Langevin equation for the extended Rayleigh model with an asymmetric bath

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In this paper a one-dimensional model of two infinite gases separated by a movable heavy piston is considered. The non-linear Langevin equation for the motion of the piston is derived from first principles for the case when the thermodynamic parameters and/or the molecular masses of gas particles on left and right sides of the piston are different. Microscopic expressions involving time correlation functions of the force between bath particles and the piston are obtained for all parameters appearing in the non-linear Langevin equation. It is demonstrated that the equation has stationary solutions corresponding to directional fluctuation-induced drift in the absence of systematic forces. In the case of ideal gases interacting with the piston via a quadratic repulsive potential, the model is exactly solvable and explicit expressions for the kinetic coefficients in the non-linear Langevin equation are derived. The transient solution of the non-linear Langevin equation is analyzed perturbatively and it is demonstrated that previously obtained results for systems with the hard-wall interaction are recovered.

I. INTRODUCTION

The Brownian motion of a massive piston in a cylinder filled with an ideal gas is one of the oldest models of non-equilibrium statistical physics. In its simplest version, both the piston (of mass $M$) and the gas molecules (of mass $m$) are confined to move in one dimension along the symmetry axis of the cylinder. The piston is assumed to be adiabatic in a sense that its heat conductivity is negligible so that there is no transfer of heat between the two compartments of the cylinder as long as the piston is held fixed. This simple model has served as a useful test of new schemes and approximations for several generations of physicists (see Ref. [1] for references). In most treatments it is assumed that the bath particles interact with the piston via the hard-wall potential, i.e. piston-molecule collisions are considered to be instantaneous. In this model the piston interacts with bath particles through a sequence of binary collisions and the possibility of simultaneous interaction of the piston with more than one molecule is neglected. This approximation is valid as long as one is interested in the asymptotic long time behavior of the system which is apparently insensitive to details of the interactions between the bath particles and the piston. On the other hand, the motion of the system on short to intermediate time scales is clearly influenced by the nature of bath particle-piston interactions, and one has to take into account the finite range of the potential and effects of multi-particle collisions. It is known that many-particle collisions are an important factor in liquid-like systems, essentially affecting the shape of the velocity correlation function, especially when a repulsive part of potential is relatively “soft” [2]. In such systems, a given particle interacts simultaneously with a relatively heavy swarm of other particles in its vicinity, leading to an enhancement of caging effects in comparison to systems with a short-ranged potential. As a result, the velocity autocorrelation function has a more pronounced negative part corresponding to an anti-correlation in the velocity induced by a particle reboncluding of its neighbors. Multi-particle collisions may also be important for tagged particle motion in a dilute gas-like medium provided the tagged particle (or “piston” in the present case) is large enough that the average number $N$ of gas molecules in the interaction shell around the particle is larger than one. Although in this case the qualitative form of correlation functions does not depend on $N$, the softness of the potential essentially influences the short-time behavior of the system leading to the non-exponential initial decay of time correlation functions [3].

Another reason why one may wish to go beyond the approximation of hard-wall interaction is methodological. It is often problematic to directly apply general analytical techniques involving differential operators for systems with a singular potential. Even if one expects multiple collisions to be unimportant, it is often convenient to model interactions via a short-ranged potential of range $l_i$ and subsequently analyze results in the hard-wall limit $l_i \to 0$.

In a earlier paper [1], a microscopic derivation of the non-linear Langevin equation was presented for a system consisting of a massive piston interacting with a bath particles via an arbitrary repulsive potential. We use the term “non-linear” to refer the Langevin equation with not only the linear dissipative term (Stokes damping) but also dissipative terms of higher orders in particle’s momentum. In Ref. [1] all generalized kinetic coefficients appearing the non-linear Langevin equation were expressed in terms of time correlation functions involving the interaction force between the piston and the bath particles and its derivatives. For some systems, such as an ideal gas interacting with the piston through a repulsive quadratic potential, the microscopic expressions for all the kinetic coefficients can...
be calculated analytically. For this reason, simple models, such as the ideal gas-piston system, provide a convenient means of studying many subtle points of Brownian motion theory, such as the role and form of non-linear damping, relative importance of non-Markovian effects, and convergence properties of small parameter expansions.

In Ref. [1] the dynamics of the piston in a homogeneous bath was examined. The purpose of this paper is to extend the analysis in Ref. [1] to the case of an asymmetric bath in which the parameters characterizing the bath to the left and to the right of the piston are different. This model has received a recent renewal of interest after it was discovered that the system may exhibit non-trivial transient and stationary behavior when there is an initial asymmetry in the thermodynamics properties of the gases to the left and to the right of the piston [4]. Among other interesting points, it was found that the piston undergoes a noise-induced directional movement in the absence of macroscopic forces, a characteristic of motion in molecular motors and stochastic ratchets. In the limit of an infinitely long cylinder, Gruber and Piasecki found [5] a stationary solution of the equations of motion of the piston corresponding to the drift of the piston in the direction of the compartment with higher temperature even when the pressure on the left and the right of the piston are the same. This result has been later confirmed by numerical simulations [6].

This fluctuation-induced motion is an effect of the first order in a small mass-ratio parameter \( \lambda \), defined as \( \lambda = \sqrt{m/M} \). It does not follow from the conventional Langevin equation with linear dissipation, and appears only when non-linear damping terms, which are of higher orders in \( \lambda \), are taken into account.

