

## Hamiltonian theory of stochastic acceleration

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Stochastic acceleration, defined in terms of a stochastic equation of motion for the acceleration, is derived from a Hamiltonian model. A free particle is coupled bilinearly to a harmonic bath through the particle's momentum and coordinate. Under appropriate conditions, momentum coupling induces velocity diffusion which is not destroyed by the spatial coupling. Spatial-momentum coupling may induce spatial subdiffusion. The thermodynamic equilibrium theory presented in this paper does not violate the second law of thermodynamics, although the average velocity squared of the particle may increase in time without bound.

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The term “stochastic acceleration” (SA) was coined by Sturrock in 1966 [1,2]. The equation of motion for the acceleration, defined as the time derivative of the velocity, is stochastic. Sturrock considered the influence of randomly time-varying electromagnetic fields on the motion of a charged test particle and concluded that they may induce a net acceleration. He showed that the effect of a random electric field on a distribution of charged particles may be represented by a diffusion equation for the velocity (a corresponding limit theorem was proven in Ref. [3]), hence the term stochastic acceleration; the mean velocity squared increases linearly in time.

To the best of our knowledge, the first physical model of SA may be found in a paper by Fermi [4] who proposed a theory for the acceleration of cosmic rays in interstellar space. In his model, charged particles collide with randomly moving magnetic clouds. Particles can gain energy in a head-on collision or lose energy in an overtaking collision. There is an average gain in energy since head-on collisions are more likely, leading to a linear increase of the average energy of the particle with time. This heating may be modeled in terms of a particle bouncing between a fixed and an oscillating wall [5–7]. Recently, Bouchet *et al.* [8] suggested a minimal stochastic model for Fermi's acceleration. Various modifications of Fermi's original idea provide explanations for several physical phenomena, as exemplified by the plasma-maser effect in a weakly turbulent plasma [9], dynamics of a nonlinear oscillator with multiplicative noise [10], and acceleration of ionospheric ions by auroral arcs [11,12].

SA is a particular example of the macroscopic manifestation of randomness in physical dynamics, first demonstrated by Einstein in his study of diffusion in space a century ago [13]. Spatial diffusion is often modeled in terms of a Hamiltonian in which the particle's coordinate is bilinearly coupled to a harmonic oscillator heat bath [14–16]. This model is fundamental to our understanding of diverse processes in dissipative media, such as chemical reactions, quantum tunneling, bulk and surface diffusion, and more. It is thus surprising that to date, SA has not been considered in the framework of this model.

There is a seemingly fundamental difficulty with such a generalization: SA implies that the average velocity squared

of the particle may increase infinitely with time suggesting the extraction of unlimited kinetic energy from a thermal heat bath, in contradiction with the second law of thermodynamics [17]. Is SA possible in a system at thermal equilibrium? What happens when one simultaneously has SA and spatial diffusion? How does one process affect the other if at all?

The purpose of this paper is to provide answers to these questions. We employ a Hamiltonian of a free particle coupled bilinearly to a harmonic oscillator bath through the momentum and the coordinate [18]. We show that under appropriate conditions on the coupling, this model leads in the continuum limit to both SA as well as spatial diffusion. In our model, SA is an equilibrium phenomenon where the term equilibrium is used throughout this paper in the sense that all relevant observables, such as diffusion coefficients, are obtained from an average over the canonical distribution  $\exp(-\beta H)$ . We find that SA is possible at thermal equilibrium, but the second law of thermodynamics is not violated since an infinite amount of energy is needed to extract the particle from the heat bath. We also show that spatial coupling does not affect the phenomenon of velocity diffusion.

