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

Galilean invariance

G.Galilei (1632): ship travelling at constant velocity on a smooth sea; any observer doing experiments below the deck would not be able to tell whether the ship was moving or stationary.

C.Huygens ($\simeq$1650): derivation of laws for elastic collisions

Inertial frames

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

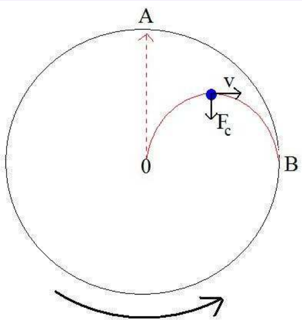
An inertial frame is a reference frame describing a **closed system** where the frame-internal physics is not affected by frame-external forces.

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

Newton's Laws are valid in all inertial frames.

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:

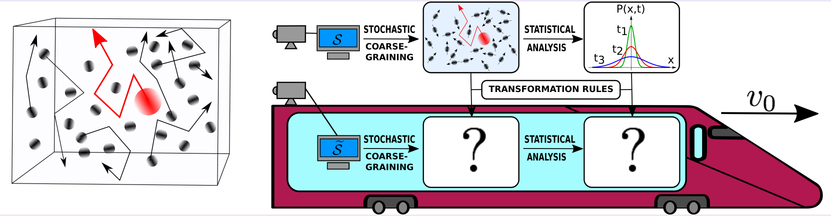
- Let $\mathcal{S}$ and $\widetilde{\mathcal{S}}$ be two different IFs. Denote by (x, v, t) and $(\widetilde{x}, \widetilde{v}, \widetilde{t}\,)$ their coordinates for position, velocity and time, respectively, in 1d.
- $\widetilde{\mathcal{S}}$ is moving with uniform velocity v_0 with respect to $\mathcal{S}$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

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

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:

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

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

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

GT into $\widetilde{\mathcal{S}}$:

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

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 $(X(t), V(t))$ interacting with a heat bath consisting of $(x_j(t), v_j(t))$, $j=1,...,N$ harmonic oscillators at angular frequency ω_j and coupling strength γ_j:

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

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

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

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

Eliminating the bath variables

solving for x_j and plugging into the equation for X yields

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

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

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

and

$$\xi(t) = \widetilde{\xi}(t) + v_0 \sum_{j=1}^{N} \frac{\gamma_j}{m\omega_j} \sin(\omega_j t)$$

yielding

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

GI persists after eliminating the bath degrees of freedom.

Deriving the stochastic Langevin equation

We had the fully deterministic tracer dynamics

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

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 $\langle \xi(t_1)\xi(t_2) \rangle = k_B T \Omega(|t_1 - t_2|)$

$\Rightarrow$ **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

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

under GT the noise was

$$\widetilde{\xi}(t) = \xi(t) - v_0 \sum_{j=1}^{N} \frac{\gamma_j}{m\omega_j} \sin(\omega_j t)$$

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

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

Deriving GT rules for stochastic dynamics

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

this implies for the probability distribution functions (PDFs)

$$P(x, v, t) = \langle \delta(x - X(t))\delta(v - V(t)) \rangle$$

$$= \left\langle \delta(x - \widetilde{X}(t) - v_0 t)\delta(v - \widetilde{V}(t) - v_0) \right\rangle$$

$$= \widetilde{P}(x - v_0 t, v - v_0, t)$$

note: in both IFs $\langle \ldots \rangle$ 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 $P(x, v, t) = \widetilde{P}(x - v_0 t, v - v_0, t)$ (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	$\left[\frac{\partial}{\partial t}+\frac{\partial}{\partial x}v-\frac{\partial}{\partial v}\Gamma(t)v\right]P$ $=\left[\frac{\partial^2}{\partial v^2}\Gamma(t)+\frac{\partial^2}{\partial x\partial v}D_{xv}(t)\right]P$	$\left[\frac{\partial}{\partial t}+\frac{\partial}{\partial x}v-\frac{\partial}{\partial v}\Gamma(t)(v+v_0)\right]\tilde{P}$ $=\left[\frac{\partial^2}{\partial v^2}\Gamma(t)+\frac{\partial^2}{\partial x\partial v}D_{xv}(t)\right]\tilde{P}$
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	$\left[\left(\frac{\partial}{\partial t}+u\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t}-u\frac{\partial}{\partial x}\right)\right]P_u$ $=-\left[\frac{1}{2}\mathcal{D}_t^{(-u,u)}+\frac{1}{2}\mathcal{D}_t^{(u,-u)}\right]P_u$	$\left[\left(\frac{\partial}{\partial t}+u_+\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t}+u_-\frac{\partial}{\partial x}\right)\right]\tilde{P}_u$ $=-\left[\frac{1}{2}\mathcal{D}_t^{(u_-,u_+)}+\frac{1}{2}\mathcal{D}_t^{(u_+,u_-)}\right]\tilde{P}_u$
Continuous time random walk	$\left[\frac{\partial}{\partial t}-\mathcal{L}\mathbb{D}_t\right]P=0$	?

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

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

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

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

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

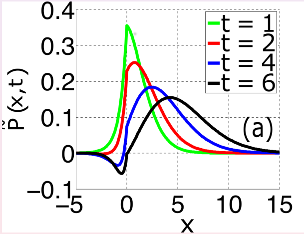
2. $$\frac{\partial}{\partial t}\widetilde{P} = v_0\frac{\partial}{\partial x}\widetilde{P} + \mathcal{L}\mathbb{D}_t\widetilde{P}$$ Metzler et al. (1998, 2000)

No WGI for CTRW

both versions violate WGI:

solve 1. in Fourier-Laplace space: violates rule 3 of WGI, which reads $P(k,\lambda) = \widetilde{P}(k, \lambda - iv_0 k)$

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

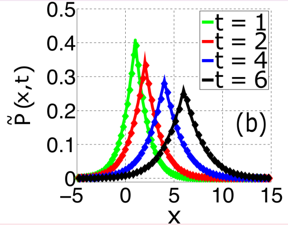
A WGI CTRW

correct WGI eq. by implemeting rule 3 in (solution of) diffusion equation in frame S: $\frac{\partial}{\partial t}\widetilde{P}(x,t) = v_0 \frac{\partial}{\partial x}\widetilde{P}(x,t) + \mathcal{L}\mathcal{D}_t^{(v_0)}\widetilde{P}(x,t)$

with fractional substantial derivative

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

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



note: a corresponding WGI Langevin equation can be derived by using the '$\overline{\xi}$-process' (Cairoli, 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.Cairoli, RK, A.Baule, *Weak Galilean invariance as a selection principle for stochastic coarse-grained diffusive models*, under review for PNAS