# Momentum Transfer in Nonequilibrium Steady States

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When a Brownian object interacts with noninteracting gas particles under nonequilibrium conditions, energy dissipation associated with Brownian motion causes an additional force on the object as a "momentum transfer deficit." This principle is demonstrated first by a new nonequilibrium steady state model and then applied to several known models such as an adiabatic piston for which a simple explanation has been lacking.

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In nonequilibrium statistical mechanics the mechanical coupling between system and environment still remains poorly understood. In the Langevin description, the framework of energetics was developed during the last decade [1,2] but there are certainly many aspects which cannot be grasped by such a level of description. For example, when a Brownian object is not symmetric, such as a cone or wedge shape, its asymmetric properties are not fully reflected in the linear friction constant or tensor $\gamma$ of the Langevin equation because $\gamma$ is nonpolar.

Related to this limitation, or due to our lack of comprehension about nonequilibrium Brownian motion, there is a class of nonequilibrium phenomena which has refused to be understood at a fundamental level. An interesting example is the *adiabatic piston* separating two gases of different temperatures under pressure equilibrium [3–5]. The laws of thermodynamics cannot tell whether the piston moves or not [3]. Feynman [4] pointed out that the fluctuations of the piston's velocity should be taken into account. However, the Langevin description with linear friction falsely predicts zero mean velocity. The adiabatic piston is, therefore, still listed among major unsolved thermodynamics problems [6]. This difficulty is also shared by some models of Brownian ratchet motors working between ideal gas reservoirs [7].

A common solution to these problems is to resort to full and general microscopic descriptions, such as the molecular dynamic (MD) simulation or master-Boltzmann equation under pertinent perturbative approximations [8]. These methods are effective in predicting the outcome. For the adiabatic piston, the MD simulations [9] and perturbative master-Boltzmann equation [5,9–11] give quite consistent results showing that the piston moves toward the *hotter* reservoir. For the ratchet models, the agreement between MD simulation and perturbative theory is excellent [7]. When higher order terms are taken into account, the perturbative theories can tell the effect of the shape of the Brownian object [7] or of the inelasticity of collisions, called the *inelastic piston* [12,13], and their combinations [14,15]. Yet, we still have no physical explanation why the nonequilibrium processes give rise to a force and what determines its direction.

In this Letter, we will develop a general theoretical framework to answer this fundamental problem. The key is to explicitly take into account the momentum and mass balances under the nonequilibrium condition, in addition to the energy balance considered by the stochastic energetics [2]. Briefly, the nonequilibrium energy transfer, or dissipation, leads to a deficiency in the momentum transfer from the environment to the Brownian object, while the gas particle (mass) flux is unchanged by the dissipation. We shall call this deficiency the *momentum transfer deficit due to dissipation* or MDD, for short. We will show that this MDD is expressed as a form of a nonequilibrium boundary condition for the momentum flow [Eq. (1) below]. With this condition, many nonequilibrium problems, which have been hitherto solved case-by-case, can be explained in a unified manner sometimes even at the semiquantitative level.

In the following, we first describe the basic principle. To demonstrate the principle we introduce a simple nonequilibrium steady state (NESS) model and its solution. Then, we will apply the basic principle to unexplained problems such as an adiabatic piston in order to show the universality of underlying physics. We extend our principle to include the weak inelasticity of collisions between the Brownian object and gas particles.

In the elementary setup, Fig. 1(a), an ideal gas of temperature $T$ and pressure $p$ fills to the left of the wall. The wall is a Brownian object and its velocity fluctuates. However, it macroscopically remains at rest. The collisions of the gas particles with the wall strictly satisfy the momentum conservation but can be either elastic or inelastic. We assume that the energy transfer by individual collision is very small so that the double collision by the wall with the same gas particle is negligible. More specifically, the mass of the wall $M$ and that of gas particles $m$ are assumed to satisfy $\epsilon^2 \equiv m/M \ll 1$.

