



Weak Galilean invariance as a selection principle for coarse-grained diffusive models

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How does the mathematical description of a system change in different reference frames? Galilei first addressed this fundamental question by formulating the famous principle of Galilean invariance. It prescribes that the equations of motion of closed systems remain the same in different inertial frames related by Galilean transformations, thus imposing strong constraints on the dynamical rules. However, real world systems are often described by coarse-grained models integrating complex internal and external interactions indistinguishably as friction and stochastic forces. Since Galilean invariance is then violated, there is seemingly no alternative principle to assess a priori the physical consistency of a given stochastic model in different inertial frames. Here, starting from the Kac–Zwanzig Hamiltonian model generating Brownian motion, we show how Galilean invariance is broken during the coarse-graining procedure when deriving stochastic equations. Our analysis leads to a set of rules characterizing systems in different inertial frames that have to be satisfied by general stochastic models, which we call “weak Galilean invariance.” Several well-known stochastic processes are invariant in these terms, except the continuous-time random walk for which we derive the correct invariant description. Our results are particularly relevant for the modeling of biological systems, as they provide a theoretical principle to select physically consistent stochastic models before a validation against experimental data.

stochastic processes | Galilean invariance | anomalous transport | coarse-graining | fractional calculus

Classical mechanics is built upon the two intimately related concepts of inertial reference frames and Galilean invariance (GI) (1). The former are coordinate systems where a freely moving particle (i.e., in the absence of external forces) either is at rest or exhibits uniform rectilinear motion. The latter principle states that in different inertial frames the equations of motion of closed systems, i.e., including all their interacting constituents, are invariant with respect to Galilean transformations (GTs). These are in general affine transformations that preserve both time intervals and distances between simultaneous events (1). For systems whose dynamical evolution can be fully characterized by microscopic deterministic models, GI plays a fundamental constitutive role, manifest in the constraints that it naturally imposes on the functional form of Newton’s equation. However, a large variety of complex systems in science and nature are not modeled on a microscopic level with Newtonian equations of motion, but rather on a mesoscopic level using, e.g., stochastic Langevin equations or Fokker–Planck diffusion equations to capture the coarse-grained effects of microscopic interactions as friction and noise on the relevant degrees of freedom. The applications of such equations and their variants are vast throughout the sciences (2–4).

Coarse-grained diffusive models are particularly relevant to describe anomalous transport phenomena, where stochasticity arises due to complex multiparticle interactions, whose precise form is usually unknown. While for normal diffusion due to Brownian motion the mean-square displacement (MSD) of an ensemble of particles with positions $X(t)$ at time t grows linearly

in the long-time limit, $\langle X^2 \rangle \sim t^\beta$ with $\beta = 1$, for anomalous diffusion it scales nonlinearly with $\beta \neq 1$. Anomalous dynamics has been observed experimentally for a wide range of physical processes like particle transport in plasmas, molecular diffusion in nanopores, and charge transport in amorphous semiconductors (5–7) that was first theoretically described in refs. 8 and 9 based on the continuous-time random walk (CTRW) (10). Likewise, anomalous diffusion was later found for biological motion (11–13) and even human movement (14). Recently, it was established as a ubiquitous characteristic of cellular processes on a molecular level (15). Here, anomalous diffusion is observed, e.g., in neuronal messenger ribonucleoprotein transport (16); in protein structural fluctuations (17); and in the intracellular transport of *Saccharomyces cerevisiae* mitochondria (18), chromosomal loci of *Escherichia coli* cells (19, 20), engulfed microspheres (21), and lipid and insulin granules (22, 23). However, because of the intrinsic difficulties in assessing the details of the microscopic interactions in experiments, theoretical models for such anomalous processes cannot be typically derived from first principles and are usually formulated on mostly phenomenological grounds. In fact, a wealth of diffusive models has been suggested in the literature, which rely on spatiotemporal memory effects and non-Gaussian power-law statistics of various observables (5, 7, 24, 25). Unfortunately so far there is no fundamental rule available that could be used to verify the physical consistency of such stochastic models a priori. To distinguish between different models it remains only the comparison with experimental data that is often imprecise due to limited sample sizes.

Significance

Galilean invariance is a cornerstone of classical mechanics. It states that for closed systems the equations of motion of the microscopic degrees of freedom do not change under Galilean transformations to different inertial frames. However, the description of real world systems usually requires coarse-grained models integrating complex microscopic interactions indistinguishably as friction and stochastic forces, which intrinsically violate Galilean invariance. By studying the coarse-graining procedure in different frames, we show that alternative rules—denoted as “weak Galilean invariance”—need to be satisfied by these stochastic models. Our results highlight that diffusive models in general cannot be chosen arbitrarily based on the agreement with data alone but have to satisfy weak Galilean invariance for physical consistency.