A particle (with mass weighted momentum  $P$  and coordinate  $Q$ ) interacting bilinearly with a harmonic oscillator heat bath both through the coordinate as well as the momentum, corresponds to the Hamiltonian

$$H = \frac{1}{2} \left[ P^2 + \sum_{j=1}^N (p_j - d_j P)^2 + \sum_{j=1}^N \omega_j^2 \left( x_j - \frac{c_j}{\omega_j^2} Q \right)^2 \right], \quad (1)$$

where  $p_j, x_j, j=1, \dots, N$  are the mass weighted momentum and coordinate of the  $j$ th bath oscillator whose frequency is  $\omega_j$ . The  $c_j$ 's and  $d_j$ 's are the respective coupling coefficients to the particle's coordinate and momentum. The formal solution of Hamilton's equations of motion for the  $j$ th bath oscillator is

$$\begin{aligned}
y_j(t) &= y_j(0)\cos(\omega_j t) + \frac{\dot{x}_j(0)}{\omega_j} \sin(\omega_j t) \\
&\quad - \frac{c_j}{\omega_j^2} \int_0^t dt' \dot{Q}(t') \cos[\omega_j(t-t')] \\
&\quad - \frac{d_j}{\omega_j} \int_0^t dt' \dot{P}(t') \sin[\omega_j(t-t')], \quad (2)
\end{aligned}$$

where we used the notation  $y_j \equiv x_j - c_j Q / \omega_j^2$ . The equations of motion for the particle are

$$\dot{Q} = P - \sum_{j=1}^N d_j \dot{x}_j \quad (3)$$

$$\dot{P} = \sum_{j=1}^N c_j y_j. \quad (4)$$

This leads to the following generalized Langevin equation for the particle:

$$\begin{aligned}
M\ddot{Q}(t) &= f_Q(t) + Mf_P(t) - \int_0^t dt' \dot{Q}(t') [\eta_Q(t-t') + M\eta_{PQ}(t-t')] \\
&\quad - \int_0^t dt' \dot{P}(t') [M\varphi_P(t-t') + \varphi_{PQ}(t-t')], \quad (5)
\end{aligned}$$

with the effective particle mass

$$M = \left( 1 + \sum_{j=1}^N d_j^2 \right)^{-1}. \quad (6)$$

The noise is represented by the coordinate  $f_Q$  and momentum  $f_P$  random forces

$$f_Q(t) = \sum_{j=1}^N c_j \left[ y_j(0)\cos(\omega_j t) + \frac{\dot{x}_j(0)}{\omega_j} \sin(\omega_j t) \right], \quad (7)$$

$$f_P(t) = \sum_{j=1}^N d_j \omega_j^2 \left[ y_j(0)\cos(\omega_j t) + \frac{\dot{x}_j(0)}{\omega_j} \sin(\omega_j t) \right]. \quad (8)$$

These random forces have zero mean and their correlation functions are

$$\beta \langle f_Q(t) f_Q(0) \rangle = \sum_{j=1}^N \frac{c_j^2}{\omega_j^2} \cos \omega_j t \equiv \eta_Q(t), \quad (9)$$

$$\beta \langle f_P(t) f_Q(0) \rangle = \sum_{j=1}^N c_j d_j \cos \omega_j t \equiv \eta_{PQ}(t), \quad (10)$$

$$\beta \langle f_P(t) f_P(0) \rangle = \sum_{j=1}^N d_j^2 \omega_j^2 \cos \omega_j t \equiv \eta_P(t). \quad (11)$$

The brackets denote averaging with respect to the thermal distribution ( $e^{-\beta H}$ ).  $\eta_Q(t)$  is the standard friction function, resulting from the spatial coupling of the particle to the bath. The other two functions are due to the momentum and

momentum-space coupling. Finally, in Eq. (5), we also used the notation:

$$\varphi_{PQ}(t) = \int_0^t dt' \eta_{PQ}(t') = \sum_{j=1}^N \frac{d_j c_j}{\omega_j} \sin(\omega_j t),$$

$$\varphi_P(t) = \int_0^t dt' \eta_P(t') = \sum_{j=1}^N d_j^2 \omega_j \sin(\omega_j t).$$

We stress that Eq. (5) is an exact equation of motion for the particle coupled to the bath via both its coordinate and momentum.

