Origin of Hyperdiffusion in Generalized Brownian Motion

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We study a minimal non-Markovian model of superdiffusion which originates from long-range velocity correlations within the generalized Langevin equation approach. The model allows for a three-dimensional Markovian embedding. The emergence of a transient hyperdiffusion, $\langle \Delta x^2(t)\rangle \propto t^{2+\lambda}$, with $\lambda \sim 1$–3 is detected in tilted washboard potentials before it ends up in a ballistic asymptotic regime. We relate this phenomenon to a transient heating of particles $T_{\rm kin}(t) \propto t^\lambda$ from the thermal bath temperature T to some maximal kinetic temperature $T_{\rm max}$. This hyperdiffusive transient regime ceases when the particles arrive at the maximal kinetic temperature.

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Anomalous diffusion is found across many different branches of physics, from charge transport processes in amorphous materials to plasma physics and biophysics, and there are many different theories reflecting a variety of underlying physical mechanisms [1–7]. One of the fundamental approaches is based on the generalized Langevin equation (GLE) [8–23], see Eq. (1) below. Remarkably, it can be derived from a Hamiltonian dynamics of a particle that bilinearly couples to a thermal bath of harmonic oscillators characterized by the bath spectral density $J(\omega)$ [9,10,12,18]. This model is capable of describing all types of anomalous diffusion $\langle \Delta x^2(t)\rangle \sim 2D_\alpha t^\alpha/\Gamma(1+\alpha)$ within a unified framework and the index α reflects just the low-frequency behavior of the spectral bath density $J(\omega) \propto \omega^\alpha$ for $0<\alpha<2$ [12,24]. Namely, the case $0<\alpha<1$ corresponds to anomalously slow diffusion, or subdiffusion, the case $\alpha=1$ to normal diffusion, and the case $1<\alpha<2$ to superdiffusion. The ballistic diffusion $\langle \Delta x^2(t)\rangle \sim D_2 t^2$ is attained for all spectral densities with $\alpha>2$ at low frequencies and the case of $J(\omega) \propto \omega^2$ is marginally ballistic (a special case). This finding is without a potential, or under a constant force. Then the occurrence of hyperdiffusion, $\langle \Delta x^2(t)\rangle \propto t^\alpha$ with $\alpha>2$, is not possible if Brownian particles are initially thermalized [25]. Several circumstances are of special interest. First, GLE diffusion is almost always ergodic, except for the ballistic case [14,17,20,22] studied also below. Similarly, anomalous diffusion based on continuous time random walks is weakly nonergodic [26]. Second, for a constant force F, the diffusion coefficient is proportional to the bath temperature, i.e., $D_\alpha \propto T$ and a generalized Einstein-Stokes relation holds [12]. For nonlinear forcing, e.g., in tilted washboard potentials, this kind of anomalous diffusion is not sufficiently investigated and offers surprises. In particular, a hyperdiffusive regime occurs with α greatly enhanced to $\alpha_{\rm eff} \sim 3$–5 [22,27]. This puzzling nonlinear and nonequilibrium effect is the focus of this study.

Such anomalous diffusion allows for Markovian embeddings of surprisingly small dimensions which suffice normally in practice [21,22]. A Markovian embedding is natural given that the underlying Hamiltonian dynamics is Markovian. However, it formally has an infinite dimension for a thermal bath considered in the thermodynamic limit. Surprisingly, the practical embedding dimension using some auxiliary stochastic variables can be quite small.

The purpose of this Letter is to give a physical explanation of the observed hyperdiffusive anomaly as a transient heating of particles with their kinetic temperature defined via the velocity variance $\langle \Delta v^2(t)\rangle \propto T_{\rm kin}$ rising in accordance to a transient power law, $T_{\rm kin}(t) \propto t^\lambda$, from the bath temperature T to a maximal kinetic temperature $T_{\rm max}$ which depends on the duration of transient period through F, T, and the amplitude of periodic potential V_0 ($T_{\rm kin}=T$, when $V_0=0$, or $F=0$). It can be very large (thousands of T). Such a nonlinear heating mechanism in fixed not alternating in time applied fields is quite unusual, and, paradoxically, smaller bias strengths F yield higher $T_{\rm max}$ values.

