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Nonequilibrium identities of granular vibrating beds



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ABSTRACT

We derive the integral fluctuation theorem around a nonequilibrium stationary state for frictionless and soft core granular particles under an external vibration achieved by a balance between an external vibration and inelastic collisions. We also derive the standard fluctuation theorem and the generalized Green–Kubo formula for this system.

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1. Introduction

One of the most remarkable achievements in recent nonequilibrium statistical mechanics is to demonstrate the existence of some nonequilibrium identities such as the generalized Green–Kubo relation [1,2], various fluctuation theorems [3–7] and the Jarzynski equality [8] as well as the mutual relationship [9]. These identities are exact and reproduce the conventional Green–Kubo formula, the second law of thermodynamics and Onsager's reciprocal relation in specific limits. Therefore, these identities are regarded as fundamental relations in nonequilibrium statistical mechanics.

Although it has been believed that these identities are supported by the local time-reversal symmetry or the detailed balance condition, some experiments suggest the existence of fluctuation theorem or related equations even in granular systems which do not have any time-reversal symmetry [10–15], though there exists a counter argument [16]. It is remarkable that Puglisi and his coworkers [17–20] clarified that granular fluids do not hold the conventional fluctuation theorem but have only the second type fluctuation theorem by Evans and Searles [21]. As long as the author's knowledge, however, there is only a paper by Chong et al. which has proven the existence of both the generalized Green–Kubo relation and the integral fluctuation theorem [7] for a granular system under a steady plane shear [11]. They also developed the representation of a nonequilibrium steady-state distribution function [22] and the liquid theory for sheared dense granular systems [23]. Recently, Hayakawa and Otsuki [24] extended their previous formulation to discuss nonequilibrium identities around a nonequilibrium steady state, and also demonstrate their validity from the direct comparison between the obtained identities and the numerical simulations.

Unfortunately, some parts of our previous theoretical studies such as the generalized Green–Kubo formula [11,24] are only valid for stationary external forces and are numerically verified for a plane shear, but the most of experiments adopt vibrating granular gases [10,12,13,15]. In this paper, thus, we re-derive the fluctuation relations for soft core granular gases under vibrations around a nonequilibrium steady state. We also derive the generalized Green–Kubo formula for vibrating beds.

The organization of this paper is as follows. In Section 2, we summarize the general framework of Liouville equation and some identities which are used in this paper. Section 3 which is the main part of this paper consists of two parts. In the first part (Section 3.1) we discuss the derivation of the integral fluctuation theorem (IFT). In the second part and the third part, we also derive a standard fluctuation theorem (Section 3.2) and the generalized Green–Kubo formula (Section 3.3),

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respectively. In Section 4 we discuss our results and we give conclusion in Section 5. In Appendix A, we briefly summarize some operators' identities.

2. Liouville equation

Let us consider a system of N identical soft spherical and smooth dissipative particles. We assume that particles are monodispersed, which are characterized by their diameter d and the mass m . The particles are influenced by the gravity with the acceleration constant g in the z -direction. If we use a box fixed frame, each particle feels the acceleration $-g + A\omega^2 \cos\omega t$ in the z -direction with the amplitude A and the angular acceleration ω . Moreover, we should introduce a confined potential which prevents particles from penetrating the bottom plate.

The basic equation for the statistical mechanics of frictionless granular particles under such a vibration is the Liouville equation [1,24–27]. The argument in this section is parallel to those in Refs. [1,24]. Let $i\mathcal{L}(t)$ be the total Liouvillian which operates an arbitrary function $A(\mathbf{\Gamma}(t))$ starting from $t = 0$ as:

$$\frac{dA(\mathbf{\Gamma}(t))}{dt} = U_{\rightarrow}(0, t)i\mathcal{L}(t)A(\mathbf{\Gamma}), \quad A(\mathbf{\Gamma}(t)) = U_{\rightarrow}(0, t)A(\mathbf{\Gamma}) \quad (1)$$

where

$$\begin{aligned} U_{\rightarrow}(0, t) &\equiv T_{\rightarrow} e^{i \int_0^t ds \mathcal{L}(s)} \\ &= \sum_{n=0}^{\infty} \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n i\mathcal{L}(s_n) \cdots i\mathcal{L}(s_2) i\mathcal{L}(s_1) \end{aligned} \quad (2)$$

and $\mathbf{\Gamma}(t) = \{\mathbf{r}_i(t), \mathbf{p}_i(t)\}_{i=1}^N$ with the abbreviation $\mathbf{\Gamma} \equiv \mathbf{\Gamma}(0)$, the position of i -th particle $\mathbf{r}_i(t)$ and the momentum of i -th particle $\mathbf{p}_i(t)$. We note that there are some trivial relations for $U_{\rightarrow}(t_0, t)$ such as:

$$U_{\rightarrow}(t_0, t) = U_{\rightarrow}(t_0, s)U_{\rightarrow}(s, t); \quad U_{\rightarrow}(t_0, t)\tilde{f}(\mathbf{\Gamma}(t_0)) = \tilde{f}(\mathbf{\Gamma}(t)) \quad (3)$$

for an arbitrary function $\tilde{f}(\mathbf{\Gamma}(t))$.

