Singular diffusion in a confined sandpile

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Abstract – We investigate the behavior of a two-state sandpile model subjected to a confining potential in one and two dimensions. From the microdynamical description of this simple model with its intrinsic exclusion mechanism, it is possible to derive a continuum nonlinear diffusion equation that displays singularities in both the diffusion and drift terms. The stationary-state solutions of this equation, which maximizes the Fermi-Dirac entropy, are in perfect agreement with the spatial profiles of time-averaged occupancy obtained from model numerical simulations in one as well as in two dimensions. Surprisingly, our results also show that, regardless of dimensionality, the presence of a confining potential can lead to the emergence of a power-law tail in the distribution of avalanche sizes.

Introduction. – Physical processes involving anomalous diffusion are typically associated with systems in which the mean square displacement of their elementary units follows a nonlinear power-law relationship with time, \( \sigma^2 \propto t^\alpha \), with an exponent \( \alpha \neq 1 \), in contrast with linear standard diffusion (\( \alpha = 1 \)). Instead of being a rare phenomenon, as suggested by its own denomination, anomalous diffusion, however, appears rather ubiquitously in Nature, playing an important role in a variety of scientific and technological applications, such as fluid flow through disordered porous media [1], surface growth [2], diffusion in fractal-like substrates [3–7], turbulent diffusion in the atmosphere [8,9], spatial spreading of cells [10] and biological populations [11], cellular transport [12], and cytoplasmic crowding in cells [13]. Anomalous diffusion can also manifest its non-Gaussian behavior in terms of nonlinear Fokker-Plank equations [14–18], which is the case, for example, of the dynamics of interacting vortices in disordered superconductors [19–22], diffusion in dusty plasma [23,24], and pedestrian motion [24].

The extreme case of nonlinear behavior in diffusive systems certainly corresponds to singular diffusion. For instance, in some physical conditions, the diffusion of adsorbates on a surface can be strongly nonlinear [25–27], with a surface diffusion coefficient that depends on the local coverage \( \theta \) as, \( D \propto (\theta - \theta_c)^{-\alpha} \). The study of surface-diffusion mechanisms is crucial for the understanding of technologically important processes related with physical adsorption [28] and catalytic surface reactions [29–31]. In particular, a singularity in the coverage dependence of the diffusion coefficient is frequently associated to continuous phase transitions [27].

A direct connection between singular diffusion and self-organized criticality [32] has been disclosed by Carlson et al. [33,34] in terms of a two-state one-dimensional sandpile model with a driving mechanism, where grains are added at one end of the pile and fall off at the other end. Besides exhibiting a self-organized state, the continuum limit of this simple model leads to a nonlinear diffusion equation, where the diffusion coefficient not only depends on the local density, but also displays a singularity at a “critical” density value [33–37]. Indeed, some aspects of this model remain to be elucidated, specially due to the fact that the most prominent sign of criticality, namely long-range power-law spatial correlations, is not present in the original setup of the simulated dynamical system. Here we show that the addition of a confining potential to the two-state sandpile model leads to power-law tails in the distribution of avalanche sizes [38] in both one- and two-dimensional versions of the theoretical model. Moreover, our results reveal that the continuum description of the model contains singular nonlinearities in both the diffusion and drift terms of the resulting partial differential equation for the transport process.

Model formulation. – The microscopic model investigated in this study consists of an one-dimensional lattice
or has a maximum in the region where $h$ on which $N$ particles are placed in such a way that the height $h(i)$ of each site is either 1 or 0 (see fig. 1). At each step, one grain is chosen randomly to move to the left or to the right with equal probability. If the nearest neighbor in the chosen direction is occupied, the grain jumps instantly to the next-nearest neighbor in the same direction. If this site is also occupied, the particle keeps jumping until it finally reaches an empty site $j$ [33]. This type of exchange driving mechanism for closed systems has been previously introduced in the context of fluctuations and local equilibrium in self-organizing systems [34,39]. Here, an external confining potential is applied to the system by introducing a non-uniform transition probability from site $i$ to $j$. Precisely, each site at a position $x_i = i\delta$, with $\delta$ being the lattice spacing, and $\phi(x_i)$ the potential energy. For a given transition, we compute $\Delta\phi_{i,j} = \phi(x_j) - \phi(x_i)$ and use the following Metropolis rules:

$$
\begin{align*}
(h(i) &\rightarrow h(i) - 1) \quad \text{if} \quad \Delta\phi_{i,j} < 0 \quad \text{or} \quad \xi < w = e^{-\beta\Delta\phi_{i,j}}, \\
(h(j) &\rightarrow h(j) + 1) \quad \text{if} \quad \Delta\phi_{i,j} > 0 \quad \text{and} \quad \xi > w,
\end{align*}
$$

where $\xi$ is a uniform random number in the interval $[0, 1]$, $\beta = 1/k_BT$, $T$ is the temperature of the thermal reservoir in contact with the system, $k_B$ is the Boltzmann constant, and we count one unit of time for every $N$ grains moved. The effect of decreasing the temperature is equivalent to increasing the strength of the external potential.

