

Galilean invariance for stochastic diffusive dynamics

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Outline

- 1 Galilean invariance in classical mechanics: brief review
- 2 Galilean invariance for stochastic systems: deriving Langevin dynamics
- 3 (weak) Galilean invariance for anomalous stochastic processes: CTRW and beyond

Galilei's classical principle of relativity

G. Galilei (1632): (thought) experiment of dropping a cannonball from the mast of a ship travelling at constant velocity



cannonball falls directly to the foot, because **an internal observer on the ship does not notice the ship's movement**
motivated by Aristotelian argument against the rotation of the earth (cannonball moves straight to the centre of the earth)

Galilean invariance and inertial frames

Galilean invariance (GI) means **the laws of motion are the same in all inertial frames** (IFs).

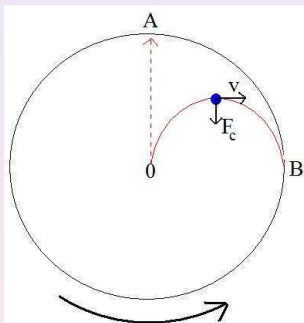
An inertial frame is a reference frame in which the **frame-internal physics is not affected by frame-external forces**, i.e. it requires a **closed system** .

Meaning as there is no external net force, particles remain at rest or move at constant velocity: **Newton's 1st Law**.

Newton's Laws are valid in all inertial frames (in the classical limit).

Example of a non-inertial frame

Coriolis force:



Non-inertial frames should be avoided, if possible, as the laws of physics are 'not simple' in them (Einstein, 1905). Otherwise you need to identify the resulting **fictitious forces**.

Galilean transformation

convert measurements in two IFs into each other by a **Galilean transformation**:

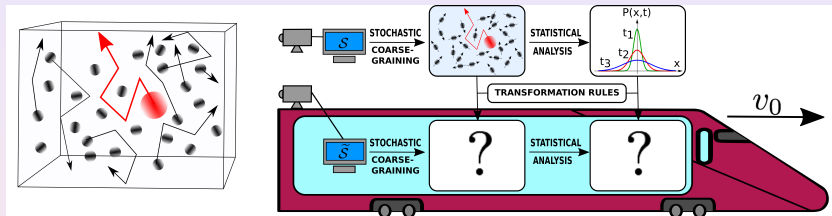
- Let \mathcal{S} and $\tilde{\mathcal{S}}$ be two different IFs. Denote by (x, v, t) and $(\tilde{x}, \tilde{v}, \tilde{t})$ their coordinates for position, velocity and time, respectively, in 1d.
- $\tilde{\mathcal{S}}$ is moving with uniform velocity v_0 with respect to \mathcal{S} and coincides with \mathcal{S} at $t = 0$. Clocks are synchronized, $\tilde{t} = t$.
- **Galilean transformation**:

$$\tilde{x} = x - v_0 t \quad , \quad \tilde{v} = v - v_0$$

If GI holds, Newton's equations of motion $F = m \ddot{x}$ (his Second Law) remain the same under a GT.

Galilean invariance for stochastic diffusive dynamics?

How does GI carry over when deriving stochastic equations via coarse graining from classical mechanical equations of motion?



not too much literature on this:

- GI for Navier-Stokes (Forster et al., 1977; Berera et al., 2007)
- KPZ equation (Wio et al., 2010)
- molecular dynamics simulations via Langevin equations (Dünweg, 1993)

Galilean transformation for Hamilton's equations

Hamiltonian for a classical system of N interacting particles:

$$H(x_1, v_1; \dots; x_N, v_N) = \sum_{i=1}^N \frac{m_i}{2} v_i^2(t) + \sum_{i < j} U(x_i(t), x_j(t))$$

with position-velocity coordinates (x_i, v_i) of the i -th particle and interaction potential U ; Hamilton's equations:

$$\dot{x}_i(t) = v_i(t), \quad m_i \dot{v}_i(t) = -\frac{\partial}{\partial x_i} \sum_{i < j} U(x_i(t), x_j(t))$$

GT into \tilde{S} :

$$\dot{\tilde{x}}_i(t) = \tilde{v}_i(t) \quad \text{and} \quad m_i \dot{\tilde{v}}_i(t) = -\frac{\partial}{\partial \tilde{x}_i} \sum_{i < j} U(\tilde{x}_i(t), \tilde{x}_j(t))$$

GI if U depends only on the relative difference between the particles' positions, $\tilde{x}_i(t) - \tilde{x}_j(t) = x_i(t) - x_j(t)$, cf. Newton's Third Law.