The total Liouvillian consists of three parts, the elastic part, the viscous part and the part from an external vibration. We write $i\mathcal{L}(t)$ as:

$$i\mathcal{L}(t) = i\mathcal{L}^{(\text{el})}(\mathbf{\Gamma}) + i\mathcal{L}^{(\text{vis})}(\mathbf{\Gamma}) + i\mathcal{L}^{(\text{ext})}(\mathbf{\Gamma}, t) \quad (4)$$

where $i\mathcal{L}^{(\text{el})}(\mathbf{\Gamma})$ is the elastic collision part,

$$i\mathcal{L}^{(\text{el})}(\mathbf{\Gamma}) = \sum_{i=1}^N \frac{\mathbf{p}_i}{m} \cdot \frac{\partial}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(\text{el})} \cdot \frac{\partial}{\partial \mathbf{p}_i} \quad (5)$$

Here, we assume that the elastic force can be represented by the summation of the pairwise force $\mathbf{F}_i^{(\text{el})} = \sum_{j \neq i} \mathbf{F}_{ij}^{(\text{el})}$ with:

$$\mathbf{F}_{ij}^{(\text{el})} = -\frac{\partial u(r_{ij})}{\partial \mathbf{r}_{ij}} = \Theta(d - r_{ij})f(d - r_{ij})\hat{\mathbf{r}}_{ij} \quad (6)$$

where we have introduced the pairwise potential $u(r_{ij})$, $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$, $r_{ij} \equiv |\mathbf{r}_{ij}|$, $\hat{\mathbf{r}}_{ij} \equiv \mathbf{r}_{ij}/r_{ij}$, and the Heaviside function $\Theta(x)$ which satisfies $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for otherwise. The elastic repulsive force $f(x)$ is proportional to x for the linear spring model, or to $x^{3/2}$ for the Hertzian contact model.

Similarly, the viscous Liouvillian $i\mathcal{L}^{(\text{vis})}$ is the contribution of inelastic collisions:

$$i\mathcal{L}^{(\text{vis})}(\mathbf{\Gamma}) = \sum_{i=1}^N \mathbf{F}_i^{(\text{vis})} \cdot \frac{\partial}{\partial \mathbf{p}_i} \quad (7)$$

where $\mathbf{F}_i^{(\text{vis})}$ is the viscous force acting on the i -th particle represented by $\mathbf{F}_i^{(\text{vis})} = \sum_{j \neq i} \mathbf{F}_{ij}^{(\text{vis})}$ with:

$$\begin{aligned} \mathbf{F}_{ij}^{(\text{vis})} &= -\hat{\mathbf{r}}_{ij}\Theta(d - r_{ij})\zeta(d - r_{ij})(\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij}) \\ &= -\hat{\mathbf{r}}_{ij}\mathcal{F}(r_{ij})(\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij}) \end{aligned} \quad (8)$$

Here we have introduced $\mathbf{v}_{ij} \equiv \dot{\mathbf{r}}_{ij} = d\mathbf{r}_{ij}/dt$, and:

$$\mathcal{F}(r) \equiv \Theta(d - r)\zeta(d - r) \quad (9)$$

with the viscous function $\zeta(x)$, which is a constant or $\zeta(x) \propto x^{1/2}$ corresponding to the linear spring model or the Hertzian contact model for the elastic contact force. The Liouville operator representing the vibration $i\mathcal{L}^{(\text{ext})}(t)$ is given by:

$$i\mathcal{L}^{(\text{ext})}(\Gamma, t) = \sum_{i=1}^N \mathbf{F}_i^{(\text{ext})}(t) \cdot \frac{\partial}{\partial \mathbf{p}_i} \tag{10}$$

where the vibrating force is given by:

$$\mathbf{F}_i^{(\text{ext})}(t) = \hat{z} \left\{ m(-g + A\omega^2 \cos \omega t) - \frac{\partial V_{\text{ext}}(z_i)}{\partial z_i} \right\} = \hat{z} F_i^{(\text{ext})}(t) \tag{11}$$

in a box fixed frame, where \hat{z} is the unit vector in the z -direction, and $V_{\text{ext}}(z)$ represents a confined potential in a box such as:

$$V_{\text{ext}}(z) = V_0 \exp[-z/\xi] \tag{12}$$

to prevent grains from penetrating the bottom plate of the container.

It should be noted that the Liouvillian is not self-adjoint, because of the violation of time-reversal symmetry for each collision. The adjoint Liouvillian is defined through the equation of the phase function or the N -body distribution function $\rho(\Gamma, t)$:

$$\rho(\Gamma, t) = \tilde{U}_{\leftarrow}(t, 0)\rho(\Gamma, 0), \quad \frac{\partial \rho(\Gamma, t)}{\partial t} = -i\mathcal{L}^\dagger(t)\rho(\Gamma, t) \tag{13}$$

where

$$\begin{aligned} \tilde{U}_{\leftarrow}(t, 0) &= T_{\leftarrow} e^{-i \int_0^t ds \mathcal{L}^\dagger(s)} \\ &\equiv \sum_{n=0}^{\infty} (-1)^n \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n i\mathcal{L}^\dagger(s_1) i\mathcal{L}^\dagger(s_2) \cdots i\mathcal{L}^\dagger(s_n) \end{aligned} \tag{14}$$