 

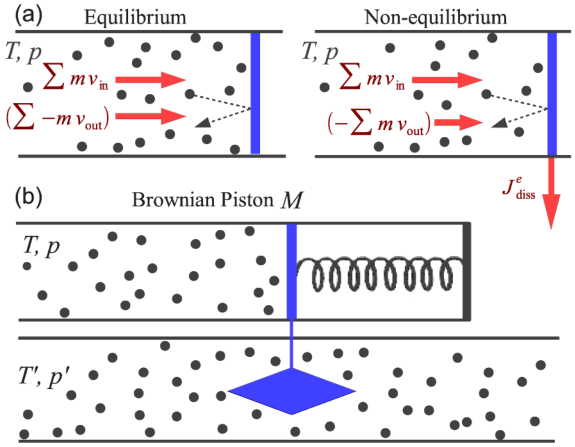


FIG. 1 (color online). (a) When the mean velocity of the piston $\bar{V}$ is zero, the net momentum transfer by the incoming particles, $\sum mv_{\rm in}$, and by the outgoing particles, $\sum(-mv_{\rm out})$, per unit time sum up to give the force on the piston.Left: Equilibrium state where no net energy is transferred to the piston. Right: Nonequilibrium case where the energy is dissipated at a rate $J^{(e)}_{\rm diss}$. When $J^{(e)}_{\rm diss} > 0[<0]$, additional force $F_{\rm MDD} < 0[>0]$ is exerted on the piston. (b) Cooled or warmed Brownian piston: The piston (thick bar) and object (diamond) are tightly bound and are held by a spring. The gas environments have temperatures $T$ and $T'$ and pressures $p$ and $p'$, respectively.

Our interest is the force exerted on the wall by the gas or equivalently the momentum transfer from the gas to the wall. We separate this momentum transfer into two parts: one due to the incoming particles toward the wall $\sum mv_{\rm in}$, and the other to the outgoing particles from the wall $\sum(-mv_{\rm out})$, where the sum is taken over a unit time. The sum of the two momentum fluxes gives the force on the wall.

When the wall's microscopic fluctuations are thermally in equilibrium with the gas [Fig. 1(a) (left)], the detailed balance condition indicates that two momentum fluxes should be equal on the time average, and the sum of the two is the hydrostatic pressure $p$ times the surface area $L$. Note that, unlike a simple kinetic theory used in elementary textbooks, the individual collisions can transfer energy between the gas and the wall at the microscopic level since the wall fluctuates. It is the detailed balance that makes the two momentum fluxes identical on the average. On the other hand, when the dissipation carries away a part of the kinetic energy of the gas upon collision to the outside of the system at the rate of $J^{(e)}_{\rm diss}$ per unit time [Fig. 1(a) (right)], the speed of the outgoing particles is, on the average, less than that of the incoming ones. Therefore, the momentum transfer by outgoing flux $\sum(-mv_{\rm out})$ should be less than the incoming one $\sum mv_{\rm in}$, which should not be influenced by the dissipation as long as the double collisions are negligible. This reduction in momentum transfer is the MDD, and the resulting force on the wall is less than that in the equilibrium by the MDD. This additional force due to MDD is exactly the point where the Langevin equation with linear friction fails to grasp the left-right asymmetry of the system.

To make this principle more concrete and quantitative, we first assume elastic collisions between gas particles and the wall. We take the thermal velocity $v_{\rm th} = \sqrt{k_BT/m}$ as a typical normal component of the velocity of incoming particles $v_{\rm in}$ up to a numerical factor (see below). The first part of the momentum transfer is $\sum mv_{\rm in} \simeq mv_{\rm th}\omega_{\rm col}$, where $\omega_{\rm col} \simeq \rho L v_{\rm th}/2$ is the collision frequency on the wall. We denote by $v'(<0)$ the typical normal component of the outgoing velocities $v_{\rm out}$. The second part of the momentum transfer is then $\sum(-mv_{\rm out}) \simeq m|v'|\omega_{\rm col}$. The conservation of mass fluxes imposed the common frequency $\omega_{\rm col}$ for both incoming and outgoing fluxes.

Now $v'$ is related to $v_{\rm th}$ though the energy balance condition, $\frac{m}{2}v_{\rm th}^2 - \frac{m}{2}v'^2 \simeq \frac{J^{(e)}_{\rm diss}}{\omega_{\rm col}}$. Here, we assumed that the parallel component of the velocity does not contribute to the energy loss. Noting $|v'| \simeq v_{\rm th}$ for weak energy transfer, the left-hand side can be approximated by $v_{\rm th}(mv_{\rm th} - m|v'|)$. Then the MDD par unit time is $(mv_{\rm th} - m|v'|)\omega_{\rm col} \simeq \frac{J^{(e)}_{\rm diss}}{v_{\rm th}}$, and the net force on the wall is

$$F = F_{\rm eq} + F_{\rm MDD}, \qquad F_{\rm MDD} \simeq -c\frac{J^{(e)}_{\rm diss}}{v_{\rm th}}, \tag{1}$$

where $F_{\rm eq} = pL$ is equilibrium hydrostatic force and the numerical constant $c$ is 1 in the above semiquantitative derivation. From the view of the gas, Eq. (1) can be considered as a boundary condition for the momentum flux. This additional force $F_{\rm MDD}$ induced by dissipation is the main result of the present Letter.

