Generalized Green-Kubo relation and integral fluctuation theorem for driven dissipative systems without microscopic time reversibility

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We derive the generalized Green-Kubo relation and an integral form of the fluctuation theorem that apply to driven dissipative systems, in which time-reversal symmetry or local detailed balance is broken. Uniformly sheared granular systems and driven inelastic Lorentz-gas model are considered as examples. It is discussed how statistical mechanical theory dealing with nonequilibrium steady-state properties can be constructed for such systems for which equilibrium state does not exist.

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Developing statistical mechanics for nonequilibrium steady states is one of the most challenging problems in physics. Indeed, quite a few studies have been devoted to such a development [1-8], and among the most remarkable outcomes have been the generalized Green-Kubo relation [3] and various forms of fluctuation theorems [4-8]. However, most of these studies rest on the use of microscopic time reversibility or local detailed balance [9], and they cannot literally be applied to macroscopic dissipative systems such as granular fluids [10] despite manifest similarities [11]. Indeed, systems lacking local detailed balance cannot reach equilibrium states because of the existence of the intrinsic dissipation in the systems, and can only reach nonequilibrium steady states via the balance between external forces and dissipations. Thus, the linear-response theory near equilibrium cannot be used for such systems in naive sense, and one needs to construct an essential nonequilibrium statistical mechanics far from equilibrium. In this paper, we explore to what extent those outcomes from previous studies hold also for this important class of systems, in which microscopic time reversibility is broken. It is demonstrated that the generalized Green-Kubo relation and an integral form of the fluctuation theorem can be derived without resorting to microscopic time reversibility. This will be exemplified for uniformly sheared granular systems and driven inelastic Lorentz-gas model.

We shall primarily deal with a system of *N* dissipative soft-sphere particles of mass *m* in a volume *V* subjected to stationary shearing characterized by the shear-rate tensor $\kappa_{\lambda\mu} = \dot{\gamma} \delta_{\lambda x} \delta_{\mu y}$ with the shear rate $\dot{\gamma}$, which we call the system A. To demonstrate the generality of our formulation, we will also consider a system, to be referred to as the system B, in which a mobile soft-sphere particle of mass *m* moves under an external force in an environment of *N* fixed spherical scatterers randomly distributed in a volume *V*, and the interaction between the mobile particle and the scatterers is dissipative.

A distinctive feature of these systems is that, due to the presence of inelastic collisions, the time-reversal symmetry is broken in the equations of motion (see below). In addition, thermal fluctuations are absent in these systems (i.e., they can be considered as the systems coupled to a heat bath of zero temperature), and their dynamics cannot be modeled by a Langevin equation. Therefore, the methods developed in [8] do not apply to the present systems. Furthermore, our formulation does not rely on the presence of the nonequilibrium steady-state distribution function, which is in contrast to the recent studies [12] for systems lacking microscopic time reversibility. In fact, it is a nontrivial problem whether a well-defined steady-state distribution function exists for such driven dissipative systems considered here [13].

The time evolution of the system A is determined by Newton's equation of motion

$$m\ddot{\mathbf{r}}_i = \sum_{j \neq i} \mathbf{F}_{ij}^{\mathrm{A}},\tag{1}$$

under a suitable boundary condition, such as the Lees-Edwards boundary condition [1], accounting for the stationary shearing. Here \mathbf{r}_i refers to the position of particle *i*. We assume pairwise-additive "smooth" contact forces acting only on the normal direction. The simplest realistic model for such a force \mathbf{F}_{ij}^{A} that particle *j* exerts on particle *i* is given by [14,15],

$$\mathbf{F}_{ij}^{\mathbf{A}} = \hat{\mathbf{r}}_{ij} \Theta(d - r_{ij}) [f_{\mathbf{A}}(d - r_{ij}) - \zeta_{\mathbf{A}}(d - r_{ij})(\mathbf{g}_{ij} \cdot \hat{\mathbf{r}}_{ij})]. \quad (2)$$

