Dynamics of a mechanical system with multiple degrees of freedom out of thermal equilibrium

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Out of thermal equilibrium, an environment imposes effective mechanical forces on nanofabricated devices as well as on microscopic chemical or biological systems. Here we address the question of how to calculate these forces together with the response of the system from first principles. We show that an ideal gaslike environment, even near thermal equilibrium, can enforce a specific steady state on the system by creating effective potentials in otherwise homogeneous space. An example of stable and unstable rectifications of thermal fluctuations is presented using a modified Feynman-Smoluchowski ratchet with two degrees of freedom. Moreover, the stability of a steady configuration depends on its chiral symmetry. The transition rate probabilities and the corresponding kinetic equations are derived for a complex mechanical system with arbitrary degrees of freedom. This work, therefore, extends the applicability of mechanical systems as a toy model playground of statistical physics for active and living matter with multiple degrees of freedom.

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I. INTRODUCTION

Macroscopic machines become unstable and disintegrate after some threshold load. Stability is, therefore, an important factor in their design. The same issue will be important for nanodevices [1] when they develop to maximum capacity. The stability of future complex devices is a fundamental question of statistical physics regarding noninear dynamics out of thermal equilibrium. Dynamics depends on the interaction between the system's degrees of freedom and the forces that drive it out of thermal equilibrium.

A nonequilibrium environment affects the degrees of freedom of a small mechanical system. A chemical or nanofabricated device out of thermal equilibrium can experience effective forces even in the absence of external potentials [2]. There exist Brownian machines with a single relevant degree of freedom, such as a Feynman-Smoluchowski ratchet [3,4], capable of utilizing these effective forces to generate useful work out of thermal fluctuations. There is a significant knowledge gap as to how the same forces affect the dynamics of a system with multiple degrees of freedom, though there are theoretical and experimental efforts in this direction [5,6].

The subject of this work is a mechanical system composed of solid bodies that are connected by a rigid axis or free rotating joints [7,8]. The different parts of the system, preserving the connectivity, are immersed in reservoirs containing ideal gases. Elastic collisions with the gas particles cause the transitions of the system between its states. In the absence of external potentials, any configuration of a mechanical system possesses the same probability at thermal equilibrium under the condition of a thermodynamic limit, meaning the temperatures of all baths are equal, their volumes are large, and the mass of a gas particle is negligible relative to the mass of the system. Let us address the question of whether a specific configuration may be favored out of thermal equilibrium and how to calculate this configuration as a function of the properties of the system.

One advantage of a mechanical framework for a thermodynamic system is the possibility of treatment from first principles by modeling the thermal bath as a gas of small elastic particles [7,9]. The disadvantage is the apparent difference of the mechanical framework from the real and artificial nanosystems that are driven by chemical or optical sources out of thermal equilibrium [1]. Nevertheless, the mechanical Feynman-Smoluchowski ratchet was an inspiration for some chemical [10,11] and mechanical devices [5,12,13]. The ratchet mechanism is considered important for verification of fundamental theorems of statistical physics [14–16], and it is an essential property of molecular motors [17–23] (though alternative hypotheses regarding the motion of molecular motors do exist).

To the best of our knowledge, only systems with a single degree of freedom have been considered from first principles so far [7,24]. A system with at least two degrees of freedom, however, is required to investigate the phenomenon of interacting degrees of freedom and the influence of this phenomenon on the dynamics of a complex system out of thermal equilibrium.

In this article, we present an *ab initio* path from the elastic scattering of a single gas particle by a mechanical system to the transition rate probability between the states of the system and to the corresponding Masters-Boltzmann equation and the average velocities of the system's degrees of freedom as functions of the macroscopic parameters of the out-of-equilibrium environment (Onsager relations) [25], including the influence of the different degrees of freedom on each other. The stability of the steady state of the system depends on the interaction between its degrees of freedom and the effective forces imposed on the system by the environment. An interesting finding is that some of these forces persist even in a single temperature environment if the thermodynamic limit does not hold. In addition, the spatial asymmetry of the system's stable state, together with the corresponding directed motion, may possess preferred chiral symmetry. To make the discussion more visual, we demonstrate all these phenomena using a modified Feynman-Smoluchowski ratchet with two degrees of freedom.

II. BROWNIAN MOTOR WITH TWO DEGREES OF FREEDOM

Consider a dumbbell-like macroscopic body consisting of symmetric and asymmetric parts; see Fig. 1. These parts are rigidly connected to each other by a thin axis. Each part

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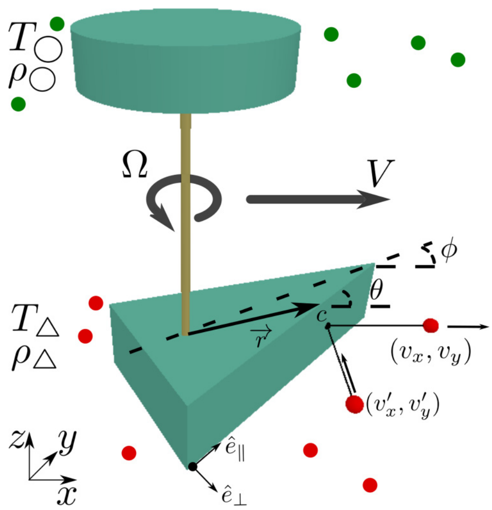