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Here, we show that GI can provide precisely such a constitutive principle. Even though the fundamental role of GI seemingly breaks down for stochastic diffusive models due to the presence of friction (26), they are nevertheless constrained by a weak form of GI to be physically consistent in different inertial frames. The weak GI rules derived below thus represent a general selection principle for stochastic coarse-grained models. Previously, the consequences of GI in the context of statistical mechanics were first explored for fluid dynamics, where it establishes specific relations between critical exponents of the characteristic parameters entering the derivation of the Navier–Stokes equation (27) [although this result has been challenged (28)]. The problem carries over to the famous Kardar-Parisi-Zhang equation (29) whose GI is equally debated (30). Whether or not these statistical equations feature GI has important practical implications for the modeling of, e.g., fluid flows (28) and nonlinear biological growth (31). Specifically, in molecular dynamics simulations of fluids using stochastic Langevin thermostats it was found that Langevin dynamics break GI by violating global momentum conservation, which makes it unsuitable to simulate hydrodynamic phenomena (32). Curing this deficiency led to novel GI algorithms, most notably dissipative particle dynamics, now widely used to simulate soft matter systems and simple liquids (33–35).

The basic setup of our problem is represented in Fig. 1: Here S and \tilde{S} are two inertial reference frames, where S is the laboratory frame at rest while \tilde{S} is moving with uniform velocity v_0 with respect to S . The GTs connecting the coordinates in the two frames are given by

$$\tilde{x} = x - v_0 t, \quad \tilde{v} = v - v_0, \quad [1]$$

where, for simplicity, we focus on the one-dimensional case. Eq. 1 is the phase space version of the classical GTs assuming an absolute time (1). A classical system of $N + 1$ interacting particles is described by the Hamiltonian function

$$H(x_1, v_1; \dots; x_{N+1}, v_{N+1}) = \sum_i \frac{m_i}{2} v_i^2(t) + \sum_{i < j} U(x_i(t), x_j(t)), \quad [2]$$

where x_i, v_i are the position-velocity coordinates of the i th particle in the reference frame S and U is the interaction potential satisfying some mild regularity conditions. Its dynamics is specified by Hamilton's equations

$$\dot{x}_i(t) = v_i(t), \quad m_i \dot{v}_i(t) = -\frac{\partial}{\partial x_i} \sum_{i < j} U(x_i(t), x_j(t)). \quad [3]$$

Transforming the coordinates to the reference frame \tilde{S} via Eq. 1, we see that $\dot{\tilde{x}}_i(t) = \tilde{v}_i(t)$ and $m_i \dot{\tilde{v}}_i(t) = -\frac{\partial}{\partial \tilde{x}_i} \sum_{i < j} U(\tilde{x}_i(t), \tilde{x}_j(t))$ if U depends only on the relative difference between the particles' positions, i.e., $U(x_i(t), x_j(t)) = U(x_i(t) - x_j(t))$, because in this case $\tilde{x}_i(t) - \tilde{x}_j(t) = x_i(t) - x_j(t)$. We thus recover Newton's equations of motion satisfying his third law, which are identical in both reference frames; i.e., they satisfy GI. Our goal is now to derive coarse-grained dynamics from systems described by Eq. 3, where some of the microscopic degrees of freedom have been eliminated, and to characterize their statistics on such a mesoscopic level in both frames S, \tilde{S} (Fig. 1).