In this paper the projection-operator method applied by Mazur and Oppenheim [7] to the theory of Brownian is adapted to the case of the asymmetric bath. We shall consider a slightly more general model of the asymmetric bath than that analyzed by Gruber and Piasecki in that not only temperatures but also the masses of the bath particles in the left and right compartment may differ. For such a system, the Langevin equation, including non-linear dissipative terms to third order in \( \lambda \), is derived from first principles. The resulting equation is general, holds for arbitrary interactions between the piston and the bath particles, and is not restricted to the ideal gas bath. The kinetic coefficients appearing in the non-linear Langevin equation are expressed as integrals of time correlation functions of the force between the piston and bath particles. For a bath of ideal gas particles interacting with the piston via the parabolic repulsive potential, the correlation functions can be computed in closed analytical form. For this model, an explicit expression describing relaxation of the momentum of the massive piston is obtained. The analysis based on the Langevin equation is much more simple than that involving the language of distribution functions adopted in other papers on the subject. The perturbative and stationary solutions are analyzed and demonstrated to be consistent with the results of Gruber and Piasecki obtained for a model of instantaneous binary collisions.

II. AN EXACT EQUATION OF MOTION FOR THE PISTON

The system consists of a piston of mass \( M \) and cross-sectional area \( S \) confined to move in one dimension (chosen to be along the \( x \) axis) in a cylinder of total length \( L \). It is assumed that the piston is initially at position \( X \) near the center of the cylinder, taken to be the origin, with the leftmost and rightmost-ends of the cylinder at positions \(-L/2\) and \( L/2\), respectively. The left and right compartments of the cylinder are filled with bath molecules of density \( n_l \) and \( n_r \), temperature \( T_l \) and \( T_r \), and mass \( m_l \) and \( m_r \), and move in one dimension along the \( x \) axis. We assume the bath molecules are confined to their respective compartments by hard-wall interactions with the immobile ends of the cylinder, and interact with the piston through a short-ranged, repulsive potential. The Hamiltonian of the piston-bath system can be written in the form

\[
H = \frac{P^2}{2M} + H_0(X),
\]

where \( X \) and \( P \) are the coordinate and the momentum of the piston, and \( H_0(X) \) is the Hamiltonian of the bath in the presence of the piston constrained at position \( X \). \( H_0(X) \) can be decomposed into the sum of two parts, \( H_0(X) = H_0^l(X) + H_0^r(X) \), corresponding to the Hamiltonian for the bath molecules on the left and right of the piston,

\[
H_0^\alpha(X) = \sum_{i=1}^{N_\alpha} \left\{ \frac{P_i^2}{2m_\alpha} + U(X - x_i) \right\}
\]

For simplicity of notation, above and throughout this paper the super- or subscript index \( \alpha = \{l, r\} \) is used to label dynamical variables in the left and right compartments of the cylinder. In the above equation \( N_\alpha \) and \( m_\alpha \) are the number and the mass of particle in a respective compartment.

In the following, we restrict our analysis to the case when differences in the thermodynamic parameters of the bath in the left and right compartments of the cylinder are small. Furthermore, the molecular masses \( m_l \) and \( m_r \) are
assumed to be of the same order of magnitude and much less than the mass of the piston $M$. Under these conditions, one might anticipate that the directional contribution to the momentum of the piston is small, and on average is of order $P \sim \sqrt{Mk_BT_p}$, where the effective temperature $T_p$ of the piston is of the same order of magnitude as the left and right temperatures $T_l$ and $T_r$. In the subsequent analysis, we show that this intuition is correct, and an explicit expression for $T_p$ will be presented.

It is convenient to express the equations of motion of the piston-bath system in scaled coordinates. To this end, we introduce the small parameter $\lambda = \sqrt{m/M}$, where $m$ is an arbitrary mass of the same order of magnitude as $m_l$ and $m_r$. One may reasonably expect that the scaled momentum of the piston $P_s = \lambda P$ will typically be of the same order of magnitude as the momentum of a bath molecule. The parameter $\lambda$ therefore serves as a quantitative measure of the time scale separation between the slow evolution of the massive piston and the fast evolution of the light bath molecules. As in the case of Brownian motion [7], it will be useful as an expansion parameter to simplify the physics of system [8].

In terms of the scaled piston’s momentum $P_s = \lambda P$, the Hamiltonian reads $H = P_s^2/2m + H_0$. The corresponding Liouville operator $\mathcal{L}$, which governs the evolution of an arbitrary dynamical variable via the equation $A(t) = e^{\mathcal{L}t}A$ ($A \equiv A(0)$ throughout the text), can be written in the form

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_1, \quad \mathcal{L}_0 = \mathcal{L}^d_0 + \mathcal{L}^r_0.$$  \hfill (3)

Here the Liouville operators $\mathcal{L}^\alpha_0$

$$\mathcal{L}^\alpha_0 = \sum_i \left( \frac{p_i}{m_\alpha \partial x_i} F_i \frac{\partial}{\partial p_i} \right),$$  \hfill (4)

describe dynamics of the bath molecules in the left and right compartments of the cylinder in the presence of the piston held fixed at position $X$, where the force $F_i$ acting on a molecule $i$ is $F_i = -\partial U(X - x_i)/\partial x_i$. The Liouville operator $\mathcal{L}_1$ is defined by

$$\mathcal{L}_1 = \frac{P_s}{m} \frac{\partial}{\partial X} + F \frac{\partial}{\partial P_s},$$  \hfill (5)

where $F = -\sum_i \partial U(X - x_i)/\partial X$ is the total force exerted on the piston by the bath molecules.