The adjoint Liouvillian satisfies:

$$i\mathcal{L}^\dagger(\Gamma, t) = i\mathcal{L}(\Gamma, t) + \Lambda(\Gamma) \tag{15}$$

where

$$\Lambda(\Gamma) \equiv \frac{\partial}{\partial \Gamma} \cdot \dot{\Gamma}(\Gamma) \tag{16}$$

is the phase volume contraction. We note that $\Lambda(\Gamma)$ in our system does not depend on t explicitly, which can be written as:

$$\Lambda(\Gamma) = \sum_i \frac{\partial}{\partial \mathbf{p}_i} \cdot \mathbf{F}_i^{(\text{vis})} = -\frac{1}{m} \sum_i \sum_{j \neq i} \mathcal{F}(r_{ij}) \tag{17}$$

for $t \geq 0$. The phase volume contraction $\Lambda(\Gamma)$ is directly related to the change of the Jacobian:

$$\left| \frac{\partial \Gamma(t)}{\partial \Gamma} \right| = \exp \left[\int_0^t d\tau \Lambda(\Gamma(\tau)) \right] \tag{18}$$

where $\Lambda(\Gamma(t)) = U_{\rightarrow}(0, t)\Lambda(\Gamma)U_{\leftarrow}(t, 0)$. Note that the time evolution of an arbitrary physical function $A(\Gamma(t))$ is given by $A(\Gamma(t)) = U_{\rightarrow}(0, t)A(\Gamma)U_{\leftarrow}(t, 0)$, where we have introduced $U_{\leftarrow}(t, 0) \equiv T_{\leftarrow} \exp[-i \int_0^t ds \mathcal{L}(s)] = U_{\rightarrow}^{-1}(0, t)$.

The average of a physical quantity is defined as:

$$\langle A(\Gamma(t)) \rangle \equiv \int d\Gamma \rho(\Gamma, 0) A(\Gamma(t)) = \int d\Gamma A(\Gamma) \rho(\Gamma, t) \tag{19}$$

From Eqs. (1), (13) and (19), we obtain the relations:

$$\int d\Gamma \rho(\Gamma) U_{\rightarrow}(0, t) A(\Gamma) = \int d\Gamma A(\Gamma) \tilde{U}_{\leftarrow}(t, 0) \rho(\Gamma, 0) \tag{20}$$

and

$$\int d\Gamma \rho(\Gamma) i\mathcal{L}(t) A(\Gamma) = - \int d\Gamma A(\Gamma) i\mathcal{L}^\dagger(t) \rho(\Gamma, 0) \tag{21}$$

Let us introduce a stationary distribution to characterize the quasi-periodic motion of granular particles under the periodic vibration. In the stationary process, the initial distribution function $\rho(\mathbf{\Gamma}, 0)$ may have the form:

$$\rho(\mathbf{\Gamma}, 0) = \rho_{\text{ini}}(\mathbf{\Gamma}) \equiv \frac{e^{-I_0(\mathbf{\Gamma})}}{\mathcal{Z}} \quad (22)$$

where $I_0(\mathbf{\Gamma}) \equiv I(\mathbf{\Gamma}, t = 2n\pi/\omega)$ with an arbitrary integer n and an effective potential $I(\mathbf{\Gamma}, t)$, and $\mathcal{Z} \equiv \int d\mathbf{\Gamma} e^{-I_0(\mathbf{\Gamma})}$. Note that $I_0(\mathbf{\Gamma})$ is an arbitrary function of $\mathbf{\Gamma}$, and thus, this choice is quite general for the argument. In the stationary process, we assume that an average of an arbitrary function $A(\mathbf{\Gamma}(t))$ satisfies the periodic condition:

$$\left\langle A\left(\mathbf{\Gamma}\left(t + \frac{2n\pi}{\omega}\right)\right) \right\rangle = \langle A(\mathbf{\Gamma}(t)) \rangle \quad (23)$$

for any nonzero integer n . This assumption is reasonable because of the periodicity of the Liouvillian:

$$i\mathcal{L}\left(t + \frac{2n\pi}{\omega}\right) = i\mathcal{L}(t) \quad (24)$$

for an arbitrary integer n . We should note that $U_{\leftarrow}(0, -t) = U_{\rightarrow}^{-1}(-t, 0)$ and $\tilde{U}_{\rightarrow}(-t, 0) = \tilde{U}_{\leftarrow}^{-1}(0, -t)$ are, respectively, not equal to $U_{\leftarrow}(t, 0) = U_{\rightarrow}^{-1}(0, t)$ and $\tilde{U}_{\rightarrow}(0, t) = \tilde{U}_{\leftarrow}^{-1}(t, 0)$ in general, where $U_{\leftarrow}(t, 0) \equiv T_{\leftarrow} e^{-i \int_0^t ds \mathcal{L}(s)}$ and $\tilde{U}_{\rightarrow}(0, t) \equiv T_{\rightarrow} \exp[i \int_0^t ds \mathcal{L}^\dagger(s)]$. However, we can use:

$$U_{\leftarrow}(t, 0) = U_{\leftarrow}(0, -t) \quad \text{and} \quad \tilde{U}_{\rightarrow}(-t, 0) = \tilde{U}_{\rightarrow}(0, t) \quad (25)$$

for stationary state for $t = 2n\pi/\omega$ with an integer n . Indeed, with the aid of Eq. (24), we can rewrite $U_{\leftarrow}(t, 0) = T_{\leftarrow} e^{-i \int_{-2n\pi/\omega}^{t-2n\pi/\omega} d\tau' \mathcal{L}(\tau')}$. Furthermore, if we restrict the time for the measurement to $t = 2n\pi/\omega$, we can rewrite $U_{\leftarrow}(t, 0) = T_{\leftarrow} e^{-i \int_{-t}^0 d\tau \mathcal{L}(\tau)} = U_{\leftarrow}(0, -t)$.