Here *d* denotes the particle diameter; $\Theta(x)$ is the Heaviside step function; $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ and $\mathbf{g}_{ij} \equiv \dot{\mathbf{r}}_i - \dot{\mathbf{r}}_j$; and $\hat{\mathbf{r}}_{ij} \equiv \mathbf{r}_{ij}/r_{ij}$ with $r_{ij} \equiv |\mathbf{r}_{ij}|$. The first term in Eq. (2) describes a conservative force representing the elastic repulsion: typical functional forms are $f_A(x) \propto x$ (linear model) and $f_A(x) \propto x^{3/2}$ (Hertzian model). The second term refers to a nonconservative, dissipative force due to inelastic collisions. It is proportional to the relative velocity of colliding particles, and breaks the time-reversal symmetry of Eq. (2), i.e., Eq. (1) is not invariant under the time-reversal map $\{\mathbf{r}_i, \dot{\mathbf{r}}_i\} \rightarrow \{\mathbf{r}_i, -\dot{\mathbf{r}}_i\}$. The amount of energy dissipation is characterized by the viscous function $\zeta_A(x)$ which is typically assumed to be constant or modeled as $\zeta_A(x) \propto x^{1/2}$.

From the theoretical side, however, it is quite difficult to handle such a boundary-driven system. Fortunately, it has been demonstrated that the boundary-driven shear flow can be accounted for simply by adding an external force $\mathbf{F}_i^{\text{ex},A}$ = $m\boldsymbol{\kappa}\cdot\mathbf{r}_i\delta(t-t_0)$ to the right-hand side of Eq. (1) [1,16]. Here t_0 denotes the time at which the external force is added, and we set $t_0=0$ in the following. Since the external force $\mathbf{F}_i^{\text{ex,A}}$ induces a linear streaming velocity profile $\boldsymbol{\kappa} \cdot \mathbf{r}_i$ at position \mathbf{r}_i , it is natural to introduce the peculiar, or thermal, momentum via $\mathbf{p}_i \equiv m(\dot{\mathbf{r}}_i - \boldsymbol{\kappa} \cdot \mathbf{r}_i)$. If the phase-space point of the system A is chosen as $\{\mathbf{r}_i, \mathbf{p}_i\}$, Newton's Eq. (1) for t > 0 can be rewritten as

$$\dot{\mathbf{p}}_i = \sum_{j \neq i} \mathbf{F}_{ij}^{\mathrm{A}} - \boldsymbol{\kappa} \cdot \mathbf{p}_i.$$
(3)

The internal energy of the system A is

$$H_{\rm A} = \sum_{i} \frac{1}{2m} \mathbf{p}_{i}^{2} + \frac{1}{2} \sum_{i} \sum_{j \neq i} V_{\rm A}(r_{ij}), \qquad (4)$$

where the potential energy function $V_A(r_{ij})$ satisfies $\partial V_A(r_{ij})/\partial r_{ij} = -\Theta(d-r_{ij})f_A(d-r_{ij})$. The rate of its change is computed by using Eq. (3) as

$$\dot{H}_{\rm A} = - \dot{\gamma} \sigma_{xy} - 2\mathcal{R}_{\rm A}. \tag{5}$$

Here we have used the specific form $\kappa_{\lambda\mu} = \dot{\gamma} \delta_{\lambda x} \delta_{\mu y}$ and the symmetry $\sigma_{\lambda\mu} = \sigma_{\mu\lambda}$ of the stress tensor

$$\sigma_{\lambda\mu} = \sum_{i} \left[\frac{p_{i,\lambda} p_{i,\mu}}{m} + r_{i,\lambda} \sum_{j \neq i} F^{A}_{ij,\mu} \right].$$
(6)

 \mathcal{R}_A is Rayleigh's dissipation function [17]

$$\mathcal{R}_{\mathrm{A}} = \frac{1}{4} \sum_{i} \sum_{j \neq i} \Theta(d - r_{ij}) \zeta_{\mathrm{A}} (d - r_{ij}) (\mathbf{g}_{ij} \cdot \hat{\mathbf{r}}_{ij})^{2}.$$
(7)

We next introduce corresponding equations and quantities for the system B. Newton's equation for the mobile particle (labeled "0") of position \mathbf{r}_0 under an external force $\mathbf{F}_0^{\text{ex,B}}$ is given by

$$m\ddot{\mathbf{r}}_0 = \sum_j \mathbf{F}_{0j}^{\mathrm{B}} + \mathbf{F}_0^{\mathrm{ex,B}}.$$
(8)