Our task is to express the equation of motion of the scaled momentum of the piston, $dP_s(t)/dt = \lambda F(t)$, in the form of a Langevin equation in which the instantaneous force $F(t)$ acting on the piston at time $t$ is decomposed into “dissipative” and “random” parts. To accomplish this goal, we define the projection operators $\mathcal{P}_l$, $\mathcal{P}_r$ and $\mathcal{P}$, which act on an arbitrary dynamical variable $A$ according to the rules

$$\mathcal{P}_\alpha A = \langle A \rangle_\alpha = \int d\Omega_\alpha \rho_\alpha A,$$

$$\mathcal{P} A = \mathcal{P}_l \mathcal{P}_r A = \langle A \rangle = \int d\Omega_l \rho_l \int d\Omega_r \rho_r A,$$  \hfill (7)

where $\Omega_\alpha = \{x_\alpha^i, p_\alpha^i\}$ are the phase points for the bath molecules in the left and right compartments of the cylinder, $\rho_\alpha = Z_\alpha^{-1} \exp \{-\beta_\alpha H_0^\alpha(X)\}$ are the corresponding canonical distributions for the bath molecules in the presence of the piston fixed at coordinate $X$, $\beta_\alpha = (k_B T_\alpha)^{-1}$ and $k_B$ is the Boltzmann’s constant. Note that the projection operator $\mathcal{P}$ effectively averages over initial conditions of the bath at a fixed position of the piston. Using the operator identity

$$e^{(A+B)t} = e^{At} + \int_0^t d\tau e^{A(t-\tau)}B e^{(A+B)\tau},$$  \hfill (8)

with $A = \mathcal{L}$ and $B = -\mathcal{P} \mathcal{L}$, one obtains the following decomposition for the force on the piston $F(t) = e^{\mathcal{L}t}F,

$$F(t) = F_\parallel(t) + \int_0^t d\tau \ e^{\mathcal{L}(t-\tau)}\mathcal{P} \mathcal{L} F_\parallel(\tau),$$  \hfill (9)

where $F_\parallel(t) = e^{\mathcal{Q}t}F$ and $\mathcal{Q} = 1 - \mathcal{P}$.

The structure $\mathcal{P} \mathcal{L} F_\parallel(\tau)$ in Eq.(9) can be further simplified to $\lambda \mathcal{P} \mathcal{L}_1 F_\parallel(\tau)$ due to the orthogonality property,

$$\mathcal{P}_l \mathcal{L}^d_0 = \mathcal{P}_r \mathcal{L}^r_0 = \mathcal{P} \mathcal{L}_0 = 0,$$  \hfill (10)
which follows from the relation $L^n_0 \rho_\alpha = 0$. Using this relation and the definition of the projection operators, Eq. (9) takes the form

$$F(t) = F^\dagger(t) + \lambda \int_0^t d\tau \ e^{t-t-\tau} \left\{ \frac{P_s}{m} \left( \frac{\partial}{\partial X} F^\dagger(\tau) \right) + \frac{\partial}{\partial P_s} \langle FF^\dagger(\tau) \rangle \right\}.$$ \hspace{1cm} (11)

In this expression the factor

$$\left\langle \frac{\partial}{\partial X} F^\dagger(\tau) \right\rangle = \int d\Omega_t \rho_l \int d\Omega_r \rho_r \frac{\partial}{\partial X} F^\dagger(\tau),$$ \hspace{1cm} (12)

can be simplified by pulling the differential operator out of the integral,

$$\left\langle \frac{\partial}{\partial X} F^\dagger(\tau) \right\rangle = \frac{\partial}{\partial X} \left\langle F^\dagger(\tau) \right\rangle - \int d\Omega_t \int d\Omega_r \ F^\dagger(\tau) \frac{\partial}{\partial X} (\rho_l \rho_r).$$ \hspace{1cm} (13)

Using properties of the projection operator, the first term on the right-hand side of Eq. (13) can be simplified using the fact that

$$\left\langle F^\dagger(t) \right\rangle = \langle e^{tQ_0} F \rangle = \mathcal{P} e^{tQ_0} F = \mathcal{P} F = \left\langle F \right\rangle.$$ \hspace{1cm} (14)

For a homogeneous system, one expects $\langle F \rangle = 0$ and hence $\langle F^\dagger(t) \rangle = 0$. For an asymmetric system, on the other hand, $\langle F \rangle \neq 0$ and the first term on the right-hand side of Eq. (13) generally does not vanish.