It is instructive to consider the simple case of pure momentum coupling such that all  $c_j=0$  and the momentum of the particle is a constant of the motion [see Eq. (4)]. From Eq. (5), one finds that the equation of motion for the acceleration is stochastic:

$$\ddot{Q} = \dot{V} = f_P(t). \quad (12)$$

where  $V = \dot{Q}$ . The dynamics of the SA depends on the properties of the momentum noise  $f_P(t)$ . For Ohmic momentum noise [ $\beta \langle f_P(t) f_P(0) \rangle = \eta_P(t) = 2\eta_P \delta(t)$ ], Eq. (12) for the velocity  $V$  is formally the same as the equation of overdamped Brownian motion for the coordinate [21]. The latter describes diffusion in the coordinate space, so Eq. (12) predicts diffusion in the velocity space. Here, in contrast to other treatments of SA, the origin of the driving force is equilibrium fluctuations rather than an external nonequilibrium source. This is a first important result—SA is an equilibrium phenomenon.

This phenomenon is not intuitively obvious. The velocity squared of the particle grows linearly in time without bound. One might then think in violation of the second law of thermodynamics that it is possible to extract from a heat bath an infinite amount of energy. One would inject the particle into the stochastic medium and then wait until the particle escapes the medium with very large velocity. The fact that this will not work is evident, if one considers the energy balance. Suppose that the bath consists of a finite number of bath modes— $N$ . When the particle is inside the medium, it is in equilibrium. So, the average energy of the composite system and bath at temperature  $T$  is  $\langle E \rangle_{\text{in}} = (N+1/2)k_B T$ . When the particle leaves the medium, we have a separable system, a free particle, and a collection of  $N$  oscillators. However, the initial conditions of the bath and the free particle are distributed according to their conditions in the composite system before the particle exited the medium. The average energy of the particle and the bath after the particle exited is  $\langle E \rangle_{\text{out}} = Nk_B T + \langle P^2 \rangle / (2M)$ . The difference in energy of the composite system and bath, once when they interact and are separated, is

$$\Delta E = \langle E \rangle_{\text{out}} - \langle E \rangle_{\text{in}} = \frac{\langle P^2 \rangle}{2M} - \frac{k_B T}{2} > 0.$$

In the continuum limit when velocity diffusion occurs, we shall show below that the effective mass  $M \rightarrow 0$ . The momentum remains equilibrated  $\langle P^2 \rangle = k_B T$  [see also Eq. (23)].

So  $\Delta E \rightarrow \infty$  and an infinite amount of energy is needed to extract (inject) the particle from (to) the medium. Although the velocity squared of the particle may grow without bound [at equilibrium, one finds from Eq. (3) that  $\langle \dot{Q}^2 \rangle = k_B T / M$ ] so that its kinetic energy outside of the medium could be very large, one needs an even larger amount of energy to extract it. Thermodynamics is not violated.

It remains to be shown that spatial coupling does not destroy the velocity diffusion as found in the presence of pure momentum coupling. It is appropriate to first provide some detail on the continuum limit. As Eqs. (9)–(11) suggest, the oscillator heat bath may be considered as the discrete Fourier representation of the functions  $\eta_j$ ,  $j=P, Q, PQ$ . Choosing  $\omega_j = j\Delta\omega$  implies that these functions are periodic with period  $2\pi/\Delta\omega$ . Since typically the functions  $\eta_j$  decay as  $t \rightarrow \infty$ , the continuum limit is obtained by allowing both  $N \rightarrow \infty$  and  $\Delta\omega \rightarrow 0$ . In the continuum limit, all three functions are localized in time and represented by a Fourier integral, instead of a Fourier series. Henceforth, the term “discrete bath” will refer to a finite  $\Delta\omega$ , the continuum limit is obtained when  $\Delta\omega \rightarrow 0$ .

