

Infinite Covariant Density for Diffusion in Logarithmic Potentials and Optical Lattices

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We solve the Fokker-Planck equation for Brownian motion in a logarithmic potential. When the diffusion constant is below a critical value the solution approaches an infinite covariant density. With this non-normalizable solution we obtain the phase diagram of anomalous diffusion for this process. We briefly discuss the physical consequences for atoms in optical lattices and charges in the vicinity of long polyelectrolytes. Our work explains in what sense the infinite covariant density and not Boltzmann's equilibrium describes the long time limit of these systems.

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Brownian particles in contact with a thermal heat bath and in the presence of a binding potential field $V(x)$ attain a steady state which is the Boltzmann equilibrium distribution $W_{\text{eq}}(x) = N \exp[-V(x)/k_b T]$. An interesting case is the logarithmic potential: $V(x) \propto \epsilon_0 \ln(x)$ for $x \gg 1$. Inserting $V(x)$ into the Boltzmann distribution, one finds that the steady state solution is described by an asymptotic power law $W_{\text{eq}}(x) \sim N x^{-\epsilon_0/k_b T}$. $\epsilon_0/k_b T$ must be larger than 1 for the normalization N to exist. Brownian motion in a logarithmic potential has attracted much attention since it describes many physical systems, ranging from the diffusive spreading of the momentum of two level atoms in optical lattices [1–3], single particle models for long ranged interacting systems [4], the famous problem of Manning condensation describing a charged particle in the vicinity of a long and uniformly charged polymer [5], and recently the motion of nanoparticles in an appropriately constructed force field [6].

In this Letter we provide the long sought after [1–4,7] long time solution of the Fokker-Planck equation describing the dynamics of Brownian particles in a logarithmic potential. Naively one would expect that in the long time limit the equilibrium distribution describes the statistical properties of the system. We will show that the logarithmic potential is much more interesting. To start with, we point out that the second moment in the steady state $\langle x^2 \rangle_{\text{eq}}$ may diverge, namely $\langle x^2 \rangle_{\text{eq}} = \infty$ if $1 < \epsilon_0/k_b T < 3$. However, if we view the problem of Brownian diffusion in a logarithmic potential dynamically, starting with a compact initial state, we immediately realize that the process cannot be faster than diffusion; namely $\langle x^2 \rangle \leq 2Dt$ where D is the diffusion constant. In this sense the steady state solution, e.g., the Boltzmann distribution, for a particle in a logarithmic potential, does not describe well the statistical properties of the problem, for any long though finite time. Thus we must consider the time dependent solution.

Here we show that Brownian particles in a logarithmic potential are characterized by an infinite covariant density. This density is not normalizable (hence the term infinite); however as we show, it does describe the anomalous

behavior of the system. For example it can be used to obtain correctly the moments of the process, while the normalizable Boltzmann distribution completely fails to do so. Similar infinite invariant densities were used by mathematicians to describe low dimensional deterministic dynamical models [8], while our work implies that these type of densities arise naturally in several physical systems. We examine these issues first in the context of diffusive spreading of momenta for atoms in an optical lattice, since this system is an excellent candidate to experimentally test our predictions. Our results with small notational changes describe a wide class of Brownian trajectories in the presence of a logarithmic potential, as discussed below.

Fokker-Planck equation.—The equation for the probability density function (PDF) $W(p, t)$ of the momentum p of an atom in an optical trap is modeled within the semi-classical approximation according to [1–3]

$$\frac{\partial W}{\partial t} = D \frac{\partial^2}{\partial p^2} W - \frac{\partial}{\partial p} F(p)W. \quad (1)$$

The cooling force

$$F(p) = -\frac{p}{1+p^2} \quad (2)$$

restores the momentum to its minimum while D describes stochastic momentum fluctuations which lead to heating. From the Sisyphus effect, interaction of atoms with the counter propagating laser beams means that D is determined by the depth of the optical potential [1–3], which in turn leads to experimental control of the unusual statistical properties of this system [9]. For $p \ll 1$ the force is harmonic, $F(p) \sim -p$, while in the opposite limit, $p \gg 1$, $F(p) \sim -1/p$. The effective potential $V(p) = -\int^p F(p)dp = (1/2) \ln(1+p^2)$ is symmetric $V(p) = V(-p)$ and $V(p) \sim \ln(p)$ when $p \gg 1$ (we use a dimensionless representation for p [3]). The minima of the effective potential $V(p)$ is at $p = 0$, the ideal cooling limit, which is not achieved due to the fluctuations.