FIG. 1. Dumbbell structure with the asymmetric part in the form of an isosceles triangle with apex angle $2\theta_0$, which is connected to a symmetric part by a rigid axis. There are two-degrees-of freedom: translation velocity $V = \partial x/\partial t$ along the x coordinate and frequency $\Omega = \partial\phi/\partial t$, where ϕ is the angle between the median of the triangle and axis x. The symmetric part is immersed in a thermal bath composed of an ideal gas with elastic particles (blue circles) of mass m at temperature $T_\bigcirc$ and density $\rho_\bigcirc$. The symmetric part is in interaction with the particles (red points) of mass m at temperature $T_\triangle$ and density $\rho_\triangle$. The dynamics of the dumbbell structure is driven by scattering of the gas particles. Scattering from velocity (v'_x, v'_y) to (v_x, v_y) may occur at any point c along the surface of the structure. Change in the velocity and rotation frequency of the structure due to a single scattering event depends on the geometry of the surface of the structure at the point of scattering c, such as an angle θ between axis x and tangential of the surface and vector $\vec{r}$ from the axis of rotation to the point c. The total change in momentum and in the energy of the structure depends on the cumulative effect of the interactions at all points c along its surface. The structure is a Brownian motor and may possess an average velocity $\langle V\rangle \neq 0$ that takes its maximum absolute values when the triangle is directed along axis x, $\phi = 0,\pi$. Velocity $\langle V\rangle$ vanishes due to symmetry at $\phi = \pi/2, -\pi/2$. The main question is as follows: What is the stable direction ϕ of the dumbbell structure as a function of the thermal bath temperatures, the shape of the asymmetric part $\theta(c)$, and the position of the rotation axis?

is in contact with a dedicated thermal bath that constitutes an infinite reservoir of the ideal gas composed of identical particles of mass m at density $\rho_\triangle$ and temperature $T_\triangle$ around the asymmetric part, and density $\rho_\bigcirc$ and temperature $T_\bigcirc$ around the symmetric part. Gas particles in each thermal bath move only in the (x,y) plane with velocities (v_x, v_y) at Maxwell distribution with temperatures $T_\triangle$ and $T_\bigcirc$, respectively. The body possesses two degrees of freedom: First, it can move along the x axis with velocity V. Second, it can rotate around the z axis with frequency Ω. The rotation angle coordinate is ϕ. The kinetic energy of the body, therefore, is $MV^2/2 + I\Omega^2/2$, where M is the mass and I is the moment of inertia. Both degrees of freedom are translation-invariant because no external potential is present. The system is a multiple-degree-of-freedom version of a single-degree-of-freedom Triangulita motor [7], which is an elegant and simple version of the Feynman-Smoluchowski ratchet.

To analyze the dynamics and stability of dumbbell structures, one should calculate the velocity V and frequency Ω as a function of the corresponding coordinates x and ϕ. The first task is to derive transition probabilities $W(V,V')$ and $W(\Omega,\Omega')$ from velocity $V' \to V$ and frequency $\Omega' \to \Omega$ due to elastic scattering of the gas particles [7,24,26]. A single particle may scatter at any point c along the perimeter of the motor; see Fig. 1. Then, the transition probability rates W are averaged over the entire interaction in all points c and all velocities of the gas particles. Finally, the average moments of $\langle V^n\rangle$ and $\langle\Omega^n\rangle$ as functions of x and ϕ are calculated from W using a Kramers-Moyal expansion.

Consider the scattering of a single gas particle with mass m by a macroscopic body with mass M and moment of inertia I. In the frame of reference of the body, the conservation of energy, the momentum, the angular momentum, and the tangential velocity of the particle along the surface of the body are

$$\begin{aligned}
&-MV^2 - I\Omega^2 + m(v'_x - v_x)(v'_x + v_x)\\
&\quad + m(v'_y - v_y)(v'_y + v_y) = 0,\\
&\quad m(v'_x - v_x) = MV,\\
&\quad I\Omega + |r \times v| = |r \times v'|,\\
&\quad v'_x \sin\theta + v'_y \cos\theta = v_x \sin\theta + v_y \cos\theta,
\end{aligned} \tag{1}$$

where (v'_x, v'_y) are the velocities of the particle prior to collision. After the collision, the velocities of the gas particle together with the velocity and the rotation frequency of the body are (v_x, v_y), V, and Ω, respectively. Angle θ and radius $\vec{r}$ depend on the body's geometry and point c of the scattering along the surface of the body; see Fig. 1.

Let us define two geometric factors:

$$\Gamma_V(c) = \sin\theta, \quad \Gamma_\Omega(c) = r_x\cos\theta + r_y\sin\theta, \tag{2}$$

where c indicates a point of the scattering on the body's surface, and, therefore, defines angle θ and radius $\vec{r} = (r_x, r_y)$; see Fig. 1. This is a natural choice because the factors (2) define linear viscous coefficients for translation and rotation degrees of freedom, respectively. As an analogy only, a connection of Γ to the linear viscous coefficients may be inferred from the similarity between the equalities:

$$m^2\Delta v_x^2 + m^2\Delta v_y^2 = M^2V^2\frac{1}{\Gamma_V^2(c)} = I^2\Omega^2\frac{1}{\Gamma_\Omega^2(c)}, \tag{3}$$

where $\Delta v_i = v_i - v'_i$, and the expression for the diffusion coefficient of the body in velocity space according to the fluctuation dissipation theorem [27] is

$$D_V = \left\langle\frac{V^2}{\Delta t}\right\rangle = \frac{T\gamma_V}{M}, \tag{4}$$

where D_V is the diffusion coefficient in velocity space, and γ_V is the linear viscous coefficient. The similarity of (3) and (4) is evident under the assumption that $\sum\Delta v_i^2 \propto T$ at thermal equilibrium. Equalities (3) follow from (1). We will see later that these equalities and their connection to the linear viscous coefficients hold rigorously in the case of an arbitrary number of degrees of freedom.