An interesting realization of MDD, which is also a new model of NESS, is illustrated in Fig. 1(b). In two dimensions, a piston with a smooth vertical wall as a Brownian object is in contact with a gas of temperature $T$ and pressure $p$. Its horizontal motion is tightly coupled to another object (rhombus) immersed in a different gas environment of temperature $T'$. We can show that when the horizontal diagonal $\ell_\parallel$ and vertical diagonal $\ell_\perp$ of the rhombus are made indefinitely large, keeping $\ell_1 \equiv 2\ell_\perp^2/\ell_\parallel$ constant, the collisional forces from the second gas converges to the ordinary force of the Langevin equation, which is the frictional $-\gamma' V$ and random force $\sqrt{2\gamma' k_B T'}\Theta_t$, with the friction constant $\gamma' = \sqrt{\pi/8}\rho\ell_1 m v_{\rm th}$ ($\rho = p/k_BT$) and Gaussian white noise $\Theta_t$ with $\langle\Theta_t\Theta_{t'}\rangle = \delta(t-t')$ [16]. Therefore, for $T' < T$, the thermal contact dissipates energy to the second gas without the net transport of momentum between the two gases on the time average.

For weak dissipation, the dissipation rate $J^{(e)}_{\rm diss}$ depends on the coupling with the environment only through the friction constants $\gamma$ with the first gas and the aforementioned $\gamma'$ with the second gas:

$$J_{\rm diss}^{(e)} = \frac{k_B T - k_B T'}{M(\gamma^{-1} + \gamma'^{-1})}. \tag{2}$$

For later use, we here show a heuristic derivation of Eq. (2). Assuming a kinetic temperature of Brownian motion, $k_B T_{\rm kin}$, we can construct dimensionally $J_{\rm diss}^{(e)}$ by the time constant $M/\gamma$ and the temperature gap, $k_B T - k_B T_{\rm kin}$, as $J_{\rm diss}^{(e)} = (\gamma/M)(k_B T - k_B T_{\rm kin})$. Applying the same argument for the second bath, i.e., $J_{\rm diss}^{(e)} = -(\gamma'/M) \times (k_B T' - k_B T_{\rm kin})$, and eliminating $T_{\rm kin}$, we obtain Eq. (2). For the standard derivation, see Ref. [2]. The linear friction, $\gamma = c' \rho L m v_{\rm th}$, can be also obtained heuristically by a Doppler shift of the momentum transfer, where $c' = \sqrt{8/\pi}$ from the standard gas kinetics.

Now substituting Eq. (2) into (1) we have a concrete form of MDD and the force in nonequilibrium. We can show that the microscopic approach with the master-Boltzmann equation gives exactly the same result if we choose $c = \sqrt{\pi/8}$. When the wall is "cooled," i.e., for $T' < T$, the mean position of the wall in NESS is displaced leftwards relative to its equilibrium position, and vice versa.

The principle (2) is also applicable to the case where the collision is weakly inelastic. In Fig. 1(b) we remove the rhombus and the second gas environment, and instead assume the restitution coefficient $e$ $(1 - e \ll 1)$ for the collision between the gas particles and the vertical wall. In this case, the dissipation rate consists of two parts:

$$J_{\rm diss}^{(e)} = J_{\rm diss,hk}^{(e)} + J_{\rm diss,ex}^{(e)}. \tag{3}$$

The "house-keeping" heat generation [17], $J_{\rm diss,hk}^{(e)}$, is due to the inelasticity of individual collisions. The "excess" dissipation $J_{\rm diss,ex}^{(e)}$ is due intrinsically to the nonequilibrium Brownian motion of the wall. If the wall were rigidly fixed, only $J_{\rm diss,hk}^{(e)}$ is nonzero. In this case the dissipation per collision is $m v_{\rm th}^2/2 - m v'^2/2 = (1 - e^2) m v_{\rm th}^2/2$ and $J_{\rm diss,hk}^{(e)} = (1 - e^2) m v_{\rm th}^2/2 \times \omega_{\rm col}$. Noting $(1 - e^2) \simeq 2(1 - e)$, the same argument leading to Eq. (1) gives

$$F_{\rm MDD} \simeq F_{\rm MDD,hk} - c\frac{J_{\rm diss,ex}^{(e)}}{v_{\rm th}}, \quad F_{\rm MDD,hk} = -\frac{1-e}{2} pL, \tag{4}$$

where $F_{\rm MDD,hk}$ is force due to the house-keeping MDD, which reduces the force even for a fixed wall. (A sand bag will receive less impact than a hard wall by a bullet.)