Steady state.—The steady state solution of $W(p, t)$ is found in the usual way: imposing $\partial W_{\text{eq}}/\partial t = 0$ from Eqs. (1) and (2) we have $W_{\text{eq}} \propto \exp[-V(p)/D]$. This solution is normalizable only if $D < 1$ in which case [3,9]

$$W_{\text{eq}}(p) = \mathcal{N}(1 + p^2)^{-1/(2D)}, \quad (3)$$

where $\mathcal{N} = \Gamma(\frac{1}{2D})/[\sqrt{\pi}\Gamma(\frac{1-D}{2D})]$ is the normalization constant. This steady state solution was observed in optical lattice experiments [9] where it was shown that this behavior is tunable, namely, one may control D to obtain different steady state solutions. Notice that Eq. (3) exhibits a power law decay for large p which is clearly related to the logarithmic potential under investigation. From Eq. (3) we have

$$\langle p^2 \rangle_{\text{eq}} = \begin{cases} \frac{D}{1-3D} & 0 < D < 1/3 \\ \infty & 1/3 < D < 1. \end{cases} \quad (4)$$

The behavior $\langle p^2 \rangle_{\text{eq}} = \infty$ implies an averaged kinetic energy which is infinite [10]; as we now show, this divergence is avoided by considering the time dependent solution.

Bounds on $\langle p^2 \rangle$.—To start our analysis we consider the dynamics of $\langle p^2 \rangle$. Multiplying the Fokker-Planck Eq. (1) with p^2 and integrating over p we have, after integrating by parts and using the natural boundary condition that $W(p, t)$ and its derivative at $p \rightarrow \pm\infty$ are zero,

$$\frac{\partial}{\partial t} \langle p^2 \rangle = 2D - 2 \left\langle \frac{p^2}{1 + p^2} \right\rangle, \quad (5)$$

where $\langle \dots \rangle = \int_{-\infty}^{\infty} \dots W(p, t) dp$. Obviously, we have $0 \leq \langle p^2/(1 + p^2) \rangle \leq 1$, hence $2D - 2 \leq \frac{\partial \langle p^2 \rangle}{\partial t} \leq 2D$, and therefore if we start with $W(p, 0) = \delta(p)$

$$(2D - 2)t \leq \langle p^2 \rangle \leq 2Dt. \quad (6)$$

The upper bound clearly implies that $\langle p^2 \rangle$ increases at most linearly as diffusion persists. The lower bound is useful when $D > 1$ since then it shows that $\langle p^2 \rangle \propto t$. We now turn to analyze the cases $D < 1$ and $D > 1$ separately since they exhibit very different behaviors.

The case $D < 1$.—We first consider the more interesting case $D < 1$ where a normalizable steady state Eq. (3) exists. For large but finite times the latter describes well the central part of $W(p, t)$ but not its tails which govern the growth of $\langle p^2 \rangle$ when $1/3 < D < 1$ (for $D < 1/3$ higher order moments diverge and the essential problem remains). We employ the scaling ansatz [11]

$$W(p, t) \sim t^\alpha f(p/\sqrt{t}) \quad (7)$$

which holds for large p and long t and the exponent α will be soon determined. Let us introduce the scaling variable $z = p/t^{1/2}$. This is the typical scaling of Brownian motion, which indicates that for large p diffusion is in control; however, as we now show, $f(z)$ is far from a Gaussian so the process is clearly not simple diffusion. Inserting Eq. (7) in the Fokker-Planck Eq. (1) and using $p \gg 1$ we find

$$D \frac{d^2 f}{dz^2} + \left(\frac{1}{z} + \frac{z}{2} \right) \frac{df}{dz} - \left(\alpha + \frac{1}{z^2} \right) f = 0. \quad (8)$$