After the transition to the laboratory frames of reference by adding velocity $(-V' + \Omega' r_y, -\Omega' r_x)$ and rotation frequency

$-\Omega$ to the degrees of freedom of the system, one gets

$$-\Delta V-\frac{M}{m}\Delta V\frac{G_V^2(c)}{\Gamma_V^2(c)}-2V'+\Omega'\frac{\Gamma_\Omega}{\Gamma_V}+2v'_x-2v'_y\frac{1}{\tan\theta}=0, \tag{5}$$

where $\Delta V=V-V'$, and

$$-\Delta\Omega-\frac{I}{m}\Delta\Omega\frac{G_\Omega^2(c)}{\Gamma_\Omega^2(c)}-2\Omega'+V'\frac{\Gamma_V}{\Gamma_\Omega}-2v'_x\frac{1}{r_y+r_x/\tan\theta}+2v'_y\frac{1}{r_y\tan\theta+r_x}=0, \tag{6}$$

where $\Delta\Omega=\Omega-\Omega'$. The coefficients G,

$$G_V^2=1+\frac{m}{I}\Gamma_\Omega^2,\quad G_\Omega^2=1+\frac{m}{M}\Gamma_V^2, \tag{7}$$

describe the interaction between degrees of freedom imposed by the environment. The terms $\Omega'\Gamma_\Omega/\Gamma_V$ and $V'\Gamma_V/\Gamma_\Omega$ correspond to the direct interaction of the degrees of freedom.

III. MECHANICAL SYSTEM WITH N DEGREES OF FREEDOM

Equations (5) and (6) can be written in a unified form for the case of an arbitrary number of degrees of freedom. For each degree of freedom, ξ holds:

$$-\Delta\dot X_\xi\left[1+\frac{M_\xi}{m}\left(\frac{G_\xi(c)}{\Gamma_\xi(c)}\right)^2\right]-2\dot X'_\xi+\sum_{\xi'\neq\xi}\frac{\Gamma_{\xi'}(c)}{\Gamma_\xi(c)}\dot X'_{\xi'}+g_{x,\xi}(c)v'_x+g_{y,\xi}(c)v'_y=0, \tag{8}$$

where $\dot X_\xi$ is the velocity such as V or Ω, and M_ξ is the mass such as M or I. Geometric factors Γ depend on the interaction channel with the thermal bath c, e.g., the point of collision in the case of the dumbbell structure; see Fig. 1. The effect of other degrees of freedom comes in the rescaling of the mass M_ξ by the factor

$$G_{\xi,i}^2(c)=1+\sum_{\xi'\neq\xi}\frac{m}{M_{\xi',i}}\Gamma_{\xi',i}^2(c), \tag{9}$$

and by the update of the velocity $\dot X'_\xi$ by other degrees of freedom, $\sum_{\xi'\neq\xi}\Gamma_{\xi'}/\Gamma_\xi\dot X'_{\xi'}$. The velocities v'_x and v'_y are velocities of the gas particle before the collision. The weights g_x and g_y fit the condition

$$g_{x,\xi}^2+g_{y,\xi}^2=\frac{1}{\Gamma_\xi^2}. \tag{10}$$

This condition holds for both (5) and (6). Later we will see that it is connected to the detailed balance at thermal equilibrium.

The averaging of (8) over all possible velocities of the colliding gas particles results in the transition rate probability W:

$$W(\dot X_\xi,\Delta\dot X_\xi)=\frac14\sum_i\rho_i\sqrt{\frac{m}{2\pi T_i}}\oint dc_i|\Delta\dot X_\xi|H\left\{\Delta\dot X_\xi\Gamma_{\xi,i}\left[1+\frac{M_\xi}{m}\left(\frac{G_{\xi,i}(c)}{\Gamma_{\xi,i}(c)}\right)^2\right]-\sum_{\xi'\neq\xi}\dot X_{\xi'}\Gamma_{\xi',i}(c)\right\}$$
$$\times\Gamma_{\xi,i}^2(c)\left[1+\frac{M_\xi}{m}\left(\frac{G_\xi(c)}{\Gamma_{\xi,i}(c)}\right)^2\right]^2\exp\left[-\frac{m\Gamma_{\xi,i}^2(c)\{\dot X_\xi-\frac12\sum_{\xi'\neq\xi}\frac{\Gamma_{\xi',i}}{\Gamma_{\xi,i}}\dot X_{\xi'}+\frac12[\Delta\dot X_\xi(\frac{M_\xi G_{\xi,i}^2(c)}{m\Gamma_{\xi,i}^2(c)}+1)]\}^2}{2T_i}\right], \tag{11}$$

where the index i goes over all thermal baths; see the Appendix for details. In the limit $G=1$ and $\sum_{\xi'\neq\xi}=0$, expression (11) converges to the results obtained for a single-degree-of-freedom system [7,24].

The transition rate probability in the form of (11) makes it possible to calculate the average velocities' momenta $\langle\dot X^n\rangle$ of a mechanical system as a function of the velocities of other degrees of freedom, the external forces, and the forces as a consequence of an out-of-equilibrium environment. This is done using a Kramers-Moyal expansion of the corresponding Masters-Boltzmann equation for the probability to possess a specific velocity:

$$\frac{\partial P(\dot X,t)}{\partial t}=\int W(\dot X-\Delta\dot X,\Delta\dot X)P(\dot X-\Delta\dot X,t)d\Delta\dot X-P(\dot X,t)\int W(\dot X,-\Delta\dot X)d\Delta\dot X, \tag{12}$$

with probability $P(\dot X,t)$ for velocity $\dot X$ at time t. This description is valid in the overdumped regime and if the velocities are uncorrelated. Therefore, we omit index ξ.

The first three moments are

$$\frac{\partial\langle\dot X\rangle}{\partial t}=\langle a_1(\dot X)\rangle,$$
$$\frac{\partial\langle\dot X^2\rangle}{\partial t}=2\langle\dot X a_1(\dot X)\rangle+\langle a_2(\dot X)\rangle,$$
$$\frac{\partial\langle\dot X^3\rangle}{\partial t}=3\langle\dot X^2a_1(\dot X)\rangle+3\langle\dot X a_2(\dot X)\rangle+\langle a_3(\dot X)\rangle, \tag{13}$$

where the coefficients a_n are defined by a Kramers-Moyal expansion:

$$\frac{\partial P(\dot X,t)}{\partial t}=\sum_{n=1}^\infty\frac{(-1)^n}{n!}\frac{d^n}{d\dot X^n}[a_n(\dot X)P(\dot X,t)], \tag{14}$$

where

$$a_n(\dot{X}) = \int \Delta\dot{X}^n W(\dot{X},\Delta\dot{X}) d\Delta\dot{X}, \tag{15}$$

and W corresponds to (A5).