In the last part of this subsection, we introduce a useful formula between $\tilde{U}_{\rightarrow}(0, t)$ and $U_{\rightarrow}(0, t)$. Any two Liouville operators even for $i\mathcal{L}(t)$ and $i\mathcal{L}^\dagger(t)$ satisfy Dyson's equation [1]:

$$\tilde{U}_{\rightarrow}(0, \tau) = U_{\rightarrow}(0, \tau) + \int_0^\tau ds \tilde{U}_{\rightarrow}(0, s) \Lambda(\mathbf{\Gamma}) U_{\rightarrow}(s, \tau) \quad (26)$$

where we have used Eq. (15). It is straightforward to rewrite Eq. (26) as [1]:

$$\tilde{U}_{\rightarrow}(0, t) = \exp\left[\int_0^t d\tau \Lambda(\mathbf{\Gamma}(\tau))\right] U_{\rightarrow}(0, t) \quad (27)$$

where $\Lambda(\mathbf{\Gamma}(t)) = U_{\rightarrow}(0, t) \Lambda(\mathbf{\Gamma}) U_{\leftarrow}(t, 0)$.

3. Fluctuation theorem and Green–Kubo formula

Now, let us derive some important identities such as fluctuation relations and the generalized Green–Kubo formula for vibrating granular materials. For the demonstration of the existence of the above mentioned identities, we explain the derivations as follows. The first part is dedicated to the derivation of the integral fluctuation theorem (IFT). We also derive both the standard fluctuation theorem in the second part and the generalized Green–Kubo formula in the third part.

3.1. Integral fluctuation theorem

The integral fluctuation theorem (IFT) is one of representations of the fluctuation theorem, which is directly related to Jarzynski's equality [8]. The relation between Jarzynski's equality and the fluctuation theorem has been investigated extensively [7,9]. Although IFT is an important identity for the stationary sheared granular systems [11], and this equality plays a fundamental role even in granular systems under a vibration.

To demonstrate the existence of the IFT, we consider a system characterized by the following time-dependent Hamiltonian:

$$H_0(\mathbf{\Gamma}(t)) = \sum_i \frac{\mathbf{p}_i(t)^2}{2m} + \frac{1}{2} \sum_{i,j \neq i} u(r_{ij}(t)) \quad (28)$$

We also assume that the initial condition satisfies the canonical distribution:

$$\rho_{\text{eq}}(\boldsymbol{\Gamma}) = \frac{e^{-\beta H_0(\boldsymbol{\Gamma})}}{Z(\beta)} \tag{29}$$

where β is the inverse temperature and $Z(\beta) \equiv \int d\boldsymbol{\Gamma} e^{-\beta H_0(\boldsymbol{\Gamma})}$.

In this case, it is easy to verify the conservation of the normalization factor, i.e. $Z(\beta) = \int d\boldsymbol{\Gamma} e^{-\beta H_0(\boldsymbol{\Gamma})} = \int d\boldsymbol{\Gamma}(t) e^{-\beta H_0(\boldsymbol{\Gamma}(t))}$. Because the time derivative of $H_0(\boldsymbol{\Gamma}(t))$ is given by:

$$\dot{H}_0(\boldsymbol{\Gamma}(t)) = \sum_i v_{i,z}(t) F_i^{\text{(ext)}}(t) - 2\mathcal{R}(\boldsymbol{\Gamma}(t)) \tag{30}$$

with $\dot{H}_0 \equiv dH_0/dt$, $\mathbf{v}_i(t) \equiv d\mathbf{r}_i(t)/dt$,

$$\mathcal{R}(\boldsymbol{\Gamma}) \equiv -\frac{1}{4} \sum_{i,j} \mathbf{v}_{ij} \cdot \mathbf{F}_{ij}^{\text{(vis)}} = \frac{1}{4} \sum_{i,j} \mathcal{F}(r_{ij}) (\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij})^2 \tag{31}$$

and $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$, the conservation of the probability leads to:

$$\begin{aligned} 1 &= \int d\boldsymbol{\Gamma}(t) \frac{e^{-\beta H_0(\boldsymbol{\Gamma}(t))}}{Z(\beta)} \\ &= \int d\boldsymbol{\Gamma} \left| \frac{\partial \boldsymbol{\Gamma}(t)}{\partial \boldsymbol{\Gamma}} \right| \frac{e^{-\beta H_0(\boldsymbol{\Gamma})}}{Z(\beta)} \exp \left[\beta \int_0^t d\tau \left\{ \sum_i v_{i,z}(\tau) F_i^{\text{(ext)}}(\tau) - 2\mathcal{R}(\boldsymbol{\Gamma}(\tau)) \right\} \right] \\ &= \int d\boldsymbol{\Gamma} \frac{e^{-\beta H_0(\boldsymbol{\Gamma})}}{Z(\beta)} \exp \left[- \int_0^t d\tau \Omega_{\text{eq}}(\boldsymbol{\Gamma}(\tau)) \right] \\ &= \left\langle \exp \left[- \int_0^t d\tau \Omega_{\text{eq}}(\boldsymbol{\Gamma}(\tau)) \right] \right\rangle_{\text{eq}} \end{aligned} \tag{32}$$

where we have used Eq. (18) for the third equality, and introduced:

$$\Omega_{\text{eq}}(\boldsymbol{\Gamma}(t)) \equiv \beta \sum_i v_{i,z}(t) F_i^{\text{(ext)}}(t) - 2\beta \mathcal{R}(\boldsymbol{\Gamma}(t)) - \Lambda(\boldsymbol{\Gamma}(t)) \tag{33}$$

and the average $\langle \cdot \rangle_{\text{eq}} \equiv \frac{1}{Z(\beta)} \int d\boldsymbol{\Gamma} e^{-\beta H_0(\boldsymbol{\Gamma})} \cdot$. Note that this derivation differs from those presented in Ref. [24].

Eq. (32) associated with Eq. (33) is the IFT for granular fluids under the vibration. It is a characteristic feature for dissipative systems that the phase volume contraction $\Lambda(\boldsymbol{\Gamma})$ is involved in $\Omega_{\text{eq}}(\boldsymbol{\Gamma}(t))$. Thus, the right-hand side of the IFT (32) for dissipative cases cannot be represented by the work done by the external force.