The second term in the right-hand side of Eq. (13), involving $\frac{\partial}{\partial X} \rho_l \rho_r$, can be worked out taking into account that in the distributions $\rho_\alpha = Z_\alpha^{-1} e^{-\beta_\alpha H_0^\alpha}$ not only the Hamiltonians but also the partition functions $Z_\alpha$ depend parametrically on $X$,  

$$\frac{\partial}{\partial X} (\rho_l \rho_r) = \rho_l \rho_r \left( \beta_1 F_l + \beta_r F_r - \frac{1}{Z_l} \frac{\partial Z_l}{\partial X} - \frac{1}{Z_r} \frac{\partial Z_r}{\partial X} \right).$$ \hspace{1cm} (15)

It is straightforward to show that

$$\frac{1}{Z_\alpha} \frac{\partial Z_\alpha}{\partial X} = \beta_\alpha \left\langle F_\alpha \right\rangle,$$ \hspace{1cm} (16)

where $F_l$ and $F_r$ are the forces on the left and right surfaces of the fixed piston such that $F_l + F_r = F$. Therefore, Eq. (13) takes the form

$$\left\langle \frac{\partial}{\partial X} F^\dagger(t) \right\rangle = \frac{d\left\langle F \right\rangle}{dX} - \beta_1 \left\langle F_l F^\dagger(t) \right\rangle - \beta_r \left\langle F_r F^\dagger(t) \right\rangle,$$ \hspace{1cm} (17)

where the double brackets denote the cumulants, $\left\langle AB \right\rangle = \left\langle AB \right\rangle - \left\langle A \right\rangle \left\langle B \right\rangle$. Substituting this result into Eq. (11), we get the following exact equation of motion of the piston

$$\frac{dP_s}{dt} = \lambda F^\dagger(t) + \lambda^2 \int_0^t d\tau \ e^{t-t-\tau} \left\{ \frac{\partial}{\partial P_s} \langle FF^\dagger(\tau) \rangle - \frac{P_s}{m} \frac{d\langle F \rangle}{dX} \right\}.$$ \hspace{1cm} (18)

For some systems, such as the extended Rayleigh model discussed in Section 4, the parametric dependence of $\langle F \rangle$ on the position $X$ of the piston is weak, and the derivative of $\langle F \rangle$ scales as $1/L$ in the limit of large $L$. In fact for the Rayleigh model, the bath is comprised of ideal gas molecules, and the parametric dependence of $\langle F \rangle$ on $X$ arises through the dependence of $\langle F \rangle$ on the concentrations of bath molecules in the respective compartments of the cylinder, $n_\alpha$. Since

$$n_l = \frac{N_l}{L/2 + X} S, \hspace{1cm} n_r = \frac{N_r}{L/2 - X} S,$$

where $N_l$ and $N_r$ are the total number of bath molecules in the left and right compartments, respectively, $dn_\alpha/dX \sim n_\alpha/L$ for large $L$, and hence $d\langle F \rangle/dX \sim 1/L$. Thus, for large cylinders, this term may be dropped in the equation of motion of the piston and we obtain
\begin{equation}
\frac{dP_x(t)}{dt} = \lambda F(t) + \lambda^2 \int_0^t d\tau e^{\mathcal{L}(t-\tau)} \left\{ \frac{\partial}{\partial P_x} \langle F F(t) \rangle - \frac{P_x \beta t}{m} \langle F F(t) \rangle \right\},
\end{equation}

which is exact for such systems in the thermodynamic limit. By expanding Eq. (19) in powers of the square root of the mass ratio \( \lambda \), one can derive the Langevin equation to any order in \( \lambda \).

### III. The Non-linear Langevin Equation

The force \( F(t) = e^{\mathcal{L}_0} F \) in the Eq. (19) can be expanded in powers of \( \lambda \) using the fact that \( \mathcal{P} \mathcal{L}_0 = 0 \) and the operator identity (8), to yield

\begin{equation}
F(t) = F_0(t) + \lambda \int_0^t d\tau e^{\mathcal{L}_0(t-\tau)} \mathcal{Q} \mathcal{L}_1 F_0(\tau) + O(\lambda^2),
\end{equation}

where \( F_0(t) = e^{\mathcal{L}_0} F \) is the force exerted by the bath molecules on the fixed piston. Since \( \mathcal{L}_1 F_0(t) = \frac{P_x \beta t}{m} F_0(t) \), the above equation takes the form

\begin{equation}
F(t) = F_0(t) + \frac{\lambda P_x}{m} \int_0^t d\tau \delta G(t, \tau) + O(\lambda^2),
\end{equation}

where

\begin{equation}
G(t, \tau) = e^{\mathcal{L}_0(t-\tau)} \frac{\partial}{\partial X} F_0(\tau)
\end{equation}

and \( \delta G = G - \langle G \rangle \). Using this result, one can extract the leading order approximation in \( \lambda \) of the correlation functions \( \langle FF(t) \rangle \) and \( \langle F \alpha F(t) \rangle \) appearing in the equation of motion (19). Since the evolution of the dynamical functions \( F_0(t) \) and \( G(t) \) is governed by the Liouville operator \( \mathcal{L}_0 \), the left and right components of \( F_0(t) \) and \( G(t) \) are independent, which implies that the cumulants \( \langle F_1 F_0^\alpha \rangle, \langle F \alpha F_0 \rangle, \langle F_1 G_1 \rangle, \langle F \alpha G_1 \rangle \) are all zero. Taking this into account, one obtains

\begin{equation}
\langle F \alpha F^\dagger(t) \rangle = \langle F \alpha F_0^\alpha(t) \rangle + \frac{\lambda P_x}{m} \int_0^t d\tau \langle F_\alpha G_\alpha(t, t') \rangle,
\end{equation}

and

\begin{equation}
\langle FF^\dagger(t) \rangle = \langle FF_0(t) \rangle + \frac{\lambda P_x}{m} \int_0^t d\tau \left\{ \langle F_\alpha G_\alpha(t, t') \rangle + \langle F_\alpha G_\alpha(t, t') \rangle \right\}.
\end{equation}