The transition from Eq. 3 to an effective description in the form of a stochastic diffusion equation can be made quantitatively precise for the specific scenario where one of the particles, for simplicity let it be the $(N + 1)$ th, is a tagged (tracer) particle of mass $m_{N+1} = M$ that interacts with the remaining particles of equal mass $m_j = m$ via a harmonic potential of coupling strength $m\omega_j^2$, thus defining the environment as a heat bath; i.e., $U(X, x_j) = \sum_{j=1}^N m\omega_j^2 [X(t) - x_j(t)]^2 / 2$. Conversely, interactions between different bath particles are switched off. This is a Galilean invariant version of the classical Kac–Zwanzig model (36), whose relevance has been recently addressed (37). Denoting by $(X(t), V(t))$ and $(x_j(t), v_j(t))$, $j = 1, \dots, N$ the position and velocity variables of the tracer and heat bath particles, respectively, in the frame S , their Hamilton's equations become $M \ddot{X}(t) = \sum_{j=1}^N m\omega_j^2 [x_j(t) - X(t)]$ and $m \ddot{x}_j(t) = -m\omega_j^2 [x_j(t) - X(t)]$. These equations specify the time evolution of all $N + 1$ particles of the system (arrows in the box in Fig. 1A) in S once the initial conditions are prescribed, which we take as $(X(0), V(0)) = (0, 0)$ and $(x_j(0), v_j(0)) = (x_{j0}, v_{j0})$, without loss of generality. The great advantage of this model is that the effective dynamics for the tracer can be derived by integrating out the bath degrees of freedom. This yields (36)

$$M \ddot{X}(t) = -\int_0^t \Omega(t-t') \dot{X}(t') dt' + \xi(t), \quad [4]$$

where the memory kernel Ω and what later will become the "noise" ξ in Langevin dynamics are exactly (36)

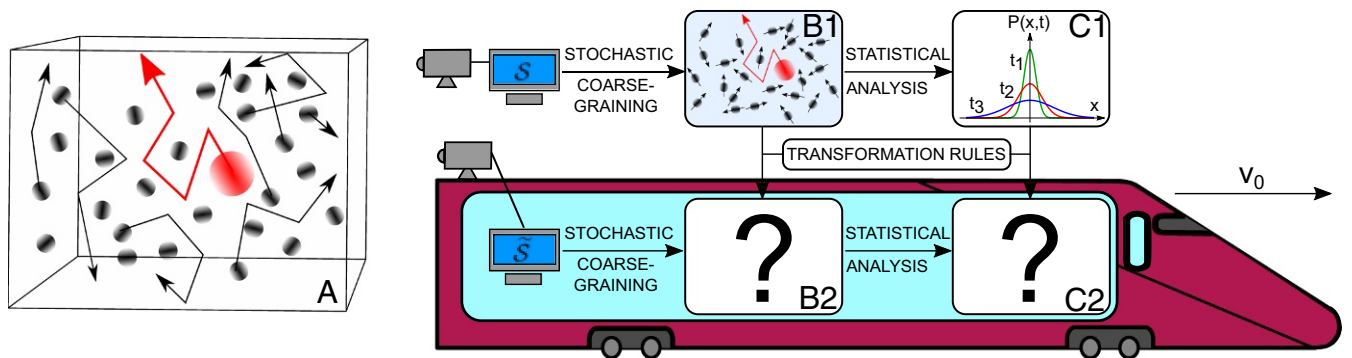


Fig. 1. Pictorial representation of the setup: A system of N heat bath particles (black) and one tracer (red) is observed from two different reference frames S and \tilde{S} . While S is at rest, \tilde{S} is moving with velocity v_0 with respect to S . We consider three different levels of description of the original system: (A) The microscopic system of $N + 1$ particles is described by deterministic equations of motion leading to trajectories fully specified by the initial conditions. (B1) Alternatively, one can provide a stochastic coarse-grained model of the tracer dynamics in terms of effective dissipative friction forces and random collisions with the N bath particles (arrowed spheres), which account for their original microscopic interactions with the probe. (C1) Finally, the system can be studied in terms of its position and velocity statistics, whose distributions are determined by either experimental measurements or a prescribed stochastic model. While the relationship between the dynamical evolutions in S and \tilde{S} for A is specified by Galilean transformations of the position and velocity degrees of freedom, here we derive the corresponding relationships for $B1 \leftrightarrow B2$ and $C1 \leftrightarrow C2$, yielding what we call weak Galilean invariance.

$$\Omega(t) = \sum_{j=1}^N \omega_j^2 \cos(\omega_j t), \quad [5]$$

$$\xi(t) = \sum_{j=1}^N \omega_j v_{j0} \sin(\omega_j t) + \sum_{j=1}^N \omega_j^2 x_{j0} \cos(\omega_j t). \quad [6]$$