A continuum limit for this microscopic model can be obtained rigorously. If we let $\rho_t = \rho(x, t)$, move to the probability that site $i$ located at $x_i$ is occupied at time $t$ and $\phi_t = \phi(x_i)$, a master equation can then be written as

$$
\frac{\partial \rho_t}{\partial t} = -\frac{\rho_t}{\tau} \left\{ \frac{1}{2} \left[ 1 - \rho_{t-j} \right] \min[1, e^{-\beta(\phi_{t-j} - \phi_t)}] \prod_{k=1}^{j-1} \rho_{t+k} \right. \\
+ \left. \frac{1}{2} \sum_{j=1}^{\infty} \left[ 1 - \rho_{t-j} \right] \min[1, e^{-\beta(\phi_{t-j} - \phi_t)}] \prod_{k=1}^{j-1} \rho_{t+k} \right\} \\
+ \frac{1}{2} \sum_{j=1}^{\infty} \left[ 1 - \rho_{t-j} \right] \min[1, e^{-\beta(\phi_{t-j} - \phi_t)}] \prod_{k=1}^{j-1} \rho_{t-k} \\
+ \frac{1}{2} \sum_{j=1}^{\infty} \min[1, e^{-\beta(\phi_{t-j} - \phi_t)}] \prod_{k=1}^{j} \rho_{t+k} \\
+ \frac{1}{2} \sum_{j=1}^{\infty} \min[1, e^{-\beta(\phi_{t-j} - \phi_t)}] \prod_{k=1}^{j} \rho_{t-k}
\right\},
$$

where $\tau$ is the average time between transitions. The first term on the right side is the transition rate corresponding to site $i$ being occupied at time $t$ and loosing the grain, while the second term accounts for the transition rate for an empty site $i$ to gain a grain. To obtain a continuum equation, we take the limit of (1) where $\delta$ and $\tau$ go to zero, while $D = \delta^2/(2\tau)$ is kept constant. In this way, and keeping terms of order up to $\delta^2$, we arrive at the following non-linear diffusion equation:

$$
\frac{\partial \rho}{\partial t} = D \frac{\partial}{\partial x} \left\{ (1 + \rho) \frac{\partial \rho}{\partial x} + (1 + \rho) \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} \right] \phi \right\}.
$$

Details of this derivation can be found in next section. Equation (2) can be related to a nonlinear Fokker-Planck equation (FPE) of the form,

$$
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left\{ \Omega(\rho) \frac{\partial \rho}{\partial x} \right\} - \frac{\partial}{\partial x} [A(x) \Psi(\rho)],
$$

with $\Omega(\rho) = D(1 + \rho)/(1 - \rho)^2$, $A(x) = -d\phi(x)/dx$, and $\Psi(\rho) = D\beta(1 + \rho)/(1 - \rho)^2$. Considering the FPE (3), with $dF/d\rho \leq 0$, where $F = U - \gamma S$, $U = \int d\rho \rho(x,t) \phi(x)$, and the entropy taken in a general form as $S[\rho] = \int dx \gamma(\rho(x))$, with $g(0) = g(1) = 0$ and $d^2g/d\rho^2 \leq 0$, we obtain [22,40]

$$
-\gamma \frac{d^2g(\rho)}{d\rho^2} = \frac{\Omega(\rho)}{\Psi(\rho)} = \frac{1}{\beta \rho(1 - \rho)},
$$

for which the entropy $S[\rho] = \int dx g[\rho(x)]$ reduces to the entropy of a Fermi gas, with $\gamma = T$. The functional $\Omega(\rho)$ physically corresponds to a diffusion coefficient which depends on $\rho(x, t)$. Clearly it diverges for $\rho = 1$ and the diffusion coefficient has the same form as for the case without the external potential [33]. The functional $\Psi(\rho)$ is related to a drift due to the external potential, and also diverges for $\rho = 1$.