The Kac-Zwanzig model for a tracer in a heat bath

tracer particle of mass M at $(X(t), V(t))$ interacts with a heat bath of $j=1, \dots, N$ harmonic oscillators of masses m_j at $(x_j(t), v_j(t))$ with angular frequencies ω_j and coupling strengths γ_j :

$$M\ddot{X}(t) = \sum_{j=1}^N \gamma_j \left[x_j(t) - \frac{\gamma_j}{m_j \omega_j^2} X(t) \right],$$

$$m_j \ddot{x}_j(t) = -m_j \omega_j^2 \left[x_j(t) - \frac{\gamma_j}{m_j \omega_j^2} X(t) \right].$$

with $(X(0), V(0)) = (0, 0)$ and $(x_j(0), v_j(0)) = (x_{j0}, v_{j0})$.

note: GI only if $\gamma_j = m_j \omega_j^2$, as discussed before

Eliminating the bath variables

solving for x_j and plugging into the equation for X yields

$$M\ddot{X}(t) = - \int_0^t \Omega(t-t')\dot{X}(t') dt' + \xi(t)$$

with memory kernel

$$\Omega(t) = \sum_{j=1}^N \omega_j \cos(\omega_j t)$$

and

$$\xi(t) = \sum_{j=1}^N \omega_j v_{j0} \sin(\omega_j t) + \sum_{j=1}^N \omega_j^2 x_{j0} \cos(\omega_j t) .$$

Zwanzig (1973)

GI of the deterministic KZ model

Under GT we have

$$\int_0^t \Omega(t-t') \dot{X}(t') dt' = \int_0^t \Omega(t-t') \tilde{\dot{X}}(t') dt' + v_0 \int_0^t \Omega(t') dt'$$

and

$$\xi(t) = \tilde{\xi}(t) + v_0 \sum_{j=1}^N \omega_j \sin(\omega_j t)$$

yielding

$$M\ddot{X}(t) = - \int_0^t \Omega(t-t') \tilde{\dot{X}}(t') dt' + \tilde{\xi}(t)$$

GI persists after eliminating the bath degrees of freedom.

Deriving the stochastic Langevin equation

We had the fully deterministic tracer dynamics

$$M\ddot{X}(t) = - \int_0^t \Omega(t-t')\dot{X}(t') dt' + \xi(t)$$

first term yields **friction**, second term **collisions with bath particles** depending on initial conditions (x_{j0}, v_{j0})

now specify $\xi(t)$ as a **random force** by choosing a suitable initial distribution of the bath particles

assume the **heat bath is at equilibrium** in \mathcal{S} : velocity distribution is Maxwellian at bath temperature T implying $\langle \xi(t) \rangle = 0$ and fluctuation-dissipation relation $\langle \xi(t_1)\xi(t_2) \rangle = k_B T \Omega(|t_1 - t_2|)$

⇒ **generalized Langevin equation**

Breaking of GI in stochastic Langevin dynamics

note: Thermal equilibrium in \mathcal{S} is not frame invariant! A proper heat bath must be infinite violating the closedness of IFs.

⇒ the stationary reference frame \mathcal{S} is singled out for calibrating the noise ξ

under GT the noise was

$$\tilde{\xi}(t) = \xi(t) - v_0 \sum_{j=1}^N \omega_j \sin(\omega_j t)$$

acquiring a different statistics than $\xi(t)$

The noise $\tilde{\xi}(t)$ cannot be defined independently, thus inevitably GI is broken.