As can be seen from Eq. 6, ξ depends explicitly on the initial conditions of the bath particles, which are related to those in $\tilde{\mathcal{S}}$ by $\tilde{x}_{j0} = x_{j0}$, $\tilde{v}_{j0} = v_{j0} - v_0$ and $\tilde{X}(0) = 0$, $\tilde{V}(0) = -v_0$. Since everything is exact, the dynamics in $\tilde{\mathcal{S}}$ follow by applying the GTs of Eq. 1 to Eqs. 4–6. Ω is unchanged under the transformation, but Eq. 6 is changed due to the GTs of the initial velocities of the bath particles. If we call $\tilde{\xi}$ the noise term in the transformed frame, i.e., Eq. 6 in \sim variables, the two noises are related by

$$\xi(t) = \tilde{\xi}(t) + v_0 \sum_{j=1}^N \omega_j \sin(\omega_j t) = \tilde{\xi}(t) + v_0 \int_0^t \Omega(t') dt'. \quad [7]$$

Overall, the deterministic coarse-grained equation of the tracer in $\tilde{\mathcal{S}}$ is then just Eq. 4 in \sim variables

$$M \ddot{\tilde{X}}(t) = - \int_0^t \Omega(t-t') \dot{\tilde{X}}(t') dt' + \tilde{\xi}(t) \quad [8]$$

$$= - \int_0^t \Omega(t-t') (\dot{\tilde{X}}(t') + v_0) dt' + \xi(t), \quad [9]$$

using Eq. 7. The deterministic effective equation of motion for the tracer thus maintains the GI of the original microscopic dynamics even after projecting out the degrees of freedom of the bath particles.

For deriving stochastic Langevin dynamics the next step is to simplify this coarse-grained description by specifying $\xi(t)$ as a random force instead of the deterministic force Eq. 6. On the Langevin level, the dynamics of the tracer then effectively originates from both dissipative friction forces and random collisions with the bath particles, accounting for their original microscopic interactions with the probe. The statistics of $\xi(t)$ are specified by the distribution of x_{j0} , v_{j0} . Assuming that the heat bath is at equilibrium in \mathcal{S} , the velocity distribution is Maxwellian at the temperature of the system T , implying $\langle \xi(t) \rangle = 0$ and $\langle \xi(t_1) \xi(t_2) \rangle = k_B T \Omega(|t_1 - t_2|)$ (36). Consequently, the fluctuation–dissipation relation holds (38). Eq. 4 then defines a generalized Langevin equation (LE) in \mathcal{S} . Crucially, the notion of thermal equilibrium is not frame invariant such that the stochastic coarse graining is not possible directly for Eq. 8. Specifying the properties of the random force that way per se singles out a reference frame and thus inevitably breaks GI, because according to Eq. 7 the noise $\tilde{\xi}$ acquires a different statistic than ξ . However, after having specified ξ via the equilibrium assumption in \mathcal{S} , Eq. 9 is still valid. Eqs. 4 and 9 then both represent the same microscopic dynamics in two different inertial frames. We see that Eq. 9 contains an additional drift term, which could be obtained directly from Eq. 4 by performing a GT on the coordinates of its deterministic part only while leaving the noise term unchanged.

The transformation rules of the stochastic equations of motion imply that the resulting position–velocity processes (X, V) and (\tilde{X}, \tilde{V}) are related via a GT, even in the presence of stochasticity, which can be shown by explicitly solving Eqs. 4 and 9, while correctly accounting for the different initial conditions in the two frames (*SI Appendix, section 1*). Consequently, also the probability density functions (PDFs) for position and velocity in different inertial frames can be related to each other directly. Including

the position coordinates as $\dot{X}(t) = V(t)$ and $\dot{\tilde{X}}(t) = \tilde{V}(t)$ we have for underdamped dynamics the PDF transformation rule

$$\begin{aligned} P(x, v, t) &= \langle \delta(x - X(t)) \delta(v - V(t)) \rangle \\ &= \langle \delta(x - \tilde{X}(t) - v_0 t) \delta(v - \tilde{V}(t) - v_0) \rangle \\ &= \tilde{P}(x - v_0 t, v - v_0, t), \end{aligned} \quad [10]$$

since the expected value in both inertial frames is over the fluctuations of the same heat bath defined in \mathcal{S} . In terms of its Fourier–Laplace transform [from now on denoted by different independent variables according to $(x, v, t) \rightarrow (k, p, \lambda)$] the connection is $P(k, p, \lambda) = e^{-ipv_0} \tilde{P}(k, p, \lambda - ikv_0)$. For overdamped dynamics the respective results are $P(x, t) = \tilde{P}(x - v_0 t, t)$ and in Fourier–Laplace space

$$P(k, \lambda) = \tilde{P}(k, \lambda - iv_0 k). \quad [11]$$

The evolution equations of $P(x, v, t)$ and $\tilde{P}(x, v, t)$ can also be shown to transform via a GT on their independent variables (*SI Appendix, section 2*).