Substitution of these expressions into the equation of motion (19) leads to the non-Markovian (generalized) non-linear Langevin equation,

\begin{equation}
\frac{dP_x(t)}{dt} = \lambda F(t) - \lambda^2 \int_0^t d\tau P_x(t-\tau) M_1(\tau) - \lambda^3 \int_0^t d\tau P_x^2(t-\tau) M_2(\tau)
+ \lambda^3 \int_0^t d\tau M_3(\tau) + O(\lambda^4),
\end{equation}

where the memory functions are given by

\begin{align}
M_1(\tau) &= \frac{1}{m} \left\{ \lambda \langle F_1 F_0(\tau) \rangle + \beta_r \langle F_1 F_0(\tau) \rangle \right\}, \\
M_2(\tau) &= \frac{1}{m^2} \int_0^\tau d\tau' \left\{ \lambda \langle F_1 G_1(\tau, \tau') \rangle + \beta_r \langle F_r G_r(\tau, \tau') \rangle \right\}, \\
M_3(\tau) &= \frac{1}{m} \int_0^\tau d\tau' \left\{ \langle F_1 G_1(\tau, \tau') \rangle + \langle F_r G_r(\tau, \tau') \rangle \right\}.
\end{align}
Note that for a totally symmetric system in which all parameters characterizing the bath to the left and to the right of the piston are the same, \( \langle \mathcal{F}(G_l(t, \tau')) \rangle = -\langle \mathcal{F}(G_r(t, \tau')) \rangle \). In this case the functions \( M_2(t), M_3(t) \) vanish, and the Langevin equation (23) is linear. Furthermore, for a symmetric bath it can be shown that the first non-linear correction term is of order \( \lambda^4 \) and proportional to \( \mathcal{P}^3 \) [1].

Assuming that the memory functions \( M_i(t) \) decay with a characteristic time \( \tau_c \), which is short on the time-scale for relaxation of the momentum of the piston, the generalized Langevin equation (23) can be written in form that is local in time. In fact, on a time scale \( \tau < \tau_c \) the momentum changes primarily due to the random force while the effect of the damping force is of higher order in \( \lambda \),

\[
P_\ast(t - \tau) = P_\ast(t) - \int_{t - \tau}^{t} \, d\tau' \dot{P}_\ast(\tau') = P_\ast(t) - \lambda \int_{t - \tau}^{t} \, d\tau' F^1(\tau') + O(\lambda^2).
\]

Substitution of this expression and a similar one for \( P^2(t - \tau) \) into Eq.(23) leads to an expression that is local in time and of the form,

\[
\frac{dP_\ast(t)}{dt} = \lambda \ddot{P}_\ast(t) - \lambda^2 \mathcal{C}_1(t) P_\ast(t) - \lambda^3 \mathcal{C}_2(t) P^2_\ast(t) + \lambda^3 \mathcal{C}_3(t) + O(\lambda^4),
\]

where \( \mathcal{C}_i(t) = \int_0^t \, d\tau M_i(\tau) \) and \( \dot{F}^1(t) \) is the random force modified with a correction of second order in \( \lambda \)

\[
\dot{F}^1(t) = F^1(t) - \frac{\lambda^2}{m} \int_0^t \, d\tau M_1(\tau) \int_{t - \tau}^{t} \, d\tau' F^1(\tau').
\]

Since this correction is small and does not change statistical properties of the force, it will be neglected below. In what follows the dynamics of the piston on a time-scale longer than the bath correlation time \( \tau_c \) is considered. When \( t \gg \tau_c \), the kinetic coefficients \( \mathcal{C}_i(t) \) assume their limiting values \( \mathcal{C}_i = \int_0^\infty \, d\tau M_i(\tau) \). Re-expressing this equation in terms of the unscaled momentum of the piston \( P = P_\ast/\lambda \) yields

\[
\frac{dP(t)}{dt} = F^1(t) - \gamma_1 P(t) - \gamma_2 P^2(t) + \gamma_3,
\]

where the kinetic coefficients \( \gamma_i \) are given by

\[
\gamma_1 = \lambda^2 \mathcal{C}_1 = \frac{1}{M} \int_0^\infty \, dt \left\{ \beta_i \langle \mathcal{F}(F^1_0(\tau)) \rangle + \beta_r \langle \mathcal{F}(F^1_r(\tau)) \rangle \right\},
\]

\[
\gamma_2 = \lambda^2 \mathcal{C}_2 = \frac{1}{M^2} \int_0^\infty \, dt \int_0^t \, d\tau' \left\{ \beta_i \langle \mathcal{F}(G(t, \tau)) \rangle + \beta_r \langle \mathcal{F}(G_r(t, \tau)) \rangle \right\},
\]

\[
\gamma_3 = \lambda^2 \mathcal{C}_3 = \frac{1}{M} \int_0^\infty \, dt \int_0^t \, d\tau \left\{ \langle \mathcal{F}(G(t, \tau)) \rangle + \langle \mathcal{F}(G_r(t, \tau)) \rangle \right\}.
\]

It is important to note that Eq. (30) with the kinetic coefficients given by Eqs. (31) - (33) is a general result that is valid for arbitrary interaction potentials for the bath and that is also independent of the specific form of the interactions between the piston and the bath molecules.