To demonstrate the influence of thermal fluctuations in the system and to simplify the presentation, let us consider Kramers-Moyal expansion (13) in the case $\dot{X}_{\xi'} = 0$ for $\xi' \neq \xi$. Velocities of other degrees of freedom impose drag force that can be added later. The first three moments of the Kramers-Moyal expansion in this case are

$$\frac{\partial\langle\dot{X}\rangle}{\partial t} = \sum_i \rho_i \sqrt{\frac{T_i}{m}}\left[-\sqrt{\frac{T_i}{M_X}}\oint \frac{\Gamma_{\dot{X},i}(c)}{G^2_{\dot{X},i}(c)}\epsilon^1_{\dot{X}} - 2\sqrt{\frac{2}{\pi}}\oint \frac{\Gamma^2_{\dot{X},i}(c)}{G^2_{\dot{X},i}(c)}\langle\dot{X}\rangle\epsilon^2_{\dot{X}} + \left(\oint \frac{\Gamma^3_{\dot{X},i}}{G^4_{\dot{X},i}}\sqrt{\frac{T_i}{M_X}} - \oint \frac{\Gamma^3_{\dot{X},i}}{G^2_{\dot{X},i}}\sqrt{\frac{M_X}{T_i}}\langle\dot{X}^2\rangle\right)\epsilon^3_{\dot{X}}\right], \tag{16}$$

the second order:

$$\frac{\partial\langle\dot{X}^2\rangle}{\partial t} = \sum_i \rho_i \sqrt{\frac{T_i}{m}}\left[-2\sqrt{\frac{T_i}{M_X}}\oint \frac{\Gamma_{\dot{X},i}}{G^2_{\dot{X},i}}\langle\dot{X}\rangle\epsilon^1_{\dot{X}} + 4\sqrt{\frac{2}{\pi}}\left(\oint \frac{\Gamma^2_{\dot{X},i}}{G^4_{\dot{X},i}}\frac{T_i}{M_X} - \oint \frac{\Gamma^2_{\dot{X},i}}{G^2_{\dot{X},i}}\langle\dot{X}^2\rangle\right)\epsilon^2_{\dot{X}} \right.$$
$$\left. - 2\left(-4\oint \frac{\Gamma^3_{\dot{X},i}}{G^4_{\dot{X},i}}\sqrt{\frac{T_i}{M_X}}\langle\dot{X}\rangle + \sqrt{\frac{M_X}{T_i}}\oint \frac{\Gamma^3_{\dot{X},i}}{G^2_{\dot{X},i}}\langle\dot{X}^3\rangle\right)\epsilon^3_{\dot{X}}\right], \tag{17}$$

and the third order:

$$\frac{\partial\langle\dot{X}^3\rangle}{\partial t} = \sum_i \rho_i \sqrt{\frac{T_i}{m}}\left[-3\sqrt{\frac{T_i}{M_X}}\oint \frac{\Gamma_{\dot{X},i}}{G^2_{\dot{X},i}}\langle\dot{X}^2\rangle\epsilon^1_{\dot{X}} + 6\sqrt{\frac{2}{\pi}}\left(2\oint \frac{\Gamma^2_{\dot{X},i}}{G^4_{\dot{X},i}}\frac{T_i}{\sqrt{M_X}}\langle\dot{X}\rangle - \sqrt{M_X}\oint \frac{\Gamma^2_{\dot{X},i}}{G^2_{\dot{X},i}}\langle\dot{X}^3\rangle\right)\epsilon^2_{\dot{X}}\right], \tag{18}$$

where X is a coordinate, M_X is the mass of the corresponding degree of freedom, $\epsilon_{\dot{X}} = m/M_X$, the index i goes over the thermal baths, and the index ξ is omitted. The expressions (16), (17), and (18) are derived with the help of Wolfram MATHEMATICA software.

If there is no interaction between degrees of freedom, then $G = 1$ and Eqs. (16), (17), together with (18) converge to the corresponding results of the system with a single degree of freedom [26], taking into account that $\oint \Gamma = 0$. The nonvanishing term proportional to Γ/G^2 is, therefore, a unique property of systems with multiple degrees of freedom.

The leading term for the average velocity at a steady state follows from (16), (17), and (18), after neglecting the time derivatives, as

$$\langle\dot{X}_\xi\rangle_\Gamma = -\frac{1}{2\sqrt{M_\xi}}\sqrt{\frac{\pi}{2}}\frac{\sum_i \rho_i T_i \oint \frac{\Gamma_{\dot{X}_\xi,i}(c)}{G^2_{\dot{X}_\xi,i}(c)}}{\sum_i \rho_i T_i^{\frac{1}{2}} \oint \frac{\Gamma^2_{\dot{X}_\xi,i}(c)}{G^2_{\dot{X}_\xi,i}(c)}}\epsilon^{-1}_{\dot{X}_\xi}. \tag{19}$$

It is of the order $\epsilon^2_{\dot{X}_{\xi'}}/\epsilon_{\dot{X}_\xi}$ taking into account that $\oint \Gamma = 0$ and $1/G^2_{\dot{X}_\xi} \approx 1 - \epsilon^2_{\dot{X}_{\xi'}}\Gamma^2_{\dot{X}_{\xi'}}$. This result vanishes when $G = 1$, e.g., in the systems with a single degree of freedom.