The IFT (32) is directly reduced to an inequality:

$$\int_0^t d\tau \langle \Omega_{\text{eq}}(\boldsymbol{\Gamma}(\tau)) \rangle \geq 0 \tag{34}$$

with the aid of Jensen's inequality. This inequality ensures the existence of an entropy-like quantity even for granular systems under the vibration.

Now, let us extend the IFT to the case of starting from an arbitrary distribution $\rho_{\text{ini}}(\boldsymbol{\Gamma})$. In this case, the IFT can be rewritten as:

$$\begin{aligned} 1 &= \int d\boldsymbol{\Gamma}(t) \frac{e^{-I_0(\boldsymbol{\Gamma}(t))}}{\mathcal{Z}} \\ &= \int d\boldsymbol{\Gamma} \left| \frac{\partial \boldsymbol{\Gamma}(t)}{\partial \boldsymbol{\Gamma}} \right| \frac{e^{-I_0(\boldsymbol{\Gamma})}}{\mathcal{Z}} \exp \left[- \int_0^t d\tau \dot{I}_0(\boldsymbol{\Gamma}(\tau)) \right] \\ &= \int d\boldsymbol{\Gamma} \frac{e^{-I_0(\boldsymbol{\Gamma})}}{\mathcal{Z}} \exp \left[- \int_0^t d\tau \Omega(\boldsymbol{\Gamma}(\tau)) \right] \\ &= \left\langle \exp \left[- \int_0^t d\tau \Omega(\boldsymbol{\Gamma}(\tau)) \right] \right\rangle \end{aligned} \tag{35}$$

where $\Omega(\boldsymbol{\Gamma}(t)) = \dot{I}_0(\boldsymbol{\Gamma}(t)) - \Lambda(\boldsymbol{\Gamma}(t))$, and $\mathcal{Z} \equiv \int d\boldsymbol{\Gamma} e^{-I_0(\boldsymbol{\Gamma})} = \int d\boldsymbol{\Gamma}(t) e^{-I_0(\boldsymbol{\Gamma}(t))}$ and $\langle \cdot \rangle = \int d\boldsymbol{\Gamma} \frac{e^{-I_0(\boldsymbol{\Gamma})}}{\mathcal{Z}} \cdot$. Eq. (35) is also reduced to the entropy-like relation:

$$\int_0^t d\tau \langle \Omega(\boldsymbol{\Gamma}(\tau)) \rangle \geq 0 \tag{36}$$

3.2. The standard fluctuation theorem

The direct consequences of Eq. (35) are two important relations, the conventional fluctuation theorem and the generalized Green–Kubo formula, from Eq. (35). Here, let us illustrate how to derive these relations.

It is straightforward to derive the conventional fluctuation theorem (FT) from IFT (32) or (35), where FT is the relation of the probability of the entropy production between the forward path and the inverse path [1]. Because the derivation of FT starting from a canonical distribution has already been discussed in Ref. [24], we, here, present the derivation of FT from Eq. (22) under the assumption that $\rho_{\text{ini}}(\boldsymbol{\Gamma})$ is invariant by the time-reversal operation. Of course, the outline of the derivation is unchanged.

Now let us consider the process from time 0 to time t by the time evolution operator $U_{\rightarrow}(0, t)$ and the trajectory of the phase variable $\boldsymbol{\Gamma}(\tau) = U_{\rightarrow}(0, t)\boldsymbol{\Gamma}$ for $0 \leq \tau \leq t$. The inverse process, thus, is characterized by the time evolution operator $U_{\leftarrow}(t, 0)$ and the inverse phase variable $\boldsymbol{\Gamma}^*(\tau) \equiv \{\mathbf{r}_i(t - \tau), -\mathbf{p}_i(t - \tau)\}_{i=1}^N = \{\boldsymbol{\Gamma}(t - \tau)\}^T$ for $0 \leq \tau \leq t$, where the operation $\{\boldsymbol{\Gamma}(t)\}^T$ represents the change of the sign of the momenta $\{\boldsymbol{\Gamma}(t)\}^T \equiv \{\mathbf{r}_i(t), -\mathbf{p}_i(t)\}_{i=1}^N$. Because the probability of the inverse trajectories $\rho_{\text{ini}}(\boldsymbol{\Gamma}^*)$ is still normalized as $\int d\boldsymbol{\Gamma}^* \rho_{\text{ini}}(\boldsymbol{\Gamma}^*) = 1$ with the abbreviation $\boldsymbol{\Gamma}^* \equiv \boldsymbol{\Gamma}^*(0)$, Eq. (35) can be rewritten as:

$$\int d\boldsymbol{\Gamma} \rho_{\text{ini}}(\boldsymbol{\Gamma}) e^{-t\overline{\Omega}_t} = \int d\boldsymbol{\Gamma}^* \rho_{\text{ini}}(\boldsymbol{\Gamma}^*) \tag{37}$$