So far we have shown that a stochastic coarse-grained description inherently violates GI. Nevertheless, Eq. 7 characterizes the stochastic dynamics in all different Galilean frames uniquely as follows: (i) Stochastic equations of motion transform via a GT on their position and velocity processes only; consequently, (ii) Fokker–Planck (FP) and Klein–Kramers equations also transform via a GT on their independent variables, and (iii) PDFs transform as in Eqs. 10 and 11. The validity of the properties *i–iii* is nontrivial and needs in principle to be shown for any specific stochastic model at hand following a coarse-graining procedure. These three Galilean transformation rules for coarse-grained stochastic dynamics and their statistical counterparts yield what we call weak GI: Apart from a shift of v_0 or $v_0 t$ for velocity and position variables, respectively, the corresponding PDFs in $\tilde{\mathcal{S}}$ remain unchanged compared with the ones in \mathcal{S} . It is important to distinguish these weak GI rules from conventional microscopic GI. In systems satisfying the latter, the equations of motion are strictly identical in all inertial frames, while their stochastic coarse-grained equivalents are different.

Clearly, all processes described by the generalized LE (Eq. 4) satisfy *i–iii*, which includes normal diffusive processes. In this case the FP equation in $\tilde{\mathcal{S}}$ is the well-known advection–diffusion equation. Eq. 4 also models anomalous diffusion if one uses for Ω a power-law kernel in time (39), which highlights that these properties are preserved in the anomalous regime. However, in modeling anomalous diffusion a large variety of processes are used for which a similarly rigorous coarse-graining procedure is not available (5, 7, 24, 40). While the accurate determination of an underlying anomalous stochastic process ultimately relies on the comparison of statistical quantities beyond the MSD with experimental data (11), we propose that weak GI can serve as an important criterion to assess the physical consistency of stochastic models from a purely theoretical first-principles perspective.

In fact, we verified the validity of our conjecture for several other stochastic models generating both sub- and superdiffusion that are commonly used in the literature, such as fractional and scaled Brownian motion (41–43), the fractional LE (42–44), Lévy flights (45–47), Lévy walks (24, 48–50), and the CTRW (5, 10, 51). An overview is presented in *SI Appendix, Table S1*, where for simplicity we demonstrate only the validity of property *ii* (details of the calculations are discussed in *SI Appendix, section 2*). Remarkably, apart from the CTRW, all representations exhibit weak GI; i.e., applying a GT to the given Langevin or FP description yields solutions in agreement with Eqs. 10 and 11. For fractional Brownian motion, scaled Brownian motion, and

the fractional LE (as a special case of the generalized LE), this result can be proved based on the Gaussian nature of the process. For Lévy flights it is a direct consequence of the Lévy–Khintchine representation of Lévy processes (52). In these examples, the Langevin dynamics can be expressed in terms of an additive noise process and thus the transformation into frame $\tilde{\mathcal{S}}$ by GT is unproblematic, leading to an advective term $v_0 \partial/\partial x$ as for normal diffusion. Even though such a simple structure does not apply to Lévy walks, surprisingly the same consistency is satisfied, as can be checked by imposing a GT onto the respective FP equation (50) and verifying that the solutions in each frame are related by Eq. 11. The FP equation in $\tilde{\mathcal{S}}$ describes a Lévy walk with asymmetric velocity jumps switching between $-v_0 + u$ and $-v_0 - u$, where $\pm u$ is the velocity in \mathcal{S} , which clearly is physically correct.

We now clarify the situation for the CTRW, a model that has huge applications across all branches of the sciences (5–7, 40). In the overdamped regime the PDF P of a CTRW in the frame \mathcal{S} is the solution of the diffusion equation (53, 54)

$$\frac{\partial}{\partial t} P(x, t) = \mathcal{L} \mathbb{D}_t P(x, t), \quad \mathcal{L} = \sigma \frac{\partial^2}{\partial x^2}, \quad [12]$$