The stationary state solution for eq. (2) can be readily obtained by imposing that $\partial \rho/\partial t = 0$, and both $\partial \rho/\partial x$ and $\partial \rho/\partial x$ go to zero as $x \to \pm \infty$. Also, since the dynamics of eq. (2) should maximize the Fermi entropy (5), we should expect the stationary distribution of the confined system to converge to equilibrium, therefore, $\rho(x)$ should converge to the Fermi distribution

$$
\rho_{\text{st}}(x) = \frac{1}{1 + e^{\beta(\phi(x) - \mu)}},
$$

where the integration constant $\mu$ relates to the chemical potential, and can be determined by the normalization

$$
\int_{-\infty}^{\infty} \rho(x,t)\, dx = N.
$$
Derivation of the continuous equation. – Treating \( \rho \) as a continuous function in time \( \rho_i(t = n\tau) \equiv \rho_i(n) \), we can write explicitly the master equation of our process as shown in eq. (1),

\[
\frac{\partial \rho_i}{\partial t} = \frac{1}{2\tau}(1 - \rho_i) \sum_{k=1}^{\infty} [S_k^+ + e^{-\beta\Delta\phi_{i-k,1}}S_k^-] - \frac{1}{2\tau} \rho_i \sum_{k=1}^{\infty} [(1 - \rho_{i+k})e^{-\beta\Delta\phi_{i+k,1}}S_k^- - \rho_{i-k} S_k^- + (1 - \rho_{i-k})S_k^-],
\]

(8)

where \( \Delta\phi_{i,j} = \phi_j - \phi_i \), and \( S_k^\pm = \prod_{j=1}^k \rho_{i\pm j} \). We can expand the factor \( e^{-\beta\Delta\phi_{i-k,1}} \) up to second order to obtain

\[
\frac{\partial \rho}{\partial t} = \frac{1}{2\tau} \sum_{k=1}^{\infty} [S_k^+ + S_k^- - \rho(S_k^+ - S_k^-)] - \frac{\beta\delta^2}{2\tau} \sum_{k=1}^{\infty} k [S_k^- - \rho S_k^- - \rho(S_k^- - S_k^+)] + \frac{\beta\delta^2}{4\tau} \sum_{k=1}^{\infty} k^2 [S_k^- - \rho S_k^- + \rho(S_k^+ - S_k^+)] + \frac{\beta^2 \delta^4}{4\tau} \sum_{k=1}^{\infty} k^2 [S_k^- - \rho S_k^- - \rho(S_k^- - S_k^+) - (S_k^+ - S_k^+) By approximating \( \rho_i \) as a continuous function in space \( \rho(x = \delta x, t) = \rho_i(t) \), we can expand it in a Taylor series to obtain

\[
S_k^\pm = \rho^k + \rho^{k-1} \left[ \frac{\pm k(k+1)}{2!} \delta \rho' + \frac{k(k+1)(2k+1)}{6} \delta^2 \rho'' \right] + \rho^{k-2} \left[ \frac{1}{24} k(k+1)(3k^2 - k - 2) \delta^2 \rho'^2 \right],
\]

(9)

where \( \rho' = \partial \rho/\partial x \) and \( \rho'' = \partial^2 \rho/\partial x^2 \). The careful evaluation of the sums neglecting, again, terms of order superior to \( \delta^2 \) yields our continuum formulation, eq. (2), where we define \( D = \lim_{\delta \to 0} \frac{\delta^2}{8\tau} \). The case for \( \delta \rho/\delta x < 0 \) can be evaluated in a similar manner to obtain the same final result.

Results and discussion. – As shown in fig. 2, the solution (6) is in excellent agreement with the spatial profiles of time-averaged occupancy obtained from numerical simulations for distinct forms of the potential, namely, \( \phi(x) = \kappa |x|^n \), \( n = 1, 2, 3 \) and \( 4 \), and different values of \( \kappa \) (or temperature). As the strength of the confining potential increases (or the temperature decreases), the maximum occupancy density at the center of the potential approaches unity, \( \rho_{\text{ma}} \approx 1 \), and the peak in the profile becomes narrower. At this point, since the density can not increase further, any additional confinement leads to more sites with a maximum average occupancy, resulting in the characteristic step shape of the Fermi-Dirac distribution.

The confining potential substantially changes the way grains jump to the nearest empty site. Here a jump from site \( i \) to \( j \) corresponds to an avalanche of size \( |j - i| \). The average distribution of avalanches with size \( s \) is shown in fig. 3 for the case where \( \phi(x) = \kappa |x| \), and different values of \( \kappa \). As depicted, the distribution is an exponential decay.
for small values of $\kappa$, in agreement with the derivation for the two-state sandpile model without confinement [33]. By increasing $\kappa$ large avalanches become more probable, since the confinement favors the occurrence of large clusters of grains near the center of the potential. For a specific value of $\kappa \approx 12.4$ the average occupancy near the center of the potential approaches 1, and the avalanche size distribution exhibits a power-law characteristics for a wide range of sizes