where we have introduced $\overline{\Omega}_t \equiv \frac{1}{t} \int_0^t d\tau \Omega(\boldsymbol{\Gamma}(\tau))$ with $\Omega(\boldsymbol{\Gamma}(t)) = \dot{I}_0(\boldsymbol{\Gamma}(t)) - \Lambda(\boldsymbol{\Gamma}(t))$. From the definition of $\Lambda(\boldsymbol{\Gamma}(t))$ and the assumption $I_0(\boldsymbol{\Gamma}^*(\tau)) = I_0(\boldsymbol{\Gamma}(t - \tau))$, there are some trivial relations: $\Lambda(\boldsymbol{\Gamma}^*(\tau)) = -\Lambda(\boldsymbol{\Gamma}(t - \tau))$, and $\Omega(\boldsymbol{\Gamma}^*(\tau)) = -\Omega(\boldsymbol{\Gamma}(t - \tau))$ for $0 \leq \tau \leq t$. Therefore, we can write the probability of $\overline{\Omega}_t = -A$ for $\overline{\Omega}_t \equiv \frac{1}{t} \int_0^t d\tau \Omega(\boldsymbol{\Gamma}^*(\tau)) = \frac{1}{t} \int_0^t d\tau \Omega(\{\boldsymbol{\Gamma}(\tau)\}^T)$:

$$\begin{aligned} \text{Prob}(\overline{\Omega}_t = -A) &= \int d\boldsymbol{\Gamma}^* \rho_{\text{ini}}(\boldsymbol{\Gamma}^*) \delta(\overline{\Omega}_t + A) \\ &= \int d\boldsymbol{\Gamma}(t) \rho_{\text{ini}}(\boldsymbol{\Gamma}(t)) \delta(\overline{\Omega}_t - A) \\ &= \int d\boldsymbol{\Gamma} \rho_{\text{ini}}(\boldsymbol{\Gamma}) e^{-t\overline{\Omega}_t} \delta(\overline{\Omega}_t - A) \\ &= e^{-At} \int d\boldsymbol{\Gamma} \rho_{\text{ini}}(\boldsymbol{\Gamma}) \delta(\overline{\Omega}_t - A) \\ &= e^{-At} \text{Prob}(\overline{\Omega}_t = A) \end{aligned} \tag{38}$$

for the conventional fluctuation theorem, where we have used $|\partial \boldsymbol{\Gamma}^*(\tau) / \partial \boldsymbol{\Gamma}(t - \tau)| = 1$, $\rho_{\text{ini}}(\boldsymbol{\Gamma}(t)) = \rho_{\text{ini}}(\boldsymbol{\Gamma}) e^{-\beta \int_0^t d\tau \dot{H}(\tau)}$ and $d\boldsymbol{\Gamma}(t) = d\boldsymbol{\Gamma} e^{\int_0^t d\tau \Lambda(\boldsymbol{\Gamma}(\tau))}$. Note that the argument is still valid for the general starting point Eq. (22) if we have the symmetry $I(\boldsymbol{\Gamma}^*(\tau)) = I(\boldsymbol{\Gamma}(t - \tau))$.

3.3. Generalized Green–Kubo formula

Next, let us derive the generalized Green–Kubo formula from Eq. (35) following the argument in Refs. [11,24]. It should be noted that the generalized Green–Kubo formula is only valid for $t = 2n\pi/\omega$ with an arbitrary integer n , i.e. at time with an identical phase of oscillation. Nevertheless, the argument in this subsection can be used for time-dependent processes which has not be proven in Ref. [24].

Now, let us rewrite Eq. (13) as:

$$\rho_{\text{ini}}(\boldsymbol{\Gamma}) = \tilde{U}_{\rightarrow}(0, t) \rho(\boldsymbol{\Gamma}, t) = e^{\int_0^t d\tau \Lambda(\boldsymbol{\Gamma}(\tau))} \rho(\boldsymbol{\Gamma}(t), t) \tag{39}$$

where we have used the identity (27). Let us operate $U_{\leftarrow}(t, 0)$ on the both sides of Eq. (39) with the aid of Eq. (25) at $t = 2n\pi/\omega$ with an integer n , we can write:

$$\begin{aligned}
U_{\leftarrow}(t, 0)\rho_{\text{ini}}(\boldsymbol{\Gamma}) &= U_{\leftarrow}(0, -t)\rho_{\text{ini}}(\boldsymbol{\Gamma}) = \rho_{\text{ini}}(\boldsymbol{\Gamma}(-t)) \\
&= \frac{e^{-I_0(\boldsymbol{\Gamma}(-t))}}{\mathcal{Z}} = e^{\int_0^t d\tau \dot{I}_0(\boldsymbol{\Gamma}(-\tau))} \rho_{\text{ini}}(\boldsymbol{\Gamma}) \\
&= U_{\leftarrow}(t, 0) \left[e^{\int_0^t d\tau \Lambda(\boldsymbol{\Gamma}(t-\tau))} \rho(\boldsymbol{\Gamma}(t), t) \right] = e^{\int_0^t d\tau \Lambda(\boldsymbol{\Gamma}(-\tau))} \rho(\boldsymbol{\Gamma}, t)
\end{aligned} \tag{40}$$

From Eq. (40) we immediately obtain:

$$\rho(\boldsymbol{\Gamma}, t) = e^{\int_0^t d\tau \Omega(\boldsymbol{\Gamma}(-\tau))} \rho_{\text{ini}}(\boldsymbol{\Gamma}) \tag{41}$$

From the time differentiation of Eq. (19) with the help of Eq. (41), we obtain:

$$\begin{aligned}
\frac{d}{dt} \langle A(\boldsymbol{\Gamma}(t)) \rangle &= \int d\boldsymbol{\Gamma} A(\boldsymbol{\Gamma}) \Omega(\boldsymbol{\Gamma}(-t)) \rho(\boldsymbol{\Gamma}, t) = \int d\boldsymbol{\Gamma} U_{\leftarrow}(t, 0) \{ A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) \} \rho(\boldsymbol{\Gamma}, t) \\
&= \int d\boldsymbol{\Gamma} A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) \tilde{U}_{\rightarrow}(0, t) \rho(\boldsymbol{\Gamma}, t) = \int d\boldsymbol{\Gamma} A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) e^{\int_0^t d\tau \Lambda(\boldsymbol{\Gamma}(\tau))} \rho(\boldsymbol{\Gamma}(t), t) \\
&= \int d\boldsymbol{\Gamma} A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) \frac{e^{-I_0(\boldsymbol{\Gamma})}}{\mathcal{Z}} = \langle A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) \rangle
\end{aligned} \tag{42}$$