Note that the correlations \( \langle \mathcal{F}(G_l(t, \tau)) \rangle \) and \( \langle \mathcal{F}(G_r(t, \tau)) \rangle \) are of different sign, which suggests that for the asymmetric bath either \( \gamma_2 \) or \( \gamma_3 \) can vanish for certain combinations of the parameters of the bath. If \( \gamma_2 = 0 \), the Langevin equation is linear and can be easily integrated. We postpone further discussion of these issues until the next section where the general results (30)-(33) are applied for the specific model of ideal gas molecules interacting with the piston via a truncated parabolic potential.

### IV. THE EXTENDED RAYLEIGH MODEL

The kinetic constants \( \gamma_i \) in Eqs. (31)-(33) are expressed in terms of integrals of correlation functions of dynamical variables whose time evolution is described by the Liouvillian operator \( \mathcal{L}_0 \) of the bath in the presence of the fixed piston. These correlations can be calculated explicitly [1] in the case when the bath is comprised of ideal gas molecules interacting with the piston via a parabolic repulsive potential

\[
U(x - X) = \begin{cases} \frac{1}{2} k_f (x - X) \, x > X_l, \\ \frac{1}{2} k_f (x - X) \, x < X_r, \\ 0, \text{ otherwise}, \end{cases}
\]

where \( X_l \) and \( X_r \) are the positions of the piston and the right wall of the piston, respectively. In this case

\[
\mathcal{C}_1(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_1(t),
\]

\[
\mathcal{C}_2(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_2(t),
\]

\[
\mathcal{C}_3(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_3(t),
\]

and

\[
\mathcal{C}_1(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_1(t),
\]

\[
\mathcal{C}_2(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_2(t),
\]

\[
\mathcal{C}_3(t) = \int_0^t \, d\tau \mathcal{L}_0^{-1} \mathcal{L}_0 \mathcal{C}_3(t),
\]

are evaluated.
Here $x$ is the coordinate of a bath molecule, $X_l = X - a$, $X_r = X + a$ define the boundaries of interaction between the molecule and the piston, with the parameter $a$ serving as a measure of the range of the potential. In the model system, the width of the piston is neglected. In addition, it is assumed that the temperatures of the ideal gas in both compartments are sufficiently low (or the potential strength constant $k_f$ is sufficiently large) that the average penetration $(k_f \beta_\alpha)^{-1/2}$ of a bath particle into the interaction regions $(X_\alpha, X)$ is much less than $a$ [9].

In the limit of large cylinder length $L$, recollisions of the piston and gas due to the finite size of the bath can be ignored. This assumption corresponds to analyzing the motion of the piston on intermediate time scales $t \ll \tau_L$, where $\tau_L$ is the time it takes on average for a bath particle to travel half the length of the cylinder. For $t \ll \tau_L$, the force acting on the sides of the piston can be written in the form [1]

$$F_l(t) = -k_f \int_0^\infty dv \int_{-v}^{0} dq \, N(X_l + q, v; t - \tau_l) \frac{v}{\omega_l} \sin \frac{\omega_l q}{v},$$

$$F_r(t) = -k_f \int_0^\infty dv \int_{0}^{v} dq \, N(X_r + q, v; t - \tau_r) \frac{v}{\omega_r} \sin \frac{\omega_r q}{v},$$

where $\omega_\alpha = \sqrt{k_f/m_\alpha}$ is the characteristic frequency of the parabolic system, $\tau_\alpha = \pi/\omega_\alpha$, and the function $N(x, v; t)$ is the microscopic linear density of particles defined by

$$N(x, v; t) = \sum_i \delta(x - x_i(t))\delta(v - v_i(t)).$$

The average forces are:

$$\langle F_l \rangle = \frac{n_l S}{\beta_l}, \quad \langle F_r \rangle = -\frac{n_r S}{\beta_r}. \quad (35)$$

Note that as mentioned in Section 2, the average force $\langle F \rangle = \langle F_l \rangle + \langle F_r \rangle$ does not vanish in general in the asymmetric system though the derivative $d\langle F \rangle/dX \sim 1/L$ can be neglected for a long cylinder. The equation of motion of the piston is given by Eq. (19) in this limit.

For this model, it was found that [1]

$$\langle F_\alpha F_\alpha^\ast (t) \rangle = \frac{k_f}{\beta_\alpha} \langle F_\alpha \rangle \xi_\alpha^\ast (t),$$

$$\langle F_\alpha G_\alpha(t_1, t_2) \rangle = -k_f \langle F_\alpha \rangle \xi_\alpha^\ast (t_1, t_2), \quad (37)$$

where the functions $\xi_\alpha^\ast (t)$ are

$$\xi_1^\ast (t) = \frac{1}{\sqrt{2\pi}} \left\{ \sin \omega_\alpha t + (\pi - \omega_\alpha t) \cos \omega_\alpha t \right\} \theta(\tau_\alpha - t), \quad (38)$$

$$\xi_2^\ast (t_1, t_2) = \frac{1}{2} \cos \omega_\alpha t_2 (1 + \cos \omega_\alpha t_1) \theta(\tau_\alpha - t_1) \theta(\tau_\alpha - t_2), \quad (39)$$

and $\theta(t)$ is the step function.