Deriving GT rules for stochastic dynamics

solve the Langevin equation both in \mathcal{S} and $\tilde{\mathcal{S}}$: (X, V) and (\tilde{X}, \tilde{V})
 are still related via the ordinary GT

this implies for the **probability distribution functions** (PDFs)

$$\begin{aligned} P(x, v, t) &= \langle \delta(x - X(t)) \delta(v - V(t)) \rangle \\ &= \left\langle \delta(x - \tilde{X}(t) - v_0 t) \delta(v - \tilde{V}(t) - v_0) \right\rangle \\ &= \tilde{P}(x - v_0 t, v - v_0, t) \end{aligned}$$

PDFs in \mathcal{S} and $\tilde{\mathcal{S}}$ are related by a **shift** and are *not* invariant

note: in both IFs $\langle \dots \rangle$ is with respect to the same heat bath defined in \mathcal{S}

Summary

We define **weak Galilean invariance** (WGI) for stochastic coarse-grained diffusive dynamics as:

- 1 **stochastic equations of motion** transform via a GT on their position and velocity processes only
- 2 **Fokker-Planck and Klein-Kramers equations** also transform via a GT on their independent variables
- 3 **PDFs** transform as $P(x, v, t) = \tilde{P}(x - v_0 t, v - v_0, t)$
(cf. also **Meztler et al., 1998, 2000**)

Weak GI for anomalous processes

Stochastic model	Fokker-Planck/Klein-Kramers equation in \mathcal{S}	Fokker-Planck/Klein-Kramers equation in $\tilde{\mathcal{S}}$
Normal diffusion (overdamped)	$\left[\frac{\partial}{\partial t} - \mathcal{L}\right] P = 0$	$\left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} - \mathcal{L}\right] \tilde{P} = 0$
Normal diffusion (underdamped)	$\left[\frac{\partial}{\partial t} + \frac{\partial}{\partial x} v - \frac{\partial}{\partial v} \gamma v - \gamma \frac{\partial^2}{\partial v^2}\right] P = 0$	$\left[\frac{\partial}{\partial t} + \frac{\partial}{\partial x} v - \frac{\partial}{\partial v} \gamma(v + v_0) - \gamma \frac{\partial^2}{\partial v^2}\right] \tilde{P} = 0$
Fractional/Scaled Brownian motion	$\left[\frac{\partial}{\partial t} - \beta t^{\beta-1} \mathcal{L}\right] P = 0$	$\left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} - \beta t^{\beta-1} \mathcal{L}\right] \tilde{P} = 0$
Generalized Langevin equation	$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{\partial}{\partial x} v - \frac{\partial}{\partial v} \Gamma(t)v\right] P \\ = \left[\frac{\partial^2}{\partial v^2} \Gamma(t) + \frac{\partial^2}{\partial x \partial v} D_{xv}(t)\right] P \end{aligned}$	$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{\partial}{\partial x} v - \frac{\partial}{\partial v} \Gamma(t)(v + v_0)\right] \tilde{P} \\ = \left[\frac{\partial^2}{\partial v^2} \Gamma(t) + \frac{\partial^2}{\partial x \partial v} D_{xv}(t)\right] \tilde{P} \end{aligned}$
Lévy flight	$\left[\frac{\partial}{\partial t} - \nabla^\beta\right] P = 0$	$\left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} - \nabla^\beta\right] \tilde{P} = 0$
Lévy walk	$\begin{aligned} \left[\left(\frac{\partial}{\partial t} + u \frac{\partial}{\partial x}\right) \left(\frac{\partial}{\partial t} - u \frac{\partial}{\partial x}\right)\right] P_u \\ = - \left[\frac{1}{2} \mathcal{D}_t^{(-u, u)} + \frac{1}{2} \mathcal{D}_t^{(u, -u)}\right] P_u \end{aligned}$	$\begin{aligned} \left[\left(\frac{\partial}{\partial t} + u_+ \frac{\partial}{\partial x}\right) \left(\frac{\partial}{\partial t} + u_- \frac{\partial}{\partial x}\right)\right] \tilde{P}_u \\ = - \left[\frac{1}{2} \mathcal{D}_t^{(u_-, u_+)} + \frac{1}{2} \mathcal{D}_t^{(u_+, u_-)}\right] \tilde{P}_u \end{aligned}$
Continuous time random walk	$\left[\frac{\partial}{\partial t} - \mathcal{L} \mathcal{D}_t\right] P = 0$	$?$