The solution of the generalized Langevin equation (5) is obtained by means of Laplace transformation,  $\hat{f}(s) = \int_0^\infty dt e^{-st} f(t)$ . Using the relations  $\hat{\phi}_P(s) = \hat{\eta}_P(s)/s$ ,  $\hat{\phi}_{PQ}(s) = \hat{\eta}_{PQ}(s)/s$ , one finds from Eq. (5) that the Laplace transform of the time derivative of the particle’s momentum is

$$\hat{P}(s) = \frac{\hat{f}_Q(s) - \hat{\eta}_Q(s)\hat{V}(s)}{s + \hat{\eta}_{PQ}(s) + B(s)\hat{\eta}_Q(s)}, \quad (13)$$

where

$$B(s) \equiv \frac{sM^{-1} - \hat{\eta}_P(s)}{s + \hat{\eta}_{PQ}(s)} = \frac{1 + s^2 \sum_{j=1}^N d_j^2 / (s^2 + \omega_j^2)}{1 + \sum_{j=1}^N c_j d_j / (s^2 + \omega_j^2)}. \quad (14)$$

From Eq. (5), the Laplace transform of the velocity  $V(t)$  and the acceleration  $A(t) \equiv \dot{Q}(t)$  are found to be

$$\hat{V}(s) = \frac{V(0) + \hat{f}_P(s) + B(s)\hat{f}_Q(s)}{s + \hat{\eta}_{PQ}(s) + B(s)\hat{\eta}_Q(s)}, \quad (15)$$

$$\hat{A}(s) = \frac{s[B(s)\hat{f}_Q(s) + \hat{f}_P(s)] - V(0)[B(s)\hat{\eta}_Q(s) + \hat{\eta}_{PQ}(s)]}{s + \hat{\eta}_{PQ}(s) + B(s)\hat{\eta}_Q(s)}. \quad (16)$$

The velocity, acceleration, and  $\dot{P}$  are random quantities with zero mean and the Laplace transform of their autocorrelation functions are given by

$$\hat{C}_V(s) \equiv \langle \hat{V}(s)V(0) \rangle = \frac{k_B T}{\hat{\eta}_Q(s) + B^{-1}(s)[s + \hat{\eta}_{PQ}(s)]}, \quad (17)$$

$$\begin{aligned} \hat{C}_A(s) &\equiv \langle \hat{A}(s)A(0) \rangle \\ &= s \frac{\hat{\eta}_P(s) + M^{-1}B(s)\hat{\eta}_Q(s) + [M^{-1} + B(s)]\hat{\eta}_{PQ}(s)}{s + \hat{\eta}_{PQ}(s) + B(s)\hat{\eta}_Q(s)} k_B T, \end{aligned} \quad (18)$$

$$\begin{aligned} \hat{C}_{\dot{P}}(s) &\equiv \langle \hat{P}(s)\dot{P}(0) \rangle \\ &= s^2 \frac{\hat{\eta}_Q(s)}{[s + \hat{\eta}_{PQ}(s)][s + \hat{\eta}_{PQ}(s) + B(s)\hat{\eta}_Q(s)]} k_B T. \end{aligned} \quad (19)$$

The system dynamics is thus expressed in terms of the correlation functions of random forces (the  $\eta$ ’s). It is useful to note that Cauchy’s inequality  $(\sum_{k=1}^n a_k b_k)^2 \leq \sum_{k=1}^n a_k^2 \sum_{k=1}^n b_k^2$  [19] implies that  $\hat{\eta}_{PQ}(s)^2 \leq \hat{\eta}_P(s)\hat{\eta}_Q(s)$ .

The general diffusional properties of the system are determined by the small  $s$  behavior of the correlation functions. From the definition of the effective mass  $M$  and the momentum function  $\eta_P(t)$ , it follows that

$$M^{-1} = 1 + \lim_{s \rightarrow 0} \hat{\eta}_P(s)/s \quad (20)$$

and hence for small  $s$ ,  $B(s) \sim [1 + \hat{\eta}_{PQ}(s)/s]^{-1}$ . The spatial diffusion coefficient is by definition [20,21]  $D_Q = \lim_{s \rightarrow 0} \hat{C}_V(s)$ . This, together with Eq. (17), implies that [under the condition  $\hat{\eta}_Q(0) \neq 0$ ]