The above results and Eqs. (31)-(33) lead to the following expressions for the kinetic coefficients,

$$\gamma_1 = \sqrt{\frac{8}{\pi M}} \frac{1}{\beta_l} \left\{ \sqrt{m_l \beta_l \langle F_l \rangle} + \sqrt{m_r \beta_r \langle F_r \rangle} \right\}, \quad (40)$$

$$\gamma_2 = -\frac{1}{M^2} \left\{ m_l \beta_l \langle F_l \rangle + m_r \beta_r \langle F_r \rangle \right\}, \quad (41)$$

$$\gamma_3 = -\frac{1}{M} \left\{ m_l \langle F_l \rangle + m_r \langle F_r \rangle \right\}. \quad (42)$$

Note that these expressions are independent of the force constant $k_f$ of the quadratic potential.

Since $\langle F_\alpha \rangle = \pm n_\alpha S/\beta_\alpha$ one can see from (41) that $\gamma_2 = 0$ when the mass densities in both compartments are the same, $m_l = m_r$. In this case the Langevin equation (30) becomes linear and has a solution

$$P(t) = P_0 e^{-\gamma_1 t} + \int_0^t dt e^{\gamma_1 (t-\tau)} F^\dagger (\tau) + \frac{\gamma_3}{\gamma_1} \left( 1 - e^{-\gamma_1 t} \right). \quad (43)$$
which describes relaxation of the momentum to the stationary value \( \langle P \rangle = \langle F \rangle / \gamma_1 + \gamma_3 / \gamma_1 \). If \( \langle F \rangle = 0 \) it follows from (40) and (42) that the stationary momentum equals

\[
\langle P \rangle = \sqrt{\frac{\pi}{8}} \frac{m_l - m_l}{\sqrt{m_l \beta_l} + \sqrt{m_r \beta_r}},
\]

which means that the piston moves in the direction of the compartment with the heavier bath particles. Conditions of equal mass densities, \( m_l m_l = m_r n_r \), and of equal pressure, \( n_l / \beta_l = n_r / \beta_r \), are satisfied simultaneously only when \( m_l \beta_l = m_r \beta_r \). Therefore, Eq. (44) describes motion in the direction of the compartment of higher temperature.

In the general case where \( \gamma_2 \neq 0 \), the non-linear Langevin equation (30) has a form of the non-linear Riccati equation and cannot be explicitly integrated. Using the transformation \( u = \exp(\gamma_2 F) \) it can be converted into a second-order linear equation. In the following, however, this line of reasoning will not be pursued and a simple perturbation analysis of the non-linear Langevin equation will be conducted.

**V. STATIONARY AND TRANSIENT SOLUTIONS**

Let us first analyze the stationary solution of Eq. (30). Since \( \langle F^\dagger(t) \rangle = \langle F \rangle \), as demonstrated in Eq. (14), the Langevin equation (30) implies that the stationary value of the momentum of the piston is given by

\[
\langle P \rangle = \frac{1}{\gamma_1} \langle F \rangle - \frac{\gamma_2}{\gamma_1} \langle P^2 \rangle + \frac{\gamma_3}{\gamma_1} \langle \lambda \rangle.
\]

(45)

To calculate \( \langle P \rangle \) perturbatively to first order in \( \lambda \), one substitutes in Eq. (45) the lowest in \( \lambda \) approximations for \( \langle P^2 \rangle \), which can be derived solving the linear Langevin equation

\[
\dot{P}(t) = F_0(t) - \gamma_1 P(t).
\]

(46)

Note that here the “random” force \( F_0 \) generally is not zero-centered. In the long time limit, the auto-correlation functions for the force on the piston in the left and right compartments are effectively

\[
\langle F_\alpha F_\alpha^\dagger(t) \rangle = \langle F_\alpha \rangle^2 + \langle [F_\alpha, F_\alpha^\dagger(t)] \rangle \rightarrow \langle F_\alpha \rangle^2 + 2\Gamma_\alpha \delta(t),
\]

(47)

where \( \Gamma_\alpha = \int_0^\infty dt \langle [F_\alpha, F_\alpha^\dagger(t)] \rangle \). Thus, the correlation function of the total force \( F_0 = F_0^l + F_0^r \) is

\[
\langle FF_0(t) \rangle = \langle F \rangle^2 + 2\Gamma \delta(t),
\]

(48)

where \( \Gamma = \Gamma_1 + \Gamma_r \).

Using (48), one can calculate \( \langle P^2(t) \rangle \) from the solution of the linear Langevin equation (46), namely,

\[
P_0(t) = P_0 e^{-\gamma_1 t} + \int_0^t d\tau e^{-\gamma_1 (t-\tau)} F_0(\tau).
\]

(49)

For \( t \gg 1/\gamma_1 \), the result assumes the form

\[
\langle P_0^2 \rangle = \frac{\Gamma}{\gamma_1} + \frac{1}{\gamma_1^2} \langle F \rangle^2,
\]

(50)

where \( \Gamma \) is given by

\[
\Gamma = \int_0^\infty dt \langle [F_l, F_l^\dagger(t)] \rangle + \int_0^\infty dt \langle [F_r, F_r^\dagger(t)] \rangle.
\]

(51)

It has been assumed throughout our analysis that the contribution of the systematic force \( \langle F \rangle \) to the momentum of the piston is small. This implies that the second term on the right hand side of Eq. (50) is small compared to the first one. Since \( \Gamma \sim \lambda^1 \) and \( \gamma_1 \sim \lambda^3 \) this restriction requires that \( \langle F \rangle \sim \lambda^{1+\epsilon} \), for some \( \epsilon > 0 \).