The excess dissipation is expressed in terms of the aforementioned kinetic temperature, $k_B T_{\rm kin}$ as $J_{\rm diss,ex}^{(e)} = (M/\gamma)(k_B T - k_B T_{\rm kin})$. Upon a binary inelastic collision, the velocity of a Brownian object changes in the same way as that of an elastic collision if the effective mass $M_{\rm eff} \equiv 2M/(1 + e)$ is used. The Brownian object then obeys approximately the Maxwell distribution $\propto e^{-M_{\rm eff} V^2/(2k_B T)}$. It implies $k_B T_{\rm kin} = k_B T \times (1 + e)/2$ Therefore,

$$J_{\rm diss,ex}^{(e)} = \frac{\gamma}{M}\frac{1-e}{2} k_B T, \tag{5}$$

where the friction constant $\gamma$ is the same as before in the lowest order in $(1 - e)$. With the numerical factor $c = \sqrt{\pi/8}$, we recover the microscopic result. When the dominant house-keeping MDD is canceled by the same MDD from the other sides, as for an inelastic triangular Brownian object [14], it is the excess MDD that explains the origin of nonequilibrium force.

We have shown that our simple calculation gives the identical result as microscopic approaches up to a numerical factor of order one. We note that the microscopic approach is still needed to find the correct numerical factor for the Brownian object of complicated geometry and to find higher order corrections to the perturbation. However, our main goal is, rather, to show that the principle (1) is a general theory of the force under nonequilibrium conditions. Below, we will apply the basic schema, Fig. 1, to various known cases and show how our principle, based on the conserved quantities, is fundamental to understand the phenomena.

*Adiabatic piston (with elastic wall)* [5,9–11].—We apply the boundary conditions (1) to the both sides of the piston shown in Fig. 2(a), with an appropriate sign of the forces and dissipation rates, and also take account of different temperatures. By the isobaric condition, the equilibrium force $F_{\rm eq}$ on both sides cancels. On the side of temperature $T'$, the force $F'_{\rm MDD}$ should contain the dissipation rate $J_{\rm diss}^{(e)\prime} = -J_{\rm diss}^{(e)}$ to assure the energy conservation. Both $F_{\rm MDD}$ and $F'_{\rm MDD}$ are oriented toward the hot side (leftward if $T > T'$), and the total momentum balance about the piston is recovered by the frictional force, $F_{\rm MDD} + F'_{\rm MDD} - (\gamma + \gamma')\bar{V} = 0$, where $\bar{V}$ is the steady state velocity of the piston. Combining with Eqs. (1) and (2) the steady state velocity reads

$$\bar{V} = -\frac{c}{\gamma + \gamma'}\left(\frac{1}{v_{\rm th}} + \frac{1}{v'_{\rm th}}\right)\frac{k_B T - k_B T'}{M(\gamma^{-1} + \gamma'^{-1})}, \tag{6}$$

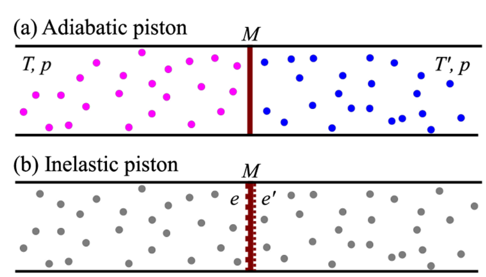


FIG. 2 (color online). (a) A microscopic "adiabatic" piston of mass $M$ (vertical bar) separates two semi-infinite gases of point-like particles with mass $m (\ll M)$. The two gases have the same pressure $p$ but different temperatures, $T$ and $T'$. (b) A macroscopic inelastic piston with restitution coefficients, $e$ (left surface) and $e'$ (right surface), is in a gas.

which is identical to the result obtained from the perturbative calculation in [10] with $c = \sqrt{\pi/8}$. ($p = \rho k_B T$ is assumed to verify it.) The correction to dissipation due to the "mesoscopic loss" $(\gamma + \gamma')\bar{V}^2$ is of a higher order by $\epsilon^2$ and, therefore, negligible. This remark applies to all other examples below.