We start from the traditional GLE model in one selected direction for a particle of mass m in the potential $V(x)$ subjected to a linear friction with memory kernel $\eta(t) = (2/\pi)\int_0^\infty d\omega J(\omega)\cos(\omega t)/\omega$ and random force $\xi(t)$ of zero mean:

$$m\ddot{x} + \int_0^t \eta(t-t')\dot{x}(t')dt' + \frac{\partial}{\partial x}V(x) = \xi(t). \qquad (1)$$

The random force is Gaussian and fully characterized by its autocorrelation function satisfying the fluctuation-dissipation relation

$$\langle \xi(t)\xi(t')\rangle = k_B T\eta(|t-t'|) \qquad (2)$$

which in turn is a consequence of the fluctuation-dissipation theorem.

A necessary condition for the emergence of superdiffusion asymptotically ($t\to\infty$) within the considered class of models is zero integral friction [14,22], i.e., $\lim_{t\to\infty}\int_0^t \eta(t')dt' = 0$. The memory kernel thus must be positive at times $t'=t$, yielding $\eta(0)>0$ cf. Eq. (2), and possess a negative part. The simplest model which satisfies these two conditions is [17]:

$$\eta(t) = \eta[2\delta(t) - \nu e^{-\nu t}]. \tag{3}$$

It will be considered in the following and corresponds to a spectral bath density $J(\omega)$ which is cubic for $\omega \ll \nu$ (typifying, e.g., acoustic bulk phonons in solids [12]) and linear for $\omega \gg \nu$. The corresponding spectral power of the noise $S(\omega)$ corresponds to the white noise (for $\omega \gg \nu$), i.e., $S(\omega) = \text{const}$, with the small-frequency part of the spectrum smoothly cut, so that $S(\omega) \propto \omega^2$ for $\omega \ll \nu$.

Furthermore, the autocorrelation function (ACF) of velocity fluctuations, $\Delta v(t) = v(t) - \langle v(t)\rangle$, in the absence of deterministic force, or under a constant forcing obeys for this minimal model

$$\langle \Delta v(t)\Delta v(t')\rangle = v_T^2\left\{\frac{\nu}{\nu+\gamma} + \frac{\gamma}{\nu+\gamma}\exp[-(\nu+\gamma)|t-t'|]\right\}, \tag{4}$$

with $\gamma = \eta/m$, provided that the velocities are initially thermally distributed with $\sqrt{\langle \Delta v^2\rangle} = v_T = \sqrt{k_B T/m}$. This follows from the Laplace-transformed result for this quantity for arbitrary kernels [8]: $\tilde{K}_v(s) = v_T^2/[s + \tilde{\eta}(s)/m]$. In other words, the ACF exponentially decays, but to a nonzero constant, which is the reason for nonergodicity and ballistic diffusion. Clearly, this is the simplest of possible models, yet physically reasonable. The model is non-Markovian, but it allows for a three-dimensional Markovian embedding [17]:

$$\begin{aligned} \dot{x}(t) &= v(t) \\ m\dot{v}(t) &= -\frac{\partial}{\partial x}V(x) - u(t) - \eta v(t) + \sqrt{2k_B T\eta}\,\zeta(t) \\ \dot{u}(t) &= -\nu\eta v(t) - \nu u(t) + \nu\sqrt{2k_B T\eta}\,\zeta(t) \end{aligned} \tag{5}$$

where $\zeta(t)$ is a zero-centered white Gaussian noise with autocorrelation function $\langle \zeta(t)\zeta(t')\rangle = \delta(t - t')$. By integrating out the auxiliary variable $u(t)$ in the above equations (projecting onto the $x - v$ plane), it is not difficult to show that this leads to the GLE in Eqs. (1) and (2) with the memory kernel of Eq. (3), if the initial value of $u(0)$ is Gaussian distributed with zero mean and variance $\langle u^2(0)\rangle = k_B T\eta$. This is assumed in the following. The initial velocities are thermally distributed.