For the truncated quadratic potential, \( \Gamma \) can be evaluated using Eq. (36) to obtain

\[
\Gamma = \sqrt{\frac{8}{\pi}} \left\{ \sqrt{\frac{m_l}{\beta_l}} \langle F_l \rangle - \sqrt{\frac{m_r}{\beta_r}} \langle F_r \rangle \right\}.
\]

(52)
It then follows that for the case \( \langle F \rangle = 0 \), one obtains
\[
\langle P_0^2 \rangle = M \sqrt{\frac{m_l/\beta_l + m_r/\beta_r}{m_l/\beta_l + m_r/\beta_r}}. \tag{53}
\]
For a random force obeying Gaussian statistics, distribution of the momentum of the piston is of Maxwellian form
\[
\langle P \rangle = \frac{1}{\gamma_1} \langle F \rangle - \frac{\gamma_2}{\gamma_1} \langle F \rangle^2 + \frac{\gamma_3}{\gamma_1} - \frac{\gamma_2 \Gamma}{\gamma_1}. \tag{54}
\]
For \( \langle F \rangle = 0 \) and with explicit expressions (40)-(42) for \( \gamma_1 \), Eq. (54) takes the form
\[
\langle P \rangle = \sqrt{\frac{\pi}{8}} \sqrt{\frac{m_l m_r}{m_l \beta_l + m_r \beta_r}} \left( \sqrt{\frac{\beta_l}{\beta_r}} - \sqrt{\frac{\beta_r}{\beta_l}} \right). \tag{55}
\]
When the masses of the bath particles are the same in both compartments, \( m_l = m_r = m \), this expression reduces to the result of Gruber and Piasecki [5]
\[
\langle P \rangle = \sqrt{\frac{\pi}{8}} \sqrt{m \left( \sqrt{k_B T_r} - \sqrt{k_B T_l} \right)}. \tag{56}
\]
Note that in this case, \( \gamma_3 \) vanishes as can be seen from Eq. (42). If \( m_l \beta_l = m_r \beta_r \) (and therefore \( \gamma_2 = 0 \)), Eq. (55) coincides with the result (44) obtained in the previous section.

In addition to the stationary solutions of the non-linear Langevin equation, perturbative solutions of the time evolution of the momentum of the piston can be examined by expanding the momentum in the form \( P(t) = P_0(t) + P_1(t) + \cdots \) where \( P_0(t) \) is the solution (49) of the linear Langevin equation (46) and \( P_1(t) \) is the next-order correction in \( \lambda \) which satisfies the equation
\[
\frac{dP_1(t)}{dt} = F_1(t) - \gamma_1 P_1(t) - \gamma_2 P_0^2(t) + \gamma_3, \tag{57}
\]
and the condition \( P_1(0) = 0 \). In this equation, the force \( F_1(t) = F(t) - F_0(t) \) is zero centered, since \( \langle F(t) \rangle = \langle P_0(t) \rangle = 0 \), as established in Eq. (14). Solving Eq. (57) and taking the average gives
\[
\langle P_1(t) \rangle = \frac{\gamma_3}{\gamma_1} \left( 1 - e^{-\gamma_1 t} \right) - \frac{\gamma_2}{\gamma_1} P^2 e^{-\gamma_1 t} \left( 1 - e^{-\gamma_1 t} \right) - \frac{2 \gamma_2}{\gamma_1} \langle F \rangle P e^{-\gamma_1 t} \left\{ \gamma_1 t - (1 - e^{-\gamma_1 t}) \right\} - \frac{2 \gamma_2}{\gamma_1} \langle F \rangle^2 e^{-\gamma_1 t} \left( \sinh \gamma_1 t - \gamma_1 t \right) - \frac{2 \gamma_2 \Gamma}{\gamma_1} e^{-\gamma_1 t} \left( \cosh \gamma_1 t - 1 \right), \tag{58}
\]
where \( P = P_0(0) \). Note that the average momentum \( \langle P \rangle = \langle P_0(t) \rangle + \langle P_1(t) \rangle \) takes the stationary value (54) in the long-time limit \( t \gg \tau_1^{-1} \). It should be emphasized that the transient solution obtained here is valid only on a time scale that is much longer than the characteristic time \( \tau_L \) for the relaxation of the bath but shorter than \( \tau_L \), the time scale for particles to move half the length of the cylinder. The above analysis may be readily extended to the short-time domain using as a starting point the Langevin equation (28) with time-dependent damping coefficients.

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[8] It is shown in Ref. [1] that for the case of the piston in a bath of ideal gas particles, $\lambda$ appears in the expansion of the generalized Langevin equation via the parameter $\lambda_* = \sqrt{N} \lambda$, where $N$ is a number of bath particles in the interaction shell around the piston (provided $N \gg 1$). The actual parameter controlling separation of time scales in this case is therefore $\lambda_*$. This assumption justifies the parabolic potential model and is similar to that used in the linear theory of lattice vibrations when displacements of atoms are assumed to be small compared to the lattice spacing.