$$\begin{aligned} \beta D_Q &= \lim_{s \rightarrow 0} \frac{s}{s \hat{\eta}_Q(s) + [s + \hat{\eta}_{PQ}(s)]^2} \\ &= \begin{cases} \hat{\eta}_Q^{-1}(0) & \text{if } \hat{\eta}_{PQ}(s) \sim s^\alpha, \alpha > \frac{1}{2} \\ (\hat{\eta}_Q(0) + \epsilon_{PQ}^2)^{-1} & \text{if } \hat{\eta}_{PQ}(s) = \epsilon_{PQ} s^{1/2} \\ 0 & \text{if } \hat{\eta}_{PQ}(s) \sim s^\alpha, \alpha < \frac{1}{2} \end{cases}. \end{aligned} \quad (21)$$

The velocity diffusion coefficient is by definition  $D_V = \lim_{s \rightarrow 0} \hat{C}_A(s)$ . Therefore, one obtains from Eq. (18)

$$D_V = \lim_{s \rightarrow 0} \langle \hat{A}(s)A(0) \rangle = k_B T \hat{\eta}_P(0). \quad (22)$$

This is a central result of this paper. It implies that irrespective of the nature of the spatial or the momentum-space coupling, the particle velocity exhibits normal diffusion  $\Delta_V^2 \equiv \langle [V(t) - V(0)]^2 \rangle = 2D_V t$  provided that  $\hat{\eta}_P(0) \neq 0$ . Note that the particle momentum does not diffuse. One finds from Eq. (19) that  $\hat{C}_{\dot{P}}(s)_{s \rightarrow 0} \sim s$  and hence

$$\Delta_{\dot{P}}^2 \equiv \langle [\dot{P}(t) - \dot{P}(0)]^2 \rangle \sim t^0, \quad (23)$$

which implies that at long times, the average kinetic energy of the particle,  $\langle P^2/2 \rangle$ , reaches its constant equilibrium value of  $k_B T/2$ . When in contact with the bath, the kinetic energy of the particle is given by its momentum squared, rather than the velocity squared, and, on average, this is a finite quantity.

The conclusion that the momentum does not diffuse even when the velocity does diffuse and the observation that the average kinetic energy of the particle is finite are crucial for understanding our results.

It is instructive to consider some further examples. For a discrete bath, one finds from Eqs. (9)–(11) that

$$\hat{\eta}_Q(s) = s \sum_{j=1}^N \frac{c_j^2}{\omega_j^2(s^2 + \omega_j^2)} \xrightarrow{s \rightarrow 0} s \sum_{j=1}^N \frac{c_j^2}{\omega_j^4}, \quad (24)$$

$$\hat{\eta}_{PQ}(s) = s \sum_{j=1}^N \frac{d_j c_j}{s^2 + \omega_j^2} \xrightarrow{s \rightarrow 0} s \sum_{j=1}^N \frac{d_j c_j}{\omega_j^2}, \quad (25)$$

$$\hat{\eta}_P(s) = s \sum_{j=1}^N \frac{d_j^2 \omega_j^2}{s^2 + \omega_j^2} \xrightarrow{s \rightarrow 0} s(M^{-1} - 1). \quad (26)$$

The fact that all the  $\hat{\eta}(s)$  go to zero as  $s$ , when  $s \rightarrow 0$ , implies that  $\hat{C}_V(s) \sim s^{-1}$  for small  $s$ . Thus at long times, the mean squared displacement behaves as  $\Delta_Q^2 \equiv \langle [Q(t) - Q(0)]^2 \rangle \sim t^2$  and the particle motion is ballistic. Similarly, the acceleration autocorrelation function is estimated by  $\hat{C}_A(s) \xrightarrow{s \rightarrow 0} \sim s$ , implying that at long times  $\langle \Delta_V^2 \rangle \sim t^0$ . The velocity dispersion stays constant, consistent with the ballistic motion for the coordinate.