We consider the case of a washboard potential with period x_0 and amplitude strength V_0 biased by a constant force F, $V(x) = -V_0\cos(2\pi x/x_0) - Fx$. It is convenient to transform Eq. (5) into dimensionless quantities by scaling time in units of γ^{-1}, distance in x_0, energy in $m(x_0\gamma)^2$ (which applies for V_0, $k_B T$, and Fx_0), u in $mx_0\gamma^2$, and ν in γ. We have integrated the system in the corresponding nondimensional variables using a standard Euler algorithm with time step $\Delta t = 10^{-4}$ for $\nu = 0.25$, $V_0 = 1$, and varying T and F. The behavior of the position variance for 10^4 particles which started at the origin with the velocities thermally distributed is depicted in Fig. 1. A striking feature is the regime of intermediate hyperdiffusion which ends in the ballistic regime. This puzzling behavior, which seems to be rather general, was not, however, explained before in physical terms.

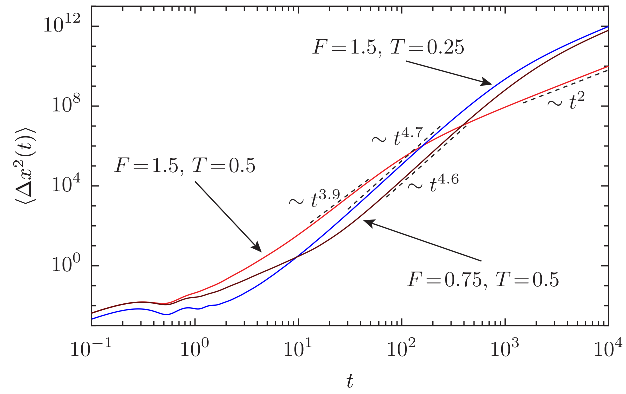

FIG. 1 (color online). Biased diffusion in a washboard potential with strength $V_0 = 1$ for different values of the bias F and the bath temperature T. The mean squared displacement exhibits transient hyperdiffusion before it reaches the asymptotically ballistic diffusion regime. The transient hyperdiffusion is enhanced upon decreasing F and T. The velocities are initially thermally distributed, $\nu = 0.25$, and $n = 10^4$ trajectories are used for the ensemble averaging.

For this we notice that the diffusive behavior can be related to the twice-integrated velocity ACF $\langle \Delta v(t)\Delta v(t')\rangle$. In the stationary limit, when the ACF depends on the difference of time arguments, the normal diffusive behavior emerges when the integral of ACF is finite. Its value defines the diffusion coefficient, which is temperature dependent. For the thermally distributed velocities and normal diffusion (singular limit for $\nu = 0$) the ACF decays exponentially to zero from $\langle \Delta v^2\rangle = k_B T/m$, with the decay rate γ. This yields the Einstein relation, $D(T) = k_B T/(m\gamma)$. For the anomalous GLE, diffusion is described by a spectral bath density $J(\omega) \propto \gamma_\alpha \omega^\alpha$ $(0 < \alpha < 2)$ which corresponds to $\tilde{\eta}(s) = \eta_\alpha s^{\alpha-1}$ and yields $\langle \Delta x^2(t)\rangle \sim 2D_\alpha(T)t^\alpha/\Gamma(1+\alpha)$ asymptotically, the integral of the ACF for $\alpha \neq 1$ either diverges (superdiffusion), or it tends to zero (either subdiffusion, or bounded motion in trapping potentials). However, in the absence of forcing, or under a constant force a generalized Einstein relation always holds, $D_\alpha(T) = k_B T/(m\gamma_\alpha)$. Furthermore, it is easy to show [from the exact expression for $\tilde{K}_v(s)$ for $V_0 = 0$] that for $\alpha > 2$, the diffusion is asymptotically always ballistic. This is why the occurrence of long-lasting hyperdiffusion is rather surprising. For the considered model we have $\langle \Delta x^2(t)\rangle \sim D_2(T)t^2$ asymptotically with $D_2(T) = k_B T/m^*$, where $m^* = m(1 + \gamma/\nu)$ is an effective mass. This asymptotics holds in the absence of a periodic potential, i.e., $V_0 = 0$.