Here $\mathbf{F}_{0j}^{\text{B}}$ describes the force between the mobile particle and the scatterer *j*, whose functional form is the same as in Eq. (2), $\mathbf{F}_{0j}^{\text{B}} = \hat{\mathbf{r}}_{0j}\Theta(d-r_{0j})[f_{\text{B}}(d-r_{0j}) - \zeta_{\text{B}}(d-r_{0j})(\dot{\mathbf{r}}_{0} \cdot \hat{\mathbf{r}}_{0j})]$, consisting of the elastic and inelastic (dissipative) terms. We do not assume particular functional forms for $f_{\text{B}}(x)$, $\zeta_{\text{B}}(x)$, and the external force $\mathbf{F}_{0}^{\text{ex,B}}$ since they are unnecessary in the following formulation. The internal energy of the system B is given by $H_{\text{B}} = \frac{1}{2}m\dot{\mathbf{r}}_{0}^{2} + V_{\text{B}}(r_{0j})$ with $V_{\text{B}}(r_{0j})$ satisfying $\partial V_{\text{B}}(r_{0j}) / \partial r_{0j} = -\Theta(d-r_{0j})f_{\text{B}}(d-r_{0j})$. The rate of the internal energy change reads $\dot{H}_{\text{B}} = (\dot{\mathbf{r}}_{0} \cdot \mathbf{F}_{0}^{\text{ex,B}}) - 2\mathcal{R}_{\text{B}}$ with \mathcal{R}_{B} $= \frac{1}{2}\Sigma_{j}\Theta(d-r_{0j})\zeta_{\text{B}}(d-r_{0j})(\dot{\mathbf{r}}_{0} \cdot \hat{\mathbf{r}}_{0j})^{2}$.

Statistical mechanical theory for both the systems A and B can be developed in parallel if one regards that the phase-space point Γ of the system A is given by $\Gamma_A = (\mathbf{r}^N, \mathbf{p}^N)$ whereas that of the system B by $\Gamma_B = (\mathbf{r}_0, m\mathbf{r}_0)$. Hence, the subscript/superscript specifying the system A or B shall be dropped in equations and quantities when they apply to both the systems. In this way, we can demonstrate the existence of universal properties of driven dissipative systems.

The time evolution of a phase variable $X(\Gamma)$ is determined by the Liouville equation [1]:

$$\frac{d}{dt}X(\Gamma) = \dot{\Gamma} \cdot \frac{\partial}{\partial \Gamma}X(\Gamma) \equiv i\mathcal{L}X(\Gamma).$$
(9)

The explicit expression for the Liouvillian $i\mathcal{L}$ for the systems A and B can easily be found from Eqs. (3) and (8), respectively. A formal solution to Eq. (9) reads $X(\Gamma(t)) = \exp(i\mathcal{L}t)X(\Gamma)$. [Hereafter, the absence of the argument *t* implies that associated quantities are evaluated at t=0, and the dependence on Γ shall often be dropped for brevity like $X(t)=X(\Gamma(t))$.] On the other hand, the Liouville equation for the phase-space distribution function $f(\Gamma, t)$ is given by [1]

$$\frac{\partial f(\Gamma, t)}{\partial t} = -\left[i\mathcal{L} + \Lambda(\Gamma)\right]f(\Gamma, t) \equiv -i\mathcal{L}^{\dagger}f(\Gamma, t).$$
(10)

Here $\Lambda(\Gamma) \equiv (\partial/\partial\Gamma) \cdot \dot{\Gamma}$ is the phase-space compression factor. From Eqs. (3) and (8), one obtains

$$\Lambda_{\mathcal{A}}(\Gamma) = -\frac{1}{m} \sum_{i} \sum_{j \neq i} \Theta(d - r_{ij}) \zeta_{\mathcal{A}}(d - r_{ij}) \le 0, \quad (11)$$

for the system A, whereas $\Lambda_{\rm B} = -\frac{1}{m} \Sigma_j \Theta(d - r_{0j}) \zeta_{\rm B}(d - r_{0j}) \leq 0$ for the system B. A formal solution to Eq. (10) is $f(\Gamma, t) = \exp(-i\mathcal{L}^{\dagger}t)f(\Gamma)$. In the following, we shall often use the relations [1]:

$$\int d\Gamma [e^{i\mathcal{L}t}X(\Gamma)]Y(\Gamma) = \int d\Gamma X(\Gamma) [e^{-i\mathcal{L}^{\dagger}t}Y(\Gamma)], \quad (12)$$

$$\exp(-i\mathcal{L}^{\dagger}t) = \exp\left[-\int_{0}^{t} ds\Lambda(-s)\right] \exp(-i\mathcal{L}t). \quad (13)$$