The next-order contribution to the velocity is

$$\langle\dot{X}_\xi\rangle_{\Gamma^3} = \frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{\sum_i \rho_i\left(T_i \oint \frac{\Gamma^3_{\dot{X}_\xi,i}}{G^4_{\dot{X}_\xi,i}} - M_\xi \dot{X}^2_{0\xi}\oint \frac{\Gamma^3_{\dot{X}_\xi,i}}{G^2_{\dot{X}_\xi,i}}\right)}{\sum_i \rho_i T_i^{\frac{1}{2}} \oint \frac{\Gamma^2_{\dot{X}_\xi,i}(c)}{G^2_{\dot{X}_\xi,i}(c)}}\frac{\epsilon_{\dot{X}_\xi}}{\sqrt{M_\xi}}, \tag{20}$$

where

$$\dot{X}^2_{0\xi} = \frac{1}{M_\xi}\frac{\sum_i \rho_i T_i^{\frac{3}{2}} \frac{\Gamma^2_{\dot{X}_\xi,i}}{G^4_{\dot{X}_\xi,i}}}{\sum_i \rho_i T_i^{\frac{1}{2}} \frac{\Gamma^2_{\dot{X}_\xi,i}}{G^2_{\dot{X}_\xi,i}}}. \tag{21}$$

This term describes rectified Brownian velocity and remains finite even in the case of a single degree of freedom [7,24].

Brownian velocity (20) vanishes if the temperatures of all thermal baths are equal, $T_i = T_j$. The velocity (19), however, remains finite. It is still an out-of-equilibrium phenomenon because (19) vanishes at the thermodynamics limit $m/M \to 0$.

The drag force imposed on the degree of freedom ξ by all other degrees of freedom $\xi' \neq \xi$ is derived by substitution of finite velocities of other degrees of freedom, $\dot{X}_\xi \to \dot{X}_\xi - \frac{1}{2}\sum_{\xi'\neq\xi}\frac{\Gamma_{\xi',i}}{\Gamma_{\xi,i}}\dot{X}_{\xi'}$, to (16):

$$\langle\dot{X}_\xi\rangle = \frac{1}{2}\frac{\sum_{\xi'\neq\xi}\sum_i \rho_i T_i \langle\dot{X}_{\xi'}\rangle \oint \frac{\Gamma_{\dot{X}_\xi,i}(c)\Gamma_{\dot{X}_{\xi'},i}(c)}{G^2_{\dot{X}_\xi,i}(c)}}{\sum_i \rho_i T_i^{\frac{1}{2}} \oint \frac{\Gamma^2_{\dot{X}_\xi,i}(c)}{G^2_{\dot{X}_\xi,i}(c)}}. \tag{22}$$

It is important to note that by substituting (25) in (22), one gets the same order of magnitude as (19).

IV. STABILITY OF BROWNIAN MOTOR WITH TWO DEGREES OF FREEDOM

Following previous general results, the dynamics of a dumbbell structure near the point $\phi = 0$ can be presented as Onsager relations [25] with nonlinear corrections due to interaction between translation and rotation degrees of freedom:

$$\frac{\partial x}{\partial t} = \frac{F_x}{\gamma_x} + L_{x,\Delta T}\frac{\Delta T}{T^2} + L_{x,\phi}\frac{\partial \phi}{\partial t},$$
$$\frac{\partial \phi}{\partial t} = \frac{M}{\gamma_\phi} + L_{\phi,\phi}\phi + L_{\phi,x}\frac{\partial x}{\partial t}, \tag{23}$$

where $L_{x,\Delta T}$, $L_{\phi,\phi}$, $L_{\phi,x}$, and $L_{x,\phi}$ are Onsager coefficients: $L_{x,\Delta T}$ corresponds to the rectified velocity (20), $L_{\phi,\phi}$ corresponds to the effective force (19), while $L_{\phi,x}$ and $L_{x,\phi}$ describe the mutual influence of degrees of freedom (22). The linear viscosity for translation and rotation degrees of freedom is γ_x and γ_ϕ, respectively. Nonlinearity emerges because $L_{x,\phi}, L_{\phi,x} \propto \phi$ in the vicinity of $\phi \approx 0$ due to symmetry considerations. As a next step, we will evaluate these Onsager coefficients with the help of Eqs. (19), (20), and (22), and we will estimate the main properties of a dumbbell structure dynamics.

The linear dissipation coefficient $\gamma_\xi = \sum_i \gamma_{\xi,i}$ follows from (16):

$$\gamma_\xi = \sum_i 4\rho_i\sqrt{\frac{mT_i}{2\pi}}\oint_c \Gamma^2_{\dot{X}_\xi,i}(c). \tag{24}$$

At this moment, one can see the connection between Γ^2 and the linear dissipation coefficient.

The translation velocity of the dumbbell structure following (20) is

$$\langle V\rangle_{\rm rec} = \sqrt{\frac{m}{M}}\sqrt{\frac{\pi}{8M}}\frac{\sum_i \rho_i\left(T_i - MV_0^2\right)\oint_c \Gamma^3_{V,i}(c)}{\sum_i \rho_i T_i^{1/2}\oint_c \Gamma^2_{V,i}(c)}. \tag{25}$$

Near thermal equilibrium, it can be presented as a function of the affinity $\Delta T/T^2$:

$$\langle V\rangle_{\rm rec} = L_{x,\phi}\frac{\Delta T}{T^2}; \tag{26}$$

see Eq. (23). It corresponds to the rectified velocity of a Triangulita motor with a single translation degree of freedom [7,24,26]. Maximum velocity is achieved when $\phi = 0$ or $\phi = \pi$. No motion occurs for $\phi = \pi/2$ and $-\pi/2$ because $\oint \Gamma_V^3$ vanishes in these cases.