If one switches on the periodic potential, the ballistic diffusion turns over into normal diffusion when $F = 0$ [22]. Upon application of a constant force $F > 0$, the particles will start to gradually accelerate when they leave the attraction domains of potential wells in the phase space due to the random kicks given by thermal noise. Their initial Maxwellian velocity distribution hence will not hold forever. Gradually accelerating, the running particles undergo drastic transient heating above the bath temperature due to multiple scattering on the periodic potential. Slower particles, however, are more strongly scattered backwards (i.e., are decelerated) by the potential wells in comparison with faster ones. This in turn yields a growing width (see Fig. 2) of the velocity distribution, which becomes also skewed towards slower particles, see Fig. 3. Indeed, the averaged kinetic energy per particle, $K = m\langle v^2\rangle/2$, can be decomposed as $K = K_m + K_T$. $K_m = m\langle v\rangle^2/2$ is the kinetic energy associated with mean velocity which asymptotically is well described by $\langle v(t)\rangle = Ft/m^*$ when the influence of periodic potential becomes negligible. The part $K_T = m\langle \Delta v^2\rangle/2 \doteqdot k_B T_{\rm kin}/2$ is used to define the effective kinetic temperature $T_{\rm kin}(t)$. Importantly, the action of F results not only in the growing mean $\langle v(t)\rangle$, but also generates a growing variance of the velocity distribution, see in Fig. 2. It is a common practice to characterize different sorts of particles with different kinetic temperatures, e.g., in plasma physics [28]. In a similar spirit, we use a "kinetic temperature" notion which should be used with care as it does not correspond to a thermodynamic temperature, but rather simply characterizes the width of a nonequilibrium velocity distribution, see in Fig. 3. Nevertheless, it is a useful concept because it reflects an important statistical aspect of the temperature, namely, that temperature characterizes the width of the kinetic energy distribution. Even if the relative spread of the velocity distribution around the mean value is rather small at the end point of simulations (by just a few percent), the mean kinetic energy is large and therefore the kinetic temperature can also be large, cf. Fig. 4.

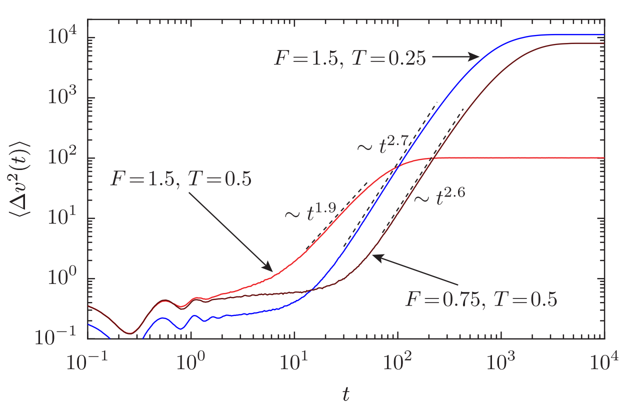

FIG. 2 (color online). The mean square fluctuation of the particles velocity for the biased diffusion in Fig. 1 exhibits a transient behavior, in which the kinetic temperature $T_{\rm kin}$ (see text) grows from bath temperature to a maximal value $T_{\rm max}$. The transient power-law growth, $T_{\rm kin}(t) \propto t^\lambda$, explains the hyperdiffusive regime with the corresponding exponent $2+\lambda$ in Fig. 1. Lower bath temperature and weaker biasing field lead surprisingly to stronger heating (see Fig. 4).

In our numerical experiments, the velocity distribution becomes broadened and strongly skewed with the "retarded" tail of distribution described by an exponential, rather than by a Gauss-Maxwell distribution, cf. in Fig. 3. The variance of the distribution grows in time in accordance with a power law, $T_{\rm kin}(t) \propto t^\lambda$, cf. Fig. 2. This explains the emergence of hyperdiffusion $\langle \Delta x^2(t)\rangle \sim D_2(T_{\rm kin})t^2 = k_B T_{\rm kin} t^2/m^* \sim t^{2+\lambda}$ in Fig. 1. This regime is, however, only transient. The duration of the transient period depends strongly on the potential amplitude V_0, the strength of the bias force F, and the bath temperature T.