For small z we get $f \sim z^{-1/D}$ or $f \sim z$; the latter is rejected since $f(z)$ cannot increase with z . To find α we require that the small z solution matches the steady state, since the latter describes well the density in the center. Using Eq. (7) with $f \propto z^{-1/D}$ we have $W(p, t) \propto t^{\alpha+1/(2D)} p^{-1/D}$ which is to be matched with the steady state solution Eq. (3) $W_{\text{eq}} \propto p^{-1/D}$. Hence; $\alpha = -\frac{1}{2D}$. Then, one solution of Eq. (8) is immediate: $f(z) = Az^{-1/D}$. While this solution has the correct small z behavior it does not decay quickly enough at large z [12], so we need the second solution:

$$f(z) = Az^{-1/D} \int_z^\infty s^{1/D} e^{-s^2/4D} ds. \quad (9)$$

The constant A is found by matching the small z solution Eq. (9) to the steady state solution Eq. (3). Solving the integral in Eq. (9) we reach our first main result

$$f(z) = \frac{\mathcal{N} z^{-1/D}}{\Gamma(\frac{1+D}{2D})} \Gamma\left(\frac{1+D}{2D}, \frac{z^2}{4D}\right), \quad (10)$$

where $\Gamma(a, x) = \int_x^\infty e^{-s} s^{a-1} ds$ is the incomplete Gamma function [13] and $\Gamma(a)$ is the Gamma function. For small and large z we find

$$f(z) \sim \begin{cases} \mathcal{N} z^{-1/D} & z \ll 2\sqrt{D} \\ \frac{\mathcal{N}(4D)^{(1/2)-(1/2D)}}{\Gamma(\frac{1+D}{2D})} z^{-1} e^{-z^2/4D} & z \gg 2\sqrt{D}. \end{cases} \quad (11)$$

Equation (10) is non-normalizable since according to Eq. (11) $f(z) \sim z^{-1/D}$ and hence $\int_0^\infty f(z) dz = \infty$.

Infinite covariant density.—We call the non-normalizable solution Eq. (10) an infinite covariant density. In Fig. 1 comparison is made between our analytical solution Eq. (10) and numerical solutions of the Fokker-Planck equation. As time increases, the solution in the scaled coordinate approaches the infinite covariant density Eq. (10), which describes the asymptotic scaling solution of the probability density. For any finite long time t , expected deviations (which we soon characterize via a uniform approximation) from the infinite covariant solution are found for small values of z (see Fig. 1). These deviations become negligible at $t \rightarrow \infty$; however they are important since they indicate that the pathological divergence of $f(z)$ on the origin is slowly approached but never actually reached; namely, the solution is of course normalizable for finite measurement times.

The variance $\langle p^2 \rangle$.—Even though the solution Eq. (10) is non-normalizable, it can be used to find the second moment $\langle p^2 \rangle$. To see this we introduce a cutoff p_c above which our solution Eq. (10) is valid. The variance is calculated using the symmetry $W(p, t) = W(-p, t)$

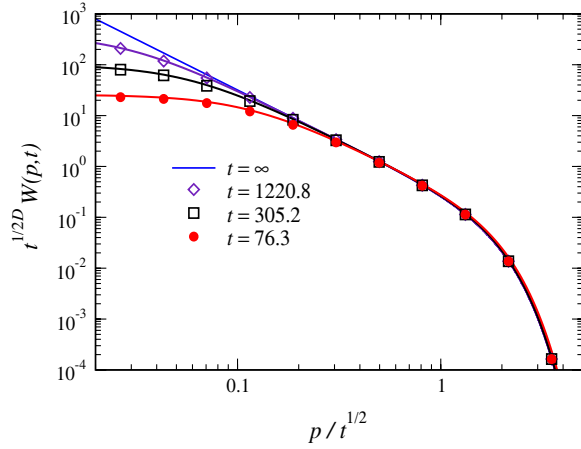


FIG. 1 (color online). We show that $f(z) = t^{1/(2D)}W(p, t)$ (with $z = p/t^{1/2}$) obtained from numerical integration of the Fokker-Planck equation converges towards the infinite covariant density [solid blue $t = \infty$ curve Eq. (10)]. Thus the asymptotic behavior of the system is *not* globally determined by the standard steady state solution. Notice that for $t \rightarrow \infty$, $f(z) \sim z^{-1/D}$ for small z and hence in the long time limit the infinite covariant density $f(z)$ is non-normalizable. For finite times simulations (symbols) and the uniform approximation Eq. (17) (curves) perfectly match. Here $D = 1/2$ and initially $W(p, t = 0)$ is a delta function centered on the origin.

$$\langle p^2 \rangle = 2 \int_0^{p_c} p^2 W(p, t) dp + 2 \int_{p_c}^{\infty} p^2 W(p, t) dp. \quad (12)$$