Let us consider the following realization of the nonequilibrium steady state. The system is first equilibrated at the inverse temperature $\beta = 1/T$ (setting Boltzmann's constant unity) in the absence of the external force and by turning off the dissipative forces (i.e., $\zeta = 0$). The latter condition is necessary since the equilibrium state is never reached in the presence of the dissipative forces. This choice of the fictitious initial state will be justified below. The initial distribution function is then given by the canonical one

$$f_{\rm c}(\Gamma;\beta) \equiv \frac{e^{-\beta H_0(\Gamma)}}{\mathcal{Z}(\beta)}, \quad \mathcal{Z}(\beta) = \int d\Gamma e^{-\beta H_0(\Gamma)}, \quad (14)$$

where H_0 denotes either H_A or H_B . At time t=0, the external force ($\mathbf{F}_i^{\text{ex,A}}$ or $\mathbf{F}_0^{\text{ex,B}}$) and dissipative forces are turned on, and thereafter the system evolves according to Eq. (3) and (8). The nonequilibrium distribution function for t>0 is then given by

$$f(\Gamma, t) = \exp(-i\mathcal{L}^{\dagger}t)f_{c}(\Gamma; \beta).$$
(15)

The steady state is assumed to be reached for $t \rightarrow \infty$.

One obtains from Eqs. (13) and (15) the so-called Kawasaki representation [1]

$$f(\mathbf{\Gamma},t) = \exp\left[-\int_{0}^{t} ds \Lambda(-s)\right] \frac{e^{-\beta H_{0}(-t)}}{\mathcal{Z}(\beta)}$$
$$= f_{c}(\mathbf{\Gamma};\beta) \exp\left[\int_{0}^{t} ds \Omega(-s)\right].$$
(16)

In the second equality we have introduced the dissipation function $\Omega(t) = e^{i\mathcal{L}t}\Omega(\Gamma)$ with

$$\Omega(\Gamma) \equiv -i\mathcal{L} \log f_{\rm c}(\Gamma;\beta) - \Lambda(\Gamma) = \beta H_0(\Gamma) - \Lambda(\Gamma).$$
(17)

One easily finds that the dissipation function $\Omega(\Gamma)$ so introduced coincides with the one in [6]. For the system A, one obtains from Eq. (5)

$$\Omega_{\rm A}(\Gamma) = -\beta \dot{\gamma} \sigma_{xy}(\Gamma) - 2\beta \mathcal{R}_{\rm A}(\Gamma) - \Lambda_{\rm A}(\Gamma), \qquad (18)$$

whereas for the system B there holds $\Omega_{\rm B}(\Gamma) = \beta(\dot{\mathbf{r}}_0 \cdot \mathbf{F}_0^{\rm ex.B})$ $-2\beta \mathcal{R}_{\rm B}(\Gamma) - \Lambda_{\rm B}(\Gamma)$. From Eq. (16) and the normalization $\int d\Gamma f(\Gamma, t) = 1$, one obtains a Jarzynski-type equality $\langle e^{\int_0^t ds \Omega(-s)} \rangle_{\beta} = 1$ [5], but a more useful form of such an equality shall be derived below. From here on, $\langle \cdots \rangle_{\beta} \equiv \int d\Gamma f_{\rm c}(\Gamma; \beta) \cdots$ refers to the averaging over the initial canonical distribution function.