The hyperdiffusive regime turns over into the ballistic diffusion regime when the particles arrive at the maximal kinetic temperature $T_{\rm max}$, compare Figs. 1 and 2. This nonlinear heating mechanism is quite unusual. The heating of plasmas by time-varying stochastic fields is well known. One of the pertinent nonlinear mechanisms is the so-called Fermi acceleration [29]. It requires but a time-varying driving field (or stochastically oscillating boundary). In our case, the "heating" field is, however, constant, and, strikingly enough, the use of weaker bias fields heats up the particles ever more strongly, see in Fig. 4(a). However, much longer times are required then. Moreover, the smaller the bath temperature is, the higher is the final kinetic temperature, cf. Fig. 4(b). Both effects are due to the fact that the transient time scale becomes longer because the particles take on the kinetic energy more slowly in the accelerating field F. The corresponding dependencies are stronger than exponential. Such a strong sensitivity is surprising. The qualitative physical explanation is as follows: The heating is caused by retardation of flying particles when they pass over the trapping domains while moving in the bias direction. It is appreciably strong as long as the averaged energy of the particles does not substantially exceed the potential barrier height. For smaller temperatures and smaller bias forces it takes an exponentially greater amount of time for the particles to escape out of potential wells and to arrive on average at

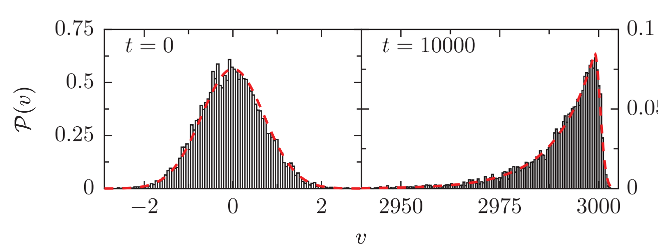

FIG. 3 (color online). Two snapshots of the velocity distribution $P(v,t)$, initial and at the end point of simulations in Figs. 1 and 2 for $F = 1.5$ and $T = 0.5$. $P(v,t)$ becomes shape invariant already for $t > 500$, after the kinetic temperature reaches its maximum, see in Fig. 2. After this happens, only the maximum of the distribution moves accelerating in time. The initial distribution is Gaussian with $\langle \Delta v^2(0)\rangle = T$. The final distribution is strongly skewed: its left slope ($v < 2999$) is well fitted by an exponential, while the right slope ($v > 2999$) remains approximately Gaussian.

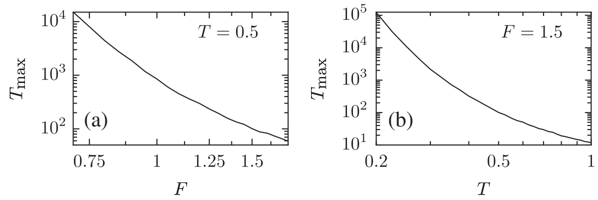

FIG. 4. Dependence of maximal kinetic temperature $T_{\max}$: (a) on applied force F for a fixed thermal bath temperature T, and (b) on T at a fixed F.

a sufficiently high kinetic energy, so that their backscattering or deceleration cease to play a role. This leads to a greater broadening of the velocity distribution [30]. The giant enhancement of ballistic diffusion reminds one of the giant enhancement of normal diffusion [31]. However, the underlying physical mechanisms are quite different.

The physical systems where the discussed hyperdiffusive heating effect might be relevant are dusty plasmas where heavy tracer particles collide with the gas of light particles serving as a thermal bath. Even if our GLE description in this case is not directly applicable, there exists some partial correspondence between the superdiffusive fractional GLE results and the fractional Kramers equation by Barkai and Silbey [6]. Such a correspondence is surprising because both descriptions are different, see, e.g., in [11]. The latter scheme derives from linear Boltzmann equations with a fractional scattering integral accounting for scattering events which are power-law distributed in time. Our physical explanation of the transient heating mechanism is more generally applicable; i.e., it is not restricted by the present GLE model. In particular, it is expected to work for the fractional kinetic equations like the fractional Kramers equation, or a more general one introduced recently by Friedrich *et al.* [7]. We are confident that our work will stimulate further studies and even an experimental validation of this intriguing hyperdiffusive behavior.

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