where σ is a generalized diffusion constant and \mathbb{D}_t is a nonlocal time operator defined as $\mathbb{D}_t P(x, t) = \frac{\partial}{\partial t} \int_0^t dt' K(t-t') P(x, t')$, which generalizes the Riemann–Liouville fractional differential operator to arbitrary waiting-time distributions. The kernel K is related to the so-called Laplace exponent Φ of the waiting-time distribution by $K(\lambda) = \Phi(\lambda)^{-1}$ (53, 54). Therefore, its Fourier–Laplace representation is $\mathbb{D}_t P(x, t) \rightarrow \lambda P(k, \lambda) / \Phi(\lambda)$. In the CTRW framework a constant drift can be incorporated by complementing the diffusion operator with $v_0 \partial/\partial x$, which would suggest that the FP equation in $\tilde{\mathcal{S}}$ is given by $\frac{\partial}{\partial t} \tilde{P} = [v_0 \frac{\partial}{\partial x} + \mathcal{L}] \mathbb{D}_t \tilde{P}$. Alternatively, another time nonlocal FP equation was previously derived, in particular for $\Phi(\lambda) = \lambda^\alpha$ ($0 < \alpha < 1$) corresponding to Lévy stable distributed waiting times, by using the transformation rule Eq. 11 and performing a Taylor expansion in the Fourier variable up to the lowest approximation order (5, 55, 56). This procedure leads to the equation $\frac{\partial}{\partial t} \tilde{P} = v_0 \frac{\partial}{\partial x} \tilde{P} + \mathcal{L} \mathbb{D}_t \tilde{P}$.

However, both equations are not correct representations of microscopic dynamics in view of the rules *i–iii* yielding weak GI. In fact, the former does not satisfy the general rule Eq. 11 as becomes clear by solving it in Fourier–Laplace space. The same is true for the latter, whose solutions are even unphysical, as they do not satisfy the requirement of positivity of a PDF (Fig. 2A

and *SI Appendix, section 3*). Therefore, a simple transformation of the fractional diffusion equation obtained by arbitrarily adding an advective term $v_0 \partial/\partial x$ as for the Gaussian models and Lévy flights (*SI Appendix, Table S1*) is not correct. Likewise, implementing GTs directly on the Langevin description of CTRWs in terms of subordination (51, 54, 57) is problematic (shown below).

Instead, the correct transformation of Eq. 12 into the frame $\tilde{\mathcal{S}}$ can be derived straightforwardly in Fourier–Laplace space. Without loss of generality, we assume $P(x, 0) = \delta(x)$. Thus, its transform is $\lambda P(k, \lambda) - 1 = -\sigma k^2 [\lambda / \Phi(\lambda)] P(k, \lambda)$. Using property *iii*, the GT is then implemented by the variable transformation $\lambda \rightarrow \lambda + ikv_0$ and the transformation rule Eq. 11 relating P, \tilde{P} . This immediately leads to a FP equation including retardation effects

$$\frac{\partial}{\partial t} \tilde{P}(x, t) = v_0 \frac{\partial}{\partial x} \tilde{P}(x, t) + \mathcal{L} \mathcal{D}_t^{(v_0)} \tilde{P}(x, t), \quad [13]$$

where the operator $\mathcal{D}_t^{(v_0)}$ is the fractional substantial derivative (49, 54, 58)

$$\mathcal{D}_t^{(v_0)} \tilde{P}(x, t) = \left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} \right] \int_0^t dt' K(t-t') \tilde{P}(x + v_0(t-t'), t'), \quad [14]$$

which has Fourier–Laplace representation $\mathcal{D}_t^{(v_0)} \tilde{P}(x, t) \rightarrow (\lambda + iv_0 k) \tilde{P}(k, \lambda) / \Phi(\lambda + iv_0 k)$. Setting $v_0 = 0$ recovers Eq. 12.

To further support our result, we also derive Eq. 13 directly in (x, t) space. This requires a careful analysis due to the nonlocal character of the operator \mathbb{D}_t . On the one hand, the left-hand side (lhs) of Eq. 12 and the time derivative in \mathbb{D}_t transform with the substitution $\partial/\partial t \rightarrow \partial/\partial t - v_0 \partial/\partial x$ (chain rule applied to Eq. 1). On the other hand, recalling the explicit definition of a PDF in terms of probability (denoted as \mathbb{P}) of events (denoted as $\{\cdot\}$), the integrand PDF is defined as $P(x, t') = \mathbb{P}(\{x \leq Y(t') \leq x + dx\})$, where $Y(t)$ denotes the position of the CTRW. According to property *i*, $Y(t')$ becomes $\tilde{Y}(t') + v_0 t'$ in the comoving frame $\tilde{\mathcal{S}}$, while the measured position x transforms at the later time t in agreement with the lhs of Eq. 12; i.e., $x \rightarrow x + v_0 t$. Therefore, $P(x, t') = \mathbb{P}(\{x + v_0(t-t') \leq \tilde{Y}(t') \leq x + v_0(t-t') + dx\}) = \tilde{P}(x + v_0(t-t'), t')$. Note that dx is invariant because the shift cancels out. Combining these arguments yields Eq. 13. The fractional substantial derivative in Eq. 14 highlights the existence of a space–time coupling, which is absent in the frame \mathcal{S} but is naturally required: Let y be the position of the CTRW in \mathcal{S} after its last jump occurred at time