If one assumes that the coupling to the bath is only through the spatial term, i.e., all  $d_j = 0$  and hence  $\eta_{PQ}(t) = \eta_P(t) = 0$ , our model reduces to the traditional model of Brownian motion. In this case, the generalized Langevin equation (5) takes its usual form  $\dot{V}(t) = f_Q(t) - \int_0^t dt' \eta_Q(t-t')V(t')$ .  $\eta_Q(t)$  is thus the standard friction (memory) function and Eq. (9) constitutes a fluctuation-dissipation theorem. In the continuum limit, equation (21) leads to the known result for the diffusion coefficient  $D_Q = k_B T \hat{\eta}_Q^{-1}(0)$  [in the specific case of Ohmic friction (white or Markovian  $f_Q$  noise),  $\eta_Q(t) = 2\eta_Q \delta(t)$ ,  $\hat{\eta}_Q(s) = \eta_Q$ ], while the velocity does not undergo diffusion,  $\hat{C}_A(s) \xrightarrow{s \rightarrow 0} \sim s$ .

In accordance with Eq. (22), the velocity undergoes normal diffusion, if  $\lim_{s \rightarrow 0} \hat{\eta}_P(s) \neq 0$ . In the particular case of Ohmic momentum memory,  $\eta_P(t) = 2\eta_P \delta(t)$  and  $\hat{\eta}_P(s) = \eta_P$ , the velocity diffusion coefficient is  $D_V = k_B T \eta_P$ . If for small  $s$ , the momentum memory behaves as  $\hat{\eta}_P(s) \sim s^\alpha$ ,  $0 \leq \alpha < 1$ , then  $\hat{C}_A(s) \xrightarrow{s \rightarrow 0} \sim s^\alpha$  so that for long times  $\Delta_V^2 \sim t^{1-\alpha}$ , i.e., the system velocity exhibits sublinear diffusion. When  $\alpha \geq 1$ , the velocity diffusion is suppressed as for a discrete bath. Note that in the case of momentum coupling only, the mean

squared displacement  $\Delta_Q^2$  increases with time as  $t^2$  since the small  $s$  behavior of the velocity autocorrelation function is  $\hat{C}_V(s) \xrightarrow{s \rightarrow 0} \sim s^{-1}$ .

In the presence of space and momentum coupling, the momentum space function critically affects the time dependence of the variance of the coordinate. Depending on the small  $s$  behavior of  $\hat{\eta}_{PQ}(s)$ , one can observe both normal and subdiffusion, or even the absence of diffusion. The evolution of the velocity is determined by the properties of the momentum correlation function. Specifically, if all memory functions are Ohmic, that is  $\eta_P(t) = 2\eta_P \delta(t)$ ,  $\eta_Q(t) = 2\eta_Q \delta(t)$ ,  $\eta_{PQ}(t) = 2\eta_{PQ} \delta(t)$ , then velocity diffusion takes place,  $D_V = k_B T \eta_P$ , even if the mean squared displacement is constant.

To summarize, a Hamiltonian model has been presented that includes bilinear spatial and momentum coupling of a free particle to a harmonic oscillator bath. We showed that along with spatial diffusion (normal or abnormal) this model exhibits velocity diffusion (or subdiffusion) under certain conditions on the properties of the ‘‘momentum’’ random force. Velocity diffusion exists even at thermal equilibrium, but it does not violate the second law of thermodynamics.

The Hamiltonian model for spatial dissipation is widely used. For example, when considering a parabolic barrier potential, it provides the main qualitative features for the effect of spatial friction on reaction rates [22]. We have limited ourselves here to the study of a free particle. It should be of some interest to study the properties of the same Hamiltonian model in the presence of a potential, such as a harmonic oscillator or parabolic barrier. In the same vein, the discussion here has been limited to classical mechanics. Quantum mechanics may profoundly affect spatial diffusion [23]. Similarly, spatial friction, in general, decreases quantum tunneling [16]. Is the same true for momentum coupling?

Not less interesting is to find systems in which momentum coupling is significant. For example, we know that the kinetic energy of coupled vibrational modes described in terms of local bond coordinates has a bilinear momentum coupling. It should be of interest to study the ‘‘momentum force’’ autocorrelation function to understand whether one should also consider momentum coupling when dealing with a particle immersed in a heat bath.

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