The rotation dynamics of the dumbbell structure depends on the interaction with the translation degree of freedom (22). The corresponding Onsager coefficient is

$$L_{\phi,x} = \frac{1}{2}\frac{S_\triangle \rho_\triangle T_\triangle^{1/2}\oint \Gamma_{\Omega,\triangle}\Gamma_{V,\triangle}}{\sum_{i=\triangle,\bigcirc}\rho_i T_i^{1/2}\oint \Gamma^2_{\Omega,i}}, \tag{27}$$

which vanishes at $\phi = 0$ due to symmetry considerations. In the vicinity of $\phi \approx 0$, one can write

$$L_{\phi,x} = K_{\phi,x}\phi, \tag{28}$$

where the coefficient K follows from (27). The effective rotation frequency imposed by the out-of-equilibrium environment (19) is

$$\langle\Omega\rangle_{\rm rec} = \frac{1}{2}\frac{\sqrt{m}}{M}\frac{S_\triangle \rho_\triangle T_\triangle^{1/2}\oint \Gamma_{\Omega,\triangle}\Gamma^2_{V,\triangle}}{\sum_{i=\triangle,\bigcirc}\rho_i T_i^{1/2}\oint \Gamma^2_{\Omega,i}}. \tag{29}$$

In the case of the dumbbell structure with the apex direction of the asymmetric part, $\phi \approx 0$, due to symmetry considerations, Eq. (29) can be rewritten as

$$\langle\Omega\rangle_{\rm rec} = L_{\phi,\phi}\phi, \tag{30}$$

where $L_{\phi,\phi}$ is an Onsager coefficient; see (23).

Following (23) and (28), in the absence of external force, the condition for the stable direction $\phi = 0$ of the dumbbell structure is

$$L_{\phi,\phi} + K_{\phi,x}\frac{\partial x}{\partial t} < 0. \tag{31}$$

The state of the system changes from stable to unstable and vice versa at a critical velocity $V_{\rm cr} = \partial x/\partial t$:

$$V_{\rm cr} = -\frac{L_{\phi,\phi}}{K_{\phi,x}} = -\lim_{\phi\to 0}\frac{\sqrt{m}}{M}\frac{\oint \Gamma_\Omega \Gamma_V^2}{\oint \Gamma_\Omega \Gamma_V}, \tag{32}$$

where the expression inside the lim function corresponds to $\langle\Omega\rangle_{\rm rec}/L_{\phi,x}$; see (29), (30), and (27). The dumbbell structure may possess transition (32) as shown later in the article.

Let us first consider the dynamic of the dumbbell structure with $\theta_0 = \pi/24$ and the axis of rotation near the apex; see Fig. 2. This figure presents velocity (25) and stability (31) as functions of the temperature difference $T_\bigcirc - T_\triangle$, under the constraint that $T_\bigcirc + T_\triangle = 20$. The velocity of the triangle with a median along the x axis ($\phi = 0$ or $\phi = \pi$) is directed

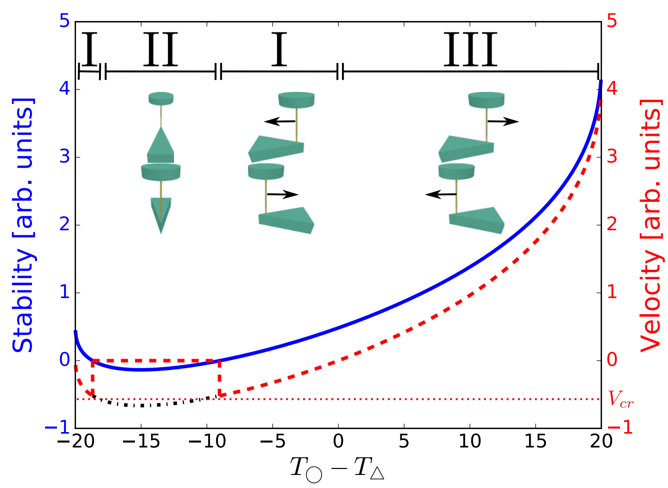

FIG. 2. Stability (blue) and velocity (red) of dumbbell structure with the asymmetric part composed of an isosceles triangle with an apex angle $\theta_0 = \pi/24$. The rotation axis is located near the apex of the triangle. Velocity (25) and stability (31) presented in arbitrary units as functions of temperature difference $T_\bigcirc - T_\triangle$ (under the assumption that $T_\bigcirc + T_\triangle = 20$). There are three regions indicated by roman numerals: First, stable motion toward the base of the triangle. Second, the motion is unstable while the symmetric orientation of the triangle part is stable, $\phi = \pm\pi/2$. The structure that enforces the direction along the x axis, $\phi = 0$ or $\phi = \pi$, would move with velocities (dashed black) beyond the critical allowed velocity $V_{\rm cr}$. This region may disappear for less acute apex angles and therefore lower velocities. Third, the stable motion toward the apex of the triangle. Stable motion toward the base is surprising because viscous forces in this case act to change the direction of the triangle. It is possible due to the potential imposed on the structure by the thermal equilibrium environment that stabilizes the motion. Nevertheless, motion toward the base is less stable than motion toward the apex. It can be considered as a chiral symmetry break.