For the nonequilibrium average $\langle X(t) \rangle_{\beta}$ defined by

$$\langle X(t) \rangle_{\beta} \equiv \int d\Gamma f_{\rm c}(\Gamma;\beta)X(t) = \int d\Gamma X(0)f(\Gamma,t),$$
 (19)

in which the second equality follows from Eq. (12), one finds using Eq. (16)

$$\langle X(t) \rangle_{\beta} = \langle X(0) e^{\int_0^t ds \Omega(-s)} \rangle_{\beta}.$$
 (20)

By differentiating and then integrating this equation with respect to time, we obtain

$$\langle X(t) \rangle_{\beta} = \langle X(0) \rangle_{\beta} + \int_{0}^{t} ds \langle X(s) \Omega(0) \rangle_{\beta}.$$
 (21)

The derivation of Eqs. (20) and (21) in terms of the dissipation function $\Omega(\Gamma)$ is called the dissipation theorem [18]. In [18], the dissipation theorem has been derived using the same conditions as required for the derivation of the fluctuation theorem, which include the requirement of microscopic time reversibility. However, as is clear from our derivation, the dissipation theorem holds also in the absence of such a symmetry.

Here, a question arises as to the utility of Eqs. (20) and (21) since they explicitly refer to the inverse temperature β of the initial equilibrium distribution. In this regard, let us prove here two important properties concerning $\lim_{t\to\infty} \langle X(t) \rangle_{\beta}$ for systems that exhibit mixing [19]. (A possibility of having symmetry breaking phenomena, such as shear banding in the case of the system A, is thus excluded from the following discussion.) First, it follows from Eq. (21) for $t\to\infty$

$$\frac{d}{dt}\langle X(t)\rangle_{\beta} = \langle X(t)\Omega(0)\rangle_{\beta} \to \langle X(t)\rangle_{\beta}\langle \Omega(0)\rangle_{\beta} = 0, \quad (22)$$

meaning that $\lim_{t\to\infty} \langle X(t) \rangle_{\beta}$ becomes a constant. Here we have used $\langle \Omega(0) \rangle_{\beta} = 0$ which can easily be confirmed for the system A from Eqs. (6), (7), and (11), and similarly for the system B. Thus, the steady-state average $\langle X \rangle_{ss} \equiv \lim_{t\to\infty} \langle X(t) \rangle_{\beta}$ is well defined, and is given by setting $t\to\infty$ in Eq. (21) as

$$\langle X \rangle_{\rm ss} = \langle X(0) \rangle_{\beta} + \int_0^\infty ds \langle X(s) \Omega(0) \rangle_{\beta}.$$
 (23)

Second, since

$$\frac{\partial}{\partial\beta} \left\{ \frac{e^{-\beta H_0(-t)}}{\mathcal{Z}(\beta)} \right\} = \left[\langle H_0 \rangle_\beta - H_0(-t) \right] \frac{e^{-\beta H_0(-t)}}{\mathcal{Z}(\beta)}, \qquad (24)$$

one obtains from Eqs. (16) and (19) for $t \rightarrow \infty$

$$\frac{\partial}{\partial\beta} \langle X(t) \rangle_{\beta} = \int d\Gamma X(0) [\langle H_0 \rangle_{\beta} - H_0(-t)] f(\Gamma, t)$$
$$= \langle X(t) \rangle_{\beta} \langle H_0 \rangle_{\beta} - \langle X(t) H_0 \rangle_{\beta} \to 0, \qquad (25)$$

i.e., $\langle X \rangle_{ss} = \lim_{t \to \infty} \langle X(t) \rangle_{\beta}$ is in fact independent of the inverse temperature β of the initial equilibrium state. Actually, we can prove a stronger statement on the insensitivity of the choice of the initial condition [20]. For the system A, $\langle X \rangle_{ss}$ is thus uniquely specified by the "thermodynamic" parameters $(N, V, \dot{\gamma})$ characterizing the nonequilibrium steady state.

Equation (23) is the generalized Green-Kubo formula relating the steady-state average to the time-correlation function describing transient dynamics from an initial equilibrium toward a final steady state. It is a natural extension of the one derived in [3] which now takes into account effects from inelastic collisions. One can easily show that Eq. (23) reduces to the conventional Green-Kubo formula if the external force is weak and the dissipative force is neglected, i.e., for small $\dot{\gamma}$ and $\zeta_A = 0$ in the case of the system A. For example, by setting $X = \sigma_{xy}$ and $\Omega = \Omega_A$ in Eq. (23), one obtains for the steady-state shear stress defined via $\sigma_{ss} \equiv -\langle \sigma_{xy} \rangle_{ss}/V$

$$\sigma_{\rm ss} = -\frac{\langle \sigma_{xy}(0) \rangle_{\beta}}{V} - \frac{1}{V} \int_0^\infty ds \langle \sigma_{xy}(s) \Omega_{\rm A}(0) \rangle_{\beta}.$$
 (26)