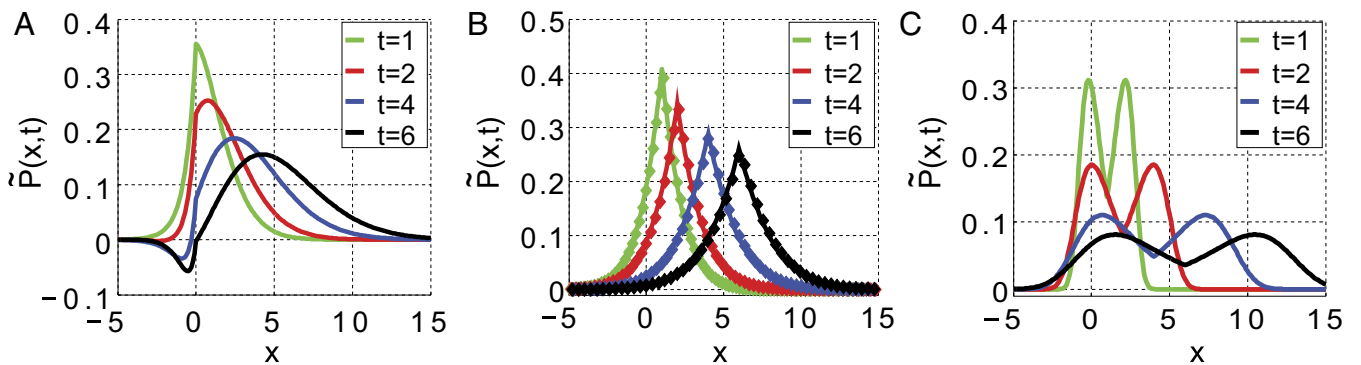


Fig. 2. Position distribution in the comoving frame $\tilde{\mathcal{S}}$. (A) Propagator of the FP equation $\frac{\partial}{\partial t} \tilde{P} = v_0 \frac{\partial}{\partial x} \tilde{P} + \mathcal{L} \mathbb{D}_t \tilde{P}$ suggested in refs. 5, 55, and 56 instead of Eq. 13. The explicit expression for the propagator is given in *SI Appendix, Eq. S47*. This function not only violates weak GI, but also exhibits nonphysical negative values. Here, $\Phi(\lambda) = \lambda^\alpha$ with $\alpha = 0.5$, $v_0 = -1$, $\sigma = 1$, $x_0 = 0$. (B) PDF solution of Eq. 13 (*SI Appendix, Eq. S68*) showing weak GI. Parameters are the same as for A. We find perfect agreement with Monte Carlo simulations of the Langevin equation $\dot{Y}(t) = -v_0 + \xi(t)$ (colored markers). (C) PDF solution of Eq. 13 (*SI Appendix, Eq. S68*) with $K(t) = t^{\alpha-1} / \Gamma(\alpha)$ and α analytically continued to yield superdiffusion at $\alpha = 1.5$. Other parameters are the same as for A. Again, weak GI is observed.

t and τ , Δy respectively be the waiting time to the next jump and its length. In \mathcal{S} its position at time $t + \tau$ is then $y + \Delta y$. In $\tilde{\mathcal{S}}$ this is $y - v_0\tau + \Delta y$ (Eq. 1, lhs). Thus, the final position in $\tilde{\mathcal{S}}$ depends on both the jump amplitude Δy and the waiting time τ . Interestingly, a similar coupling is constitutive of the Lévy walk model (24), which explains why it satisfies weak GI.