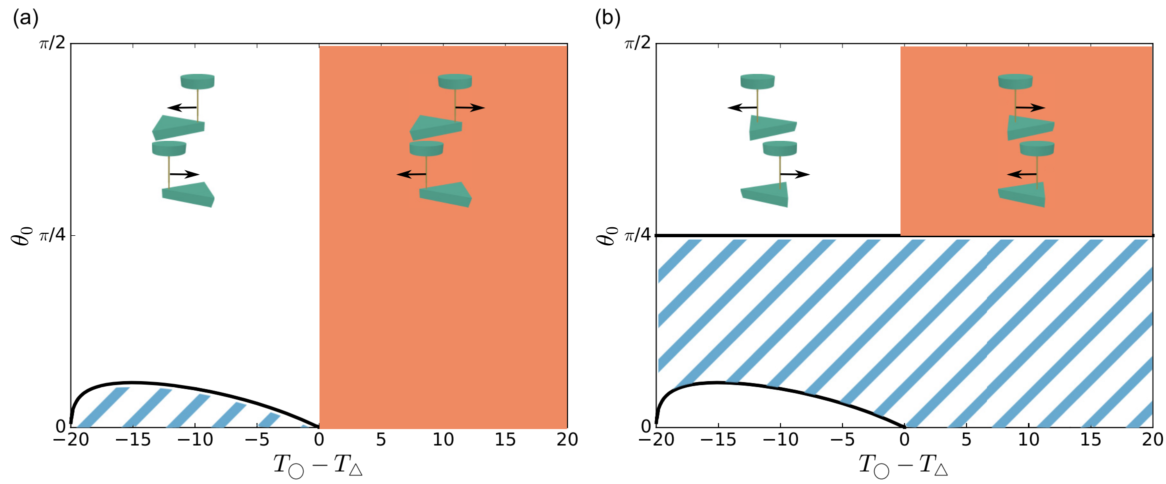

FIG. 3. Stable orientation and the corresponding translation motion of the dumbbell structure as a function of its shape and the temperatures of the thermal bathes. The asymmetric part is an isosceles triangle with an arbitrary angle of the apex $0 < \theta_0 < \pi$. The phase diagram is presented as a function of θ_0 and the difference of the temperatures, $T_{\bigcirc} - T_{\triangle}$ (under the assumption that $T_{\bigcirc} + T_{\triangle} = 20$). The white region indicates the stable motion toward the base of the triangle. The orange region corresponds to the stable motion toward the apex. No stable motion exists in the dashed region. (a) Rotation axis near the apex. The motion is stable for the majority of the temperatures and triangle shapes, but for the region of acute apex angle and negative temperature difference (dashed region). This region corresponds to high velocity toward the base of the triangle. (b) Rotation axis near the base. Motion is stable if the apex angle is obtuse, $2\theta_0 > \pi/2$. Motion toward the base is also stable in the case of a very acute apex angle that corresponds to high velocities.

toward the apex if $T_{\triangle} < T_{\bigcirc}$ and toward the base otherwise, $T_{\triangle} > T_{\bigcirc}$. Motion toward the base becomes unstable beyond the critical velocity V_{cr} (32). In this case, the stable position of the triangle's median is perpendicular to the axis x ($\phi = \pm\pi/2$). Motion in the direction of the apex is always stable.

Stability depends on the gases' temperatures, the shape of the structure, and the position of the rotation axis. Consider two cases when the axis of rotation is located on the median of the triangle either near the apex or near the base. Figure 3 presents stability in both cases as a function of apex angle θ_0 together with the temperature difference $T_{\bigcirc} - T_{\triangle}$. If the rotation axis is located near the apex of the triangle, then the motion in either direction is mainly stable, but for a small region of high velocities toward the base, as in Fig. 2. At the same region of high velocities in the direction of the base, however, the motion is stable if the axis of rotation is located near the base. In addition, in the case of the rotation axis near the base, the motion is unstable if the apex angle is acute, $2\theta_0 < \pi/2$, and it is stable for an obtuse triangle, $2\theta_0 > \pi/2$.

V. DISCUSSION

The dynamics of the dumbbell structure possesses intuitive and counterintuitive features. For instance, consider an isosceles triangle with the axis of rotation near its apex. Intuitively, the motion of this triangle is stable in the direction of the apex, while the motion of the same triangle in the direction of its base is unstable. In this case, motion toward the base creates angular momentum (27), which rotates the triangle from this direction. In a similar way, the stable motion of the triangle with the axis of rotation near its base toward the apex is counterintuitive. The motion becomes stable due to the effective potential (29) imposed on the system by the out-of-thermal-equilibrium environment. This motion becomes unstable only above some critical velocity (32) when the imposed angular momentum becomes high. This instability occurs only if the apex angle is acute enough to achieve this velocity.

The main finding of this work is the important role of local potentials imposed on the system by an out-of-thermal-equilibrium environment. The potential imposed by this environment on a mechanical system corresponds to the Onsager coefficient, such as $L_{\phi,\phi}$ in (23). Moreover, these potentials are present even if the temperatures of the thermal baths are equal (zero affinities) but the system deviates from the thermodynamic limit, e.g., the mass of gas particles is not negligibly small compared to the mass of the system.

According to (11), the mass of the ξ degree of freedom is rescaled by the factor of G (9). The average factor G is a function of linear viscous coefficients (24):

$$\langle G - 1 \rangle \propto \sum_{\xi' \neq \xi, i} \frac{1}{\rho_i \sqrt{m T_i}} \gamma_{\xi',i}. \qquad (33)$$

One can hope for experimental verification of this prediction using mass correction measurements [28]. It may be relevant for discrete transition state models [29].

The predictions for the imposed potential (19) and rectified velocity (20) are valid in the limit of $m/M \to 0$. Both expressions, however, vanish at the same limit. Nevertheless, the results of a molecular-dynamics simulation of the system with a single degree of freedom (see Fig. 9 of [30]) indicate that Eq. (20) remains valid for large ratios of $m/M \approx 1$. This work neglects memory effects in the dynamics of a thermal bath. This condition is wrong in the real world, and it is difficult to achieve in an experimental realization except with computer molecular dynamics. It is a common limitation of mechanical ratchet models. Investigation of memory effects is beyond the scope of the current work.

According to this work, the stability of a thermal ratchet depends on the relative directions of its motion and of its spatial asymmetry, e.g., the direction of the apex. It can be connected to chirality because two triangles that move toward the apex and toward the base cannot be superimposed on each other (strictly speaking, motion along a circular or at least a curved path is required) [31]. In biology, there is an open question regarding the homochirality of the living systems that are composed of L-chiral isomers, though from a chemical point of view R-chiral life would possess the same physical properties [32]. This work provides an example in which chirality is broken dynamically [33]. It may be interesting in motility-based theories on the origin of life [34,35].

This work may be useful to estimate the properties of the kinetic coefficients of active matter [36], such as asymmetric particles in an external flow [37,38]. This work, however, considers interaction with a rare gas, while the experiments are performed in a liquid. In addition, an assumption of translationally invariant degrees of freedom was made. Both of these shortcomings of the approach do not appear explicitly in the predicted dynamics (23) of a system. The results of this work may be extended to the nonlinear regime [39]. This work contributes to the recently discussed issue of the forces as well as the stability and rigidity increase for probes in an out-of-thermal-equilibrium environment [40–46].