When $\zeta_A=0$, there hold $\langle \sigma_{xy}(0) \rangle_{\beta}=0$ and $\Omega_A=-\beta \dot{\gamma} \sigma_{xy}$ [see Eq. (18)], and Eq. (26) reduces to

$$\sigma_{\rm ss} = \frac{\beta \dot{\gamma}}{V} \int_0^\infty ds \langle \sigma_{xy}(s) \sigma_{xy}(0) \rangle_\beta.$$
(27)

For small $\dot{\gamma}$, one can replace the Liouvillean governing the dynamics of $\sigma_{xy}(s)$ in the integrand with that for a quiescent equilibrium state, and hence, Eq. (27) is the conventional Green-Kubo formula for the viscosity η defined via $\eta \equiv \sigma_{ss}/\dot{\gamma}$. Notice the quite different physics exhibited by Eqs. (26) and (27). Equation (27) applies only to the linear-response regime of nondissipative systems for which equilibrium state is available, and η therefrom depends on (N, V, β) characterizing that equilibrium state. On the other hand, Eq.

(26) holds for sheared dissipative systems arbitrarily far from equilibrium, and the resulting viscosity depends on $(N, V, \dot{\gamma})$ as stated above.

We next derive a generalized Jarzynski-type equality

$$\left\langle e^{\alpha \int_{0}^{t} ds \Omega(-s)} \right\rangle_{\beta} = \left\langle e^{(\alpha-1) \int_{0}^{t} ds \Omega(s)} \right\rangle_{\beta}.$$
 (28)

Since $\int_0^t ds \Omega(-s) = \int_{-t}^0 ds \Omega(s)$, the left-hand side can be expressed as $\int d\tilde{\Gamma} f_c(\tilde{\Gamma}; \beta) e^{\alpha \int_{-t}^0 ds \Omega(\tilde{\Gamma}(s))}$. By setting $\tilde{\Gamma} = \Gamma(t)$, there holds, since $\tilde{\Gamma}(s) = \Gamma(t+s)$,

$$\left\langle e^{\alpha f_0' ds \Omega(-s)} \right\rangle_{\beta} = \int d\Gamma(t) f_{\rm c}(\Gamma(t);\beta) e^{\alpha f_0' ds \Omega(\Gamma(s))}.$$
 (29)

Using $H_0(\Gamma(t)) = H_0(\Gamma) + \int_0^t ds \dot{H}_0(\Gamma(s))$ and $d\Gamma(t) = e^{\int_0^t ds \Lambda(\Gamma(s))} d\Gamma$ [6] which follows from the conservation of the number of ensemble members within a co-moving phase volume, one derives similarly to Eq. (16)

$$d\Gamma(t)f_{\rm c}(\Gamma(t);\beta) = d\Gamma f_{\rm c}(\Gamma;\beta)e^{-\int_0^t ds\Omega(\Gamma(s))}.$$
 (30)

Substituting this into Eq. (29) yields the equality Eq. (28).

For $\alpha = 1$, the equality Eq. (28) reduces to the one noted below Eq. (18). By setting $\alpha = 0$ in Eq. (28), one obtains

$$\left\langle e^{-\int_0^t ds\Omega(s)} \right\rangle_{\beta} = 1.$$
 (31)

This equality is called the integral fluctuation theorem [7] or the nonequilibrium partition identity [18], originally derived as a corollary of the transient fluctuation theorem that rests on microscopic time reversibility. Thus, the integral form of the fluctuation theorem holds also in the absence of such a symmetry. Applying the Jensen inequality to Eq. (31), one obtains $\int_0^t ds \langle \Omega(s) \rangle_{\beta} \ge 0$, which is referred to as the secondlaw inequality [18].

In this paper, we derived the generalized Green-Kubo relation and the integral fluctuation theorem that apply to driven dissipative systems lacking microscopic time reversibility. Our formulation for granular systems, when combined with liquid-state theories as done in [21], will also be useful in studies of jammed glassy materials.

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