This equation can be integrated over t as:

$$\langle A(\boldsymbol{\Gamma}(t)) \rangle = \langle A(\boldsymbol{\Gamma}) \rangle + \int_0^t ds \langle A(\boldsymbol{\Gamma}(s)) \Omega(\boldsymbol{\Gamma}) \rangle \tag{43}$$

This result depends on $\rho_{\text{ini}}(\boldsymbol{\Gamma})$. Therefore, the formal response theory can be written as:

$$\langle \delta A(\boldsymbol{\Gamma}) \rangle = \int_0^{\infty} dt \langle A(\boldsymbol{\Gamma}(t)) \Omega(\boldsymbol{\Gamma}) \rangle \tag{44}$$

where $\delta A(\boldsymbol{\Gamma}) \equiv \lim_{t \rightarrow \infty} A(\boldsymbol{\Gamma}(t)) - A(\boldsymbol{\Gamma})$.

4. Discussion

In this paper, we obtain exact nonequilibrium relations. To verify the validity, we may need numerical simulations as in Ref. [24]. In simulations, we need to restrict our interest to the statistics for a small number of particles with a large number of sample averages. For example, Ref. [24] uses 18 grains with 800,000 samples. It should be noted that the verification of the generalized Green–Kubo formula is not difficult by the direct simulation, but the confirmation of the integral fluctuation theorem by simulations is not easy because of the limitation of numerical accuracy. We should stress that these identities can be used even for dense granular systems above the jamming transition.

Although the results obtained in this paper are exact without the limitation of applicability range, the actual confirmation for large systems is almost impossible, because the theory requires all cumulants and information for N -body distribution function, which are not correctly measured in experiments. Similarly, to prepare the general initial distribution function (22) except for the equilibrium condition (29) experimentally is almost impossible. In Ref. [24], we use the inverse trajectory in which the time flows from the future to the past, which cannot be used in experiments. These difficulties come from the fact that the derived equation is exact without using any coarsening procedure.

Thus, it is not easy to calculate the correlation function (Eq. (43) or Eq. (44)). One of the possible methods is to use the mode-coupling theory (MCT). It is helpful to apply MCT for granular liquids to characterize theology near the jamming transition [25,28–31]. It is notable that Ref. [27] develops a linear response theory for a sheared thermostat system around a nonequilibrium steady state. The application of this method will be discussed elsewhere.

5. Summary

We have developed some exact relations for frictionless granular fluids under vibrations. We derived the integral fluctuation theorem and the standard fluctuation theorem around a nonequilibrium steady state. We finally obtained the generalized Green–Kubo formula around a nonequilibrium steady state.

In this paper, we focus on the detailed analytic calculation on the granular fluids under the vibration. The systematic check in terms of the simulations will be reported elsewhere.

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Appendix A. Some operators' identities

Let us consider the time evolution of $\Gamma(t; t_0)$ defined by:

$$\Gamma(t; t_0) = U_{\rightarrow}(t_0, t)\Gamma(t_0) \quad (45)$$

where we have explicitly written the initial time t_0 .

By using $U_{\rightarrow}(t_0, t)$ and $U_{\leftarrow}(t, t_0)$ it is notable that there is an important relation for $U_{\rightarrow}(t_0, t)$:

$$A(\Gamma(t)) \equiv U_{\rightarrow}(t_0, t)A(\Gamma(t_0))U_{\leftarrow}(t, t_0) = U_{\rightarrow}(t_0, t)A(\Gamma(t_0)) \quad (46)$$

The proof of (46) is straightforward. The right-hand side of Eq. (46) can be rewritten as:

$$\begin{aligned} U_{\rightarrow}(t_0, t)A(\Gamma(t_0)) &= U_{\rightarrow}(t_0, t)A(\Gamma(t_0))U_{\leftarrow}(t, t_0)U_{\rightarrow}(t, t_0)1 = U_{\rightarrow}(t_0, t)A(\Gamma(t_0))U_{\leftarrow}(t, t_0)1 \\ &= U_{\rightarrow}(t_0, t)A(\Gamma(t_0))U_{\leftarrow}(t, t_0) \end{aligned} \quad (47)$$

where we have used $U_{\rightarrow}(t_0, t)1 = 1$ for a constant 1. When we use Eq. (46), we readily obtain:

$$U_{\rightarrow}(t_0, t)A(\Gamma(t_0))B(\Gamma(t_0)) = A(\Gamma(t; t_0)) \cdot B(\Gamma(t; t_0)) \quad (48)$$

Indeed, the left-hand side of this equation can be rewritten as:

$$\begin{aligned} U_{\rightarrow}(t_0, t)A(\Gamma(t_0))B(\Gamma(t_0)) &= U_{\rightarrow}(t_0, t)A(\Gamma(t_0))U_{\leftarrow}(t, t_0)U_{\rightarrow}(t_0, t)B(\Gamma(t_0))U_{\leftarrow}(t, t_0) \\ &= A(\Gamma(t; t_0)) \cdot B(\Gamma(t; t_0)) \end{aligned} \quad (49)$$

which is the end of the proof of Eq. (48).