The first term in Eq. (12) is a constant and can be neglected once the second term is shown to increase with time. Inserting the infinite covariant solution Eq. (10) in the second term of Eq. (12)

$$\langle p^2 \rangle \sim 2t^{(3/2)-(1/2D)} \int_{p_c/\sqrt{t}}^{\infty} z^2 f(z) dz \quad (13)$$

for $1/3 < D < 1$. The lower limit in the integral $p_c/t^{1/2}$ goes to zero when $t \rightarrow \infty$ and the diffusion is anomalous

$$\langle p^2 \rangle \sim 2t^{(3/2)-(1/2D)} \int_0^{\infty} z^2 f(z) dz. \quad (14)$$

Thus the infinite covariant density yields the anomalous diffusion in this model. While $f(z) \sim z^{-1/D}$ for small z and is hence non-normalizable, the integral in Eq. (14) is finite: the z^2 cures the pathology of the density at the origin. Solving the integral in Eq. (14) as well as the diffusive regime soon to be discussed we obtain

$$\langle p^2 \rangle \sim \begin{cases} \frac{D}{1-3D} & D < \frac{1}{3} \\ \frac{16\mathcal{N}}{2^{1/D}\Gamma(\frac{1+D}{2D})} \frac{D}{3D-1} (Dt)^{(3/2)-(1/2D)} & \frac{1}{3} < D < 1 \\ 2(D-1)t & 1 < D. \end{cases} \quad (15)$$

For $D < 1/3$, $\langle p^2 \rangle$ is time independent and is determined by the steady state solution Eq. (3). For the intermediate regime $1/3 < D < 1$ the diffusion is anomalous, while for $D > 1$ it is normal in agreement with the bounds, Eq. (6).

In Fig. 2, numerical solutions for $\langle p^2 \rangle$ versus time exhibit convergence towards these types of behavior.

A simple argument for the anomalous scaling in Eq. (15), for $1/3 < D < 1$, is found by noticing that the steady state solution Eq. (3) describes the center part of the PDF with a diffusion determined cutoff, $|p| < \sqrt{Dt}$:

$$\begin{aligned} \langle p^2 \rangle &\propto \int_{-\sqrt{Dt}}^{\sqrt{Dt}} p^2 W_{\text{eq}}(p) dp \propto 2 \int^{\sqrt{t}} p^{2-1/D} dp \\ &\propto t^{(3/2)-(1/2D)}. \end{aligned} \quad (16)$$

To characterize the distribution of p and to find $\langle p^2 \rangle$ exactly, we need the infinite covariant density which cannot be obtained by similar simple scaling arguments.

A uniform approximation is now presented which works well for long though finite times and for all p . Noticing that the solution for not too large p is given by the steady state, while the tails of $W(p, t)$ are described by the scaling solution we can match both regimes to find

$$W(p, t) \simeq \mathcal{N} (1 + p^2)^{-(1/2D)} \frac{\Gamma(\frac{1+D}{2D}, \frac{p^2}{4Dt})}{\Gamma(\frac{1+D}{2D})}. \quad (17)$$

As shown in Fig. 1 this uniform approximation perfectly agrees with numerical integration already for moderately long time. Equation (17) does not diverge at the origin, still as demonstrated in Fig. 1 the solution approaches the infinite covariant density.