GT for Continuous Time Random Walk

In the simplest case a (subdiffusive) CTRW in 1d is governed by a waiting time and a jump length distribution leading to the **generalized diffusion equation**

$$\frac{\partial}{\partial t} P(x, t) = \mathcal{L} \mathbb{D}_t P(x, t), \quad \mathcal{L} = \sigma \frac{\partial^2}{\partial x^2}$$

with $\mathbb{D}_t P(x, t) = \frac{\partial}{\partial t} \int_0^t dt' K(t-t') P(x, t')$; for power law memory kernel we recover the Riemann-Liouville fractional derivative

How to incorporate a constant drift here 'mimicking' GT?
two attempts:

$$1. \quad \frac{\partial}{\partial t} \tilde{P} = \left[v_0 \frac{\partial}{\partial x} + \mathcal{L} \right] \mathbb{D}_t \tilde{P}$$

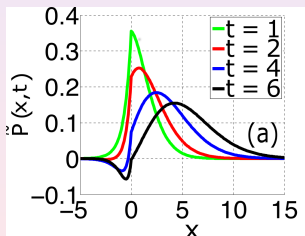
$$2. \quad \frac{\partial}{\partial t} \tilde{P} = v_0 \frac{\partial}{\partial x} \tilde{P} + \mathcal{L} \mathbb{D}_t \tilde{P} \quad \text{Metzler et al. (1998, 2000)}$$

No WGI for CTRW

both versions violate WGI:

solve 1. in Fourier-Laplace space: violates rule 3 of WGI, which reads $P(k, \lambda) = \tilde{P}(k, \lambda - iv_0k)$

similarly 2. violates rule 3 and, even worse, violates positivity of the PDFs; analytical results for power law memory kernel:



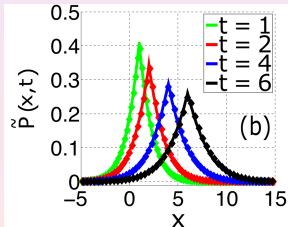
⇒ generally, do NOT try to implement GT by arbitrarily adding a drift term

A WGI CTRW

correct WGI eq. by implementing rule 3 in (solution of) diffusion equation in frame S : $\frac{\partial}{\partial t} \tilde{P}(x, t) = v_0 \frac{\partial}{\partial x} \tilde{P}(x, t) + \mathcal{L} \mathcal{D}_t^{(v_0)} \tilde{P}(x, t)$ with **fractional substantial derivative**

$$\mathcal{D}_t^{(v_0)} \tilde{P}(x, t) = \left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} \right] \int_0^t dt' K(t-t') \tilde{P}(x + v_0(t-t'), t')$$

modeling a retardation effect (Sokolov, Metzler, 2003; Friedrich et al., 2006)



note: a corresponding **WGI Langevin equation** can be derived by using the ‘ $\bar{\xi}$ -process’ (Cairolì, Baule, 2015)

Summary

- detailed analysis of the Kac-Zwanzig model shows **where and how GI is broken** for deriving the stochastic Langevin equation
- but **GI survives in the form of three selection rules**, which we called **weak Galilean invariance**
- weak GI particularly tricky for **spatio-temporally correlated (anomalous) stochastic processes**

A.Cairolì, R.K., A.Baule, *Weak Galilean invariance as a selection principle for stochastic coarse-grained diffusive models*, PNAS **115**, 5714 (2018)