*Inelastic piston*[12,13].—A piston of two inelastic faces, shown in Fig. 2(b), is in a gas of temperature $T$ and pressure $p$, and the faces have coefficients of restitution $e$ (left face) and $e'$ (right face), respectively, with $1 - e \ll 1$ and $1 - e' \ll 1$. The dissipation rate $J^{(e)}_{\rm diss}$, MDD and $F_{\rm MDD}$, on each face satisfy Eq. (1). But the MDD on the two faces has different signs, and thus the net force arises only when $e \neq e'$, as $F_{\rm MDD}|_{\rm left} + F_{\rm MDD}|_{\rm right} = (e - e')pL/2$. By balancing with the frictional force, the stationary velocity $\bar{V}$ to the lowest order in $1 - e$ and $1 - e'$ (therefore $|e - e'| \ll 1$) and in $\epsilon$ is

$$\bar{V} = \frac{1}{\gamma + \gamma'} \frac{e - e'}{2} pL = -\frac{e - e'}{4c'} v_{\rm th}, \qquad (7)$$

where $\gamma \simeq \gamma' = c' \rho L m v_{\rm th}$ with $c'$ a constant. The result (7) agrees with the perturbative results [12,13] with $c' = \sqrt{8/\pi}$. This elementary example shows, however, that our principal formula (1) is universal whether or not the origin of dissipation is kinematical or dynamical, because the momentum conservation is universally valid.

*Ratchet model in two gas environments*.—Van den Broeck *et al.* [7] proposed and analyzed a series of Brownian ratchet models that move horizontally in contact with two ideal gas environments at different temperatures $T$ and $T'$. One typical example is shown in Fig. 3 (top), where we assumed isobaric condition only to simplify the argument without losing the essential point. Microscopic methods concluded that it moves steadily with the base of the triangle in a hotter environment that is ahead, i.e., leftwards if $T > T'$. Based on our principle, the origin of the nonequilibrium force is essentially the same as the aforementioned adiabatic piston. Intuitively, if we look at only the bases of triangles, it already appears identical to the adiabatic piston, Fig. 3 (bottom). In fact, the sides of the triangle receive more frequent collisions than on the base but with much less impact on the horizontal motion. We can rigorously show that in the limit of $\theta \to 0$ (see Fig. 3), the momentum transfer rate on the sides converges to the equilibrium force $pL$ without fluctuation or frictional velocity dependence [16]. Therefore, in this limit, the effect of the side surface vanishes and the same principle as the adiabatic piston determines the motion of the ratchet model. The result agrees with their perturbative calculation [7].

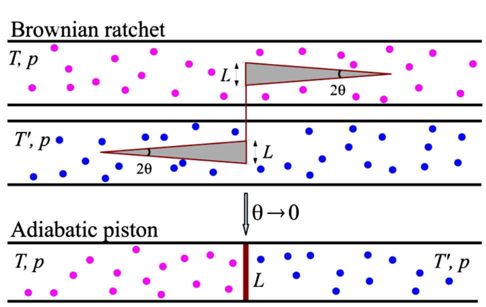


FIG. 3 (color online). A Brownian ratchet proposed in [7] (top) consists of two triangles (total mass $M$) that translate along the horizontal axis. This model can be mapped to the adiabatic piston (bottom) in the limit, $\theta \to 0$.

*Inelastic triangle*—Costantini *et al.*[12] studied a variant of the above ratchet model using a single triangle but with the inelastic surface of a restitution constant $e$. In this case, the net house-keeping component vanishes, as if the triangle is in a hydrostatic pressure, $(1 + e)p/2$. On the other hand, the excess dissipation $J^{(e)}_{\rm diss,ex}$ on the side surfaces are less important than that on the base, in the way that the contribution by the side surfaces vanishes in the limit $\theta \to 0$. In this limit, the force balance with frictional drag $-\gamma\bar{V}$ and Eq. (5) yields

$$\bar{V} = -\frac{c}{M} \frac{1 - e}{2 v_{\rm th}} k_B T. \qquad (8)$$

This result is identical to the one obtained by the microscopic approach [12] to the lowest order in $1 - e$, if we choose $c = \sqrt{\pi/8}$.

In summary, we have introduced a unified theory on the generation of nonequilibrium force as a momentum transfer deficit due to dissipation. This principle is applied to a new model of NESS, named, cooled or warmed piston, as well as to many existing models such as an adiabatic piston in a unified manner. What we clarified here is that, while the energetics at the Langevin level [2] is enough to treat the dissipation, the dissipation attributed to Brownian motion plays a decisive role [4] in the force generation through the MDD. As perspectives, the MDD should be taken as incorporated in the hydrodynamic description of the adiabatic piston [18]. It is of interest to generalize the present results to interacting gas particles, for example, the boundary thermostats [19], as well as to the contact value theorem [20] under nonequilibrium.

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