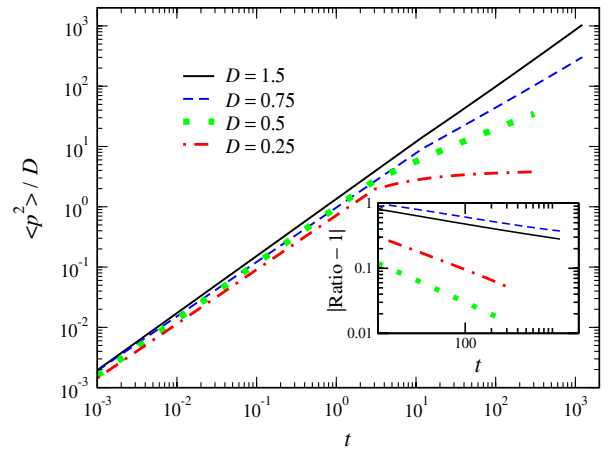


FIG. 2 (color online). In the long time limit the variance $\langle p^2 \rangle$ exhibits three behaviors: normal diffusion if $D > 1$, anomalous diffusion $\langle p^2 \rangle \sim t^{3/2-1/(2D)}$ if $1/3 < D < 1$ and steady state behavior $\langle p^2 \rangle \rightarrow \text{const}$ for $D < 1/3$. For short times $\langle p^2 \rangle \sim 2Dt$ since then the influence of the force field is negligible (initially particles are at the origin). In the inset we show $|\text{Ratio} - 1|$ versus t where Ratio is the ratio of $\langle p^2 \rangle$ obtained from numerical integration to that given by the asymptotic formula, Eq. (15). A theory (to be published) shows that $|\text{Ratio} - 1| \propto t^{-\epsilon(D)}$ with $\epsilon(D) = \min(|D - 1|/2D, 1/2)$. The inset illustrates that as time increases simulations converge to our asymptotic theory, and that the convergence is slow, e.g., $\epsilon(\frac{2}{3}) = 1/6$.

The case $D > 1$.—In analogy to the previous case, we set $W(p, t) = t^{-1/2}f(z)$ where, again $z = p/\sqrt{t}$. We find

$$f(z) = \frac{z^{-1/D} e^{(-z^2)/4D}}{(4D)^{1-\beta} \Gamma(1-\beta)}, \quad (18)$$

where $\beta = (1 + D)/(2D)$. Roughly speaking the potential is responsible for the accumulation of particles close to the origin which yields the $z^{-1/D}$ factor in Eq. (18). Although the solution Eq. (18) exhibits a divergence at $z = 0$, since now $D > 1$ the solution is normalizable and in this regime we do not find an infinite covariant density.

The role of infinite invariant densities and non-normalizable states in physics is now briefly discussed. Clearly, for particles diffusing freely in space the corresponding steady state is non-normalizable. While the motion of particles in a logarithmic potential shares some features with free particles, e.g., unbounded growth of $\langle p^2(t) \rangle$, the logarithmic potential supports a normalized steady state (when $D < 1$). Thus Brownian motion in a logarithmic potential is unique: a normalized steady state exists besides an infinite covariant density and both are needed to describe the long time behavior of this system. Mathematicians have investigated infinite invariant measures in the context of ergodic theory for many years [8]. More recently, an infinite invariant density [14] was used to calculate subexponential separation of trajectories and entropy production in the well known intermittent Pomeau-Manneville map. In the context of a model of an electron glass, the distribution of eigenvalues of a relaxation matrix was found to be non-normalizable which yields slow relaxations [15]. These routes to infinite densities are all found in systems which exhibit anomalous diffusion [16–18], a connection which demands further investigation.

Thermal systems.—As noted in the introduction, we may consider over-damped Brownian particles coupled to a thermal heat bath with temperature T and get the same results as for the optical lattice. More precisely, consider overdamped Brownian motion in the potential $\epsilon_0 \ln(a^2 + x^2)/2$ and diffusion constant \bar{D} (units m^2/s). From the fluctuation dissipation theorem we have

$$\frac{\partial P(\tilde{x}, \tilde{t})}{\partial \tilde{t}} = \left[\frac{k_b T}{\epsilon_0} \frac{\partial^2}{\partial \tilde{x}^2} + \frac{\partial}{\partial \tilde{x}} \frac{\tilde{x}}{1 + \tilde{x}^2} \right] P(\tilde{x}, \tilde{t}) \quad (19)$$

which after an obvious change of notation is the same as Eq. (1). In Eq. (19) dimensionless time $\tilde{t} = \epsilon_0 \bar{D} t / a^2 k_b T$ and space $\tilde{x} = x/a$ are used. More importantly our results are not limited to one dimension. Indeed an infinite wire of radius b , with uniform charge density per unit length λ yields the logarithmic potential $V(r) = \lambda \ln(r)$ for $r > b > 0$. Such a potential was considered by Manning [5] in the context of ion condensation on a long polyelectrolyte. It is not difficult to show that the radial

Fokker-Planck equation yields behavior similar to ours. We do note that the limit $b \rightarrow 0$ gives different behavior.

Summary.—Steady state solutions are commonly assumed to describe the long time limit of dynamics of many thermal and nonthermal systems. We find that for the widely applicable process of Brownian motion in a logarithmic potential, the infinite covariant density Eq. (10) is needed to characterize the long time solution. Thus, while Boltzmann's equilibrium concepts are important they are clearly not sufficient in this case.

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