What is now the corresponding Langevin dynamics of the anomalous diffusive process described by Eq. 13? The key is to describe the CTRW directly in physical time rather than in the widely used subordination picture (51, 54, 57). In the physical time representation a CTRW in \mathcal{S} is given as $\dot{Y}(t) = \bar{\xi}(t)$, where $\bar{\xi}$ is the derivative of a subordinated Brownian motion (59). This is equivalently written as the formal definition $\bar{\xi}(t) = \int_0^\infty \xi(s)\delta(t - T(s))ds$, where ξ is a white Gaussian noise with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t_1)\xi(t_2) \rangle = 2\sigma\delta(t_1 - t_2)$, and T is a strictly increasing Lévy process. Using this representation, we can calculate the characteristic functional G of $\bar{\xi}$ for a general test function u (SI Appendix, section 4),

$$G[u(r)] = \left\langle \exp \left[-\sigma \int_0^\infty [u(T(s))]^2 ds \right] \right\rangle, \quad [15]$$

where the brackets denote an average over the realizations of the process T . A GT can now be performed without problems, leading to $\dot{\tilde{Y}}(t) = -v_0 + \bar{\xi}(t)$. Remarkably, using functional techniques (60) together with the result in Eq. 15, we can show that the FP equation for this process is precisely given by Eq. 13, thus completing the picture (SI Appendix, section 4). The Langevin description in physical time highlights that to correctly implement the change of frame, the constant advective force exerted on the underlying random walk in the frame $\tilde{\mathcal{S}}$ needs to act at each time step, i.e., also during the trapping times. This simple physical scenario underlies the complicated space-time coupling manifest in the retardation of Eq. 13. Its modeling in terms of subordination thus inevitably couples the equations for the position and elapsed time processes, which makes any analytical treatment challenging (an example is discussed in SI Appendix, section 5, where we derive Eq. 13 for the process \tilde{Y} using its representation in terms of coupled subordinated equations). Further, using the characteristic functional of the noise $\bar{\xi}$ in Eq. 15 one can derive its analytical solution

$$\tilde{P}(k, \lambda) = \frac{1}{\lambda + ikv_0} \left[1 - \frac{\sigma k^2}{\Phi(\lambda + ikv_0) + \sigma k^2} \right], \quad [16]$$

whose inverse Fourier–Laplace transform is plotted in Fig. 2B for the particular case of T being a Lévy stable process of order α (SI Appendix, Eq. S68). We observe the typical distribution of a force-free CTRW (5) time-shifted with velocity v_0 , in perfect agreement with numerical simulations of \tilde{Y} .

Moreover, we find that \tilde{Y} can also generate a superdiffusive MSD, thus providing a unified model for both sub- and superdif-

fusion. This surprising fact relies on the Langevin description in physical time and the equivalent characterization of $\bar{\xi}$ by means of its multipoint correlation functions (59). In particular, its FP equation is still Eq. 13, which can be derived by a generalization of Novikov's theorem via functional methods (61, 62) (SI Appendix, section 6), and the resulting PDF satisfies weak GI. In Fig. 2C we plot its propagator for $K(t) = t^{\alpha-1}/\Gamma(\alpha)$, now for $1 < \alpha < 2$ (SI Appendix, Eq. S68, analytically continued in α). For $v_0 = 0$, this PDF was first discussed in ref. 63.

In summary, using a Galilean invariant version of the paradigmatic Kac–Zwanzig model, we have derived the weak GI properties *i–iii* that need to be satisfied to consistently describe the same stochastic system in different inertial frames. While these properties hold for normal diffusion based on our analytical derivation, by using these rules consistent anomalous diffusive models can be constructed for both sub- and superdiffusion, even though a precise coarse-graining procedure is missing for them. We demonstrated this by providing the missing representation for the important class of CTRW models, which shows that the correct form is not at all suggested from the representation in the rest frame. Moreover, the Langevin representation *i* discloses that in a comoving frame the heat bath leads generally to an additive flow field on the tracer particle irrespective of the details of the underlying coupling. Consequently, the definitions of work, heat, and entropy production used within the recent theory of stochastic thermodynamics (64) have to be modified to account for the contribution of the external flow (65), highlighting fundamental similarities between normal and anomalous diffusive systems, even though the stochastic thermodynamics of the latter are so far not well understood (66). Along these lines, connections between GI and the validity of fluctuation–dissipation relations on the one hand and the celebrated fluctuation relations generalizing the second law of thermodynamics (64) on the other hand have been suggested (66, 67) and need to be investigated further. But our most important statement is that ignoring our weak GI rules can easily lead to unphysical models, as exemplified by the CTRW with an ad hoc advective term (Fig. 2A). The consequences of our results are thus far reaching. Weak GI is expected to constrain all mesoscopic diffusive models whose microscopic representation is expected to satisfy conventional GI. As such, it provides an important selection principle for stochastic models preceding comparison with data, which can guide modeling approaches throughout the physical, chemical, and biological sciences.

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