References

- [1] D.J. Evans, G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids*, 2nd ed., Cambridge University Press, Cambridge, 2008.
- [2] G.P. Morriss, D.J. Evans, Application of transient correlation functions to shear flow far from equilibrium, *Phys. Rev. A* 35 (1987) 792–797.
- [3] D.J. Evans, E.G.D. Cohen, G.P. Morriss, Probability of second law violations in shearing steady states, *Phys. Rev. Lett.* 71 (1993) 2401–2404.
- [4] G. Gallavotti, E.G.D. Cohen, Dynamical ensembles in nonequilibrium statistical mechanics, *Phys. Rev. Lett.* 74 (1995) 2694–2697.
- [5] J. Kurchan, Fluctuation theorem for stochastic dynamics, *J. Phys. A: Math. Gen.* 31 (1998) 3719–3729.
- [6] D.J. Evans, D.J. Searles, The fluctuation theorem, *Adv. Phys.* 51 (2002) 1529–1585.
- [7] U. Seifert, Stochastic thermodynamics, fluctuation theorems and molecular machines, *Rep. Prog. Phys.* 75 (2012) 126001 (58 p.).
- [8] C. Jarzynski, Nonequilibrium equality for free energy differences, *Phys. Rev. Lett.* 78 (1997) 2690–2693.
- [9] G.E. Crooks, Path-ensemble averages in systems driven far from equilibrium, *Phys. Rev. E* 61 (2000) 2361–2366.
- [10] K. Feitosa, N. Mennon, Fluidized granular medium as an instance of the fluctuation theorem, *Phys. Rev. Lett.* 92 (2004) 164301 (4 p.).
- [11] S.-H. Chong, M. Otsuki, H. Hayakawa, Generalized Green–Kubo relation and integral fluctuation theorem for driven dissipative systems without microscopic time reversibility, *Phys. Rev. E* 81 (2010) 041130 (4 p.).
- [12] N. Kumar, S. Ramaswamy, A.K. Sood, Symmetry properties of the large-deviation function of the velocity of a self-propelled polar particle, *Phys. Rev. Lett.* 106 (2011) 118001 (4 p.).
- [13] S. Jaubaud, D. Lohse, D. van der Meer, Fluctuation theorems for an asymmetric rotor in a granular gas, *Phys. Rev. Lett.* 108 (2012) 210604 (5 p.).
- [14] A. Naert, Experimental study of work exchange with a granular gas: The viewpoint of the Fluctuation Theorem, *Europhys. Lett.* 97 (2012) 20010 (6 p.).
- [15] A. Mounier, A. Naert, The Hatano–Sasa equality: Transitions between steady states in a granular gas, *Europhys. Lett.* 100 (2012) 30002 (7 p.).
- [16] A. Puglisi, P. Visco, R. Barrat, E. Trizac, F. van Wijland, Fluctuations of internal energy flow in a vibrated granular gas, *Phys. Rev. Lett.* 95 (2005) 110202 (4 p.).
- [17] A. Puglisi, P. Visco, E. Trizac, F. van Wijland, Injected power and entropy flow in a heated granular gas, *Europhys. Lett.* 72 (2005) 55–61.
- [18] A. Puglisi, P. Visco, E. Trizac, F. van Wijland, Dynamics of a tracer granular particle as a nonequilibrium Markov process, *Phys. Rev. E* 73 (2006) 021301 (13 p.).
- [19] A. Puglisi, L. Rondoni, A. Vulpiani, Relevance of initial and final conditions for the fluctuation relation in Markov processes, *J. Stat. Mech.* (2006) P08001 (22 p.).
- [20] A. Sarracino, D. Villamaina, G. Gradenigo, A. Puglisi, Irreversible dynamics of a massive intruder in dense granular fluids, *Europhys. Lett.* 92 (2010) 34001 (5 p.).
- [21] D.J. Evans, D.J. Searles, Equilibrium microstates which generate second law violating steady states, *Phys. Rev. E* 50 (1994) 1645–1648.
- [22] S.-H. Chong, M. Otsuki, H. Hayakawa, Representation of the nonequilibrium steady-state distribution function for sheared granular systems, *Prog. Theor. Phys. Suppl.* 184 (2010) 72–87.
- [23] H. Hayakawa, S.-H. Chong, M. Otsuki, *AIP Conf. Proc.* 1227 (2010) 19–30.
- [24] H. Hayakawa, M. Otsuki, Nonequilibrium identities and response theory for dissipative particles, *Phys. Rev. E* 88 (2013) 032117 (9 p.).
- [25] H. Hayakawa, M. Otsuki, Mode-coupling theory of sheared dense granular liquids, *Prog. Theor. Phys.* 119 (2008) 381–402.
- [26] K. Suzuki, S.-H. Chong, M. Otsuki, H. Hayakawa, *in preparation*.
- [27] K. Suzuki, H. Hayakawa, Nonequilibrium mode-coupling theory for uniformly sheared underdamped systems, *Phys. Rev. E* 87 (2013) 012304 (27 p.).
- [28] W.T. Kranz, M. Sperl, A. Zippelius, Glass transition for driven granular fluids, *Phys. Rev. Lett.* 104 (2010) 225701 (4 p.).
- [29] W.T. Kranz, M. Sperl, A. Zippelius, Glass transition in driven granular fluids: A mode-coupling approach, *Phys. Rev. E* 87 (2013) 022207 (14 p.).
- [30] K. Suzuki, H. Hayakawa, Mode-coupling theory for sheared granular liquids, *AIP Conf. Proc.* 1542 (2013) 670–673.
- [31] K. Suzuki, H. Hayakawa, Rheology of dense sheared granular liquids: a mode-coupling approach, *arXiv:1310.3042v1* (9 p.).