An *Ab initio* microscopic approach is essential to predict the steady state of a system with multiple degrees of freedom out of thermal equilibrium. Macroscopic results such as Onsager relations [25], Prigogine's principle of minimum entropy production at steady state [47], the Onsager Machlup function [48], together with recent Jarzynski [49] and Crooks [50] relations for dissipation in a driven system describe the properties of a steady state as a function of the system's symmetries. On the contrary, the microscopic approach makes it possible to calculate the steady state's macroscopic parameters and symmetries instead of postulating them.

To conclude, even a simple dumbbell body out of thermal equilibrium possesses nonintuitive dynamics. Many hope that the dynamics of complex mechanical systems may be similar to the behavior of living matter. This work provides the tools to calculate the dynamics of a system with arbitrary degrees of freedom. The findings include phenomena such as stability and symmetry breaks imposed by an out-of-equilibrium environment. It is an advance on the path from single-degree-of-freedom Brownian motors to a multiple-degrees-of-freedom Brownian robotics.

APPENDIX

To derive the transition rate probability W (11) for an arbitrary degree of freedom X_ξ and the corresponding velocity $\dot{X}_\xi$, one should estimate the probability of a transition $\dot{X}' \to \dot{X}$ due to interactions with the gas particles. The transition rate probability $\dot{X}' \to \dot{X}$ is proportional to the amount of particles that hit the body at some point c and the amount of possible transitions to a specific velocity. Using (8) as a constraint and integrating over the entire surface c of the body, one gets

$$W(\dot{X}_\xi,\dot{X}'_\xi) = \oint dc \int_{-\infty}^{\infty} dv'_x \int_{-\infty}^{\infty} dv'_y H[(\dot{X}'_\xi - v')e_\perp]|(\dot{X}'_\xi - v')e_\perp|\rho\phi(v'_x,v'_y)\delta \\ \times \left[-\Delta\dot{X}_\xi - \frac{2\dot{X}_\xi - \sum_{\xi'\neq\xi}\frac{\Gamma_{\xi'}(c)}{\Gamma_\xi(c)}\dot{X}_{\xi'} - g_{x,\xi}(c)v'_x - g_{y,\xi}(c)v'_y}{1+\frac{M}{m}\left(\frac{G_\xi(c)}{\Gamma_\xi(c)}\right)^2}\right], \tag{A1}$$

where ρ is the density of the gas particles, H is the Heaviside step function, and ϕ is the Maxwell distribution of the gas particles' velocities:

$$\phi(v'_x,v'_y) = \frac{m}{2\pi T}\exp\left(\frac{-m\left(v'^2_x + v'^2_y\right)}{2T}\right). \tag{A2}$$

From (5), (6), and (8), it follows that

$$(\dot{X}'_\xi - v')e_\perp = -\frac{1}{2}\Delta\dot{X}_\xi\Gamma_\xi\left[1+\frac{M}{m}\left(\frac{G_\xi(c)}{\Gamma_\xi(c)}\right)^2\right] + \frac{1}{2}\sum_{\xi'\neq\xi}\dot{X}_{\xi'}\Gamma_{\xi'}(c). \tag{A3}$$

Using the following formula:

$$\int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \frac{m}{2\pi T}\exp(-\frac{m\left(v_x^2+v_y^2\right)}{2T}\delta(Av_x + Bv_y + C) = \sqrt{\frac{m}{2\pi T(A^2+B^2)}}\exp\left(-\frac{mC^2}{2T(A^2+B^2)}\right), \tag{A4}$$

one gets

$$W(\dot{X}_\xi,\Delta\dot{X}_\xi) = \frac{1}{4}\sum_i \rho_i\sqrt{\frac{m}{2\pi T_i}}\oint dc_i|\Delta\dot{X}_\xi|H\left\{\Delta\dot{X}_\xi\Gamma_{\xi,i}\left[1+\frac{M_\xi}{m}\left(\frac{G_{\xi,i}(c)}{\Gamma_{\xi,i}(c)}\right)^2\right] - \sum_{\xi'\neq\xi}\dot{X}_{\xi'}\Gamma_{\xi',i}(c)\right\}\Gamma_{\xi,i}(c)\frac{1}{\sqrt{g^2_{x,\xi,i}+g^2_{y,\xi,i}}} \\ \times\left[1+\frac{M_\xi}{m}\left(\frac{G_\xi(c)}{\Gamma_{\xi,i}(c)}\right)^2\right]^2\exp\left[-\frac{\frac{m}{g^2_{x,\xi,i}+g^2_{y,\xi,i}}\left\{\dot{X}_\xi - \frac{1}{2}\sum_{\xi'\neq\xi}\frac{\Gamma_{\xi',i}}{\Gamma_{\xi,i}}\dot{X}_{\xi'} + \frac{1}{2}\left[\Delta\dot{X}_\xi\left(\frac{M_\xi G^2_{\xi,i}(c)}{m\Gamma^2_{\xi,i}(c)}+1\right)\right]\right\}^2}{2T_i}\right], \tag{A5}$$

where the index i goes over all thermal baths.

The final expression (11) follows from (A5) using (10), which follows rigorously from the requirement of detailed balance at thermal equilibrium:

$$P^{\mathrm{eq}}(\dot{X}')W(\dot{X},\dot{X}') = P^{\mathrm{eq}}(-\dot{X})W(-\dot{X}',-\dot{X}), \tag{A6}$$

where $P^{\mathrm{eq}}(\dot{X})$ is the distribution of velocities of a single degree of freedom at equilibrium:

$$P^{\mathrm{eq}}(\dot{X}) \propto \exp\left(-\frac{M\dot{X}^2}{2T}\right), \tag{A7}$$

in the thermodynamic limit $G \to 1$.

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