combination of frequencies which denote the poles. The time domain representation of the function highlights the role of the zeros in initiating damping at the start of the process.

A Gaussian function is an approximation of a delta function which is illustrated in figure 6(a) [34]. A signal comprising a series of delta functions and its derivatives would have a form factor similar to figure 6(b). Thus, it could be argued that excitation of a system at its resonant frequencies or its poles enhance its response while the zeros impart a series of impulse like effect to the function resulting in its attenuation in the time domain.

Currently, the thermal reservoirs are defined from the perspective of comprising of a number of poles which is the characteristic feature of an oscillator. An alternative perspective of a thermal reservoir is that of a system which generates an impulse function. Both the approaches only partially represents the physical behaviour of a thermal reservoir.

The analysis also indicates that finite thermal reservoirs can be designed for specific systems having well defined oscillations. For example the transfer function of a circuit comprising a resistor R , inductor L , and a capacitor C , in series, circuit where the output is connected across the inductor and resistor element has the following transfer function [35],

$$V(s) = \frac{R + sL}{1/(sC) + R + sL} \quad (36)$$

If the circuit is coupled to an electrical oscillator of resonance mode at R/L , the output response can be made zero. Thus, the circuit would act like a finite thermal reservoir corresponding to the given oscillator. Such finite thermal reservoirs can be of used in controlling the vibrational modes of systems like optical tweezers used to control the dynamics of molecules in specific potential wells [36].

In recent years, a number of experiments have been carried out on cooling using microcantilevers using pulses of laser light [37–39]. In such experiments, the amplitude of microcantilever vibrations are slowed down

by transferring energy, which is phase displaced by 180° with the oscillator's vibrations. Thus, the system is cooled down by coupling it with some kind of active thermal reservoir, which absorbs the kinetic energy of the system, bringing it to a lower temperature. The dynamics of such a system can be represented by the following equation,

$$y(\omega) = \frac{s - \alpha}{\omega_n^2 + 2\zeta\omega_n s + s^2} \quad (37)$$

Its time domain response is,

$$e^{-\zeta\omega_n t} \left[\cosh w_n \sqrt{t(\zeta^2 - 1)} - \frac{(\alpha + w_n \zeta) \sinh w_n t \sqrt{\zeta^2 - 1}}{w_n \sqrt{\zeta^2 - 1}} \right] \quad (38)$$

The $s - \alpha$ term in the numerator plays an active role in accelerating the process of damping of the amplitude. It is similar in form to the response function derived by Metzger and Karrai on cooling a microlever using laser pulses [37] (Please see the coefficient $(1/(1 + j\omega\tau_n))$ of numerator of equation (2) in [37], which can be expressed as $(1 - j\omega\tau_n)$ under Taylor expansion). A relatively more complex heat bath can be constructed by adding related terms in the numerator.

Currently, thermal reservoirs are assumed to be of infinite physical size. However, the most important physical aspect of a thermal reservoir is the fact that it should be able to annihilate the amplitudes of a dynamic system coupled to it. Based on the transfer function based formulation of a thermal reservoir, an artificial thermal reservoir, which is comparable to the size of a dynamic system can be created by having an active system within it which generates modes corresponding to the existing resonant modes of the system. For example, if an oscillator has a set of resonant modes between f_i and f_j , a thermal reservoir of any size can be defined which has zeros lying in the range of f_i and f_j which can annihilate the momentum current associated with the resonant modes. Thus, a thermal reservoir can be designed in terms of the key resonant modes which need to be annihilated instead of a large thermal reservoir having infinite number of modes. At a physical level, all materials have finite amount of elasticity whose impulse response can be represented as a collection of simple harmonic oscillators having a set of poles. Thus, finite sized thermal reservoirs can be designed in order to suppress the selective modes.

5. Discussion

The concept of modeling a system from the perspective of a simple harmonic oscillator is widely used in quantum mechanics [40, 41] where interactions between two systems are considered as coupling between two oscillators with specific resonant modes. The principle can be used to model a macroscopic classical system comprising of different resonant modes and damping coefficients. However, a thermal reservoir is a special system, having a macroscopic collection of particles, which annihilates the trajectories of a particle with which it interacts. Although some aspects of the dynamics can be certainly modeled using a set of coupled harmonic oscillators, its global impact on a particle is to bring it down at an equilibrium where, the initial energy is transformed into heat in an irreversible manner and in the process, it loses its momentum and asymmetric trajectory in the phase space diagram.

A set of oscillators have specific resonant modes, with poles, whose frequency domain response function can be represented as $\sum_i^N 1/(s - \omega_n)$, where i varies from 1 to N . Any kind of interaction with another oscillator will generate a finite response which can be construed as work, which appears contrary to empirical observations during interaction between a particle and a thermal reservoir.

Representation of a thermal reservoir with a delta function also does not address the key problem as it would again induce finite response in the system in the time domain as well as frequency domain. Under such interactions, finite amount of work can be derived from the system, which is again, contrary to empirical observations on interaction between a particle and a thermal reservoir.

A better mathematical model of a heat bath would comprise of a system comprising a set of zeros, which interact with a harmonic oscillator to generate a response which drives the system's output to zero. In the time domain, such a system would comprise of a number of delta functions, its derivatives and related combinations, which would truly represent a give thermal reservoir. The model can more accurately represent physical interactions, where the thermal reservoir is of finite size and the system is able to transfer its energy to it within a finite amount of time.

6. Conclusion

The fundamental conclusion of the current work is the observation that phase space trajectories associated with generation of work has asymmetric form while the corresponding trajectories associated with transfer of heat has a symmetric form. In other words, during transfer of energy as work, the constituent particles comprising a system, develop finite values of phase changes and frequencies while generation of heat annihilates the phases and related frequencies. Thus, by analyzing the phase domain trajectories, a clear distinction between heat and work can be defined at the microscopic scale with limited degrees of freedom. The concept has been used to define a thermal reservoir as a dynamic system which annihilates the asymmetric phase space trajectories of a dynamic system. Thus, at a mathematical level, a thermal reservoir can be defined as a system comprising a set of poles, whose symmetry leads to annihilation of asymmetric phase space trajectories of an oscillator. The novel model of thermal reservoir addresses some of the conceptual problems related to current models which consider thermal reservoirs as comprising of a set of harmonic oscillators.

Competing interest

The author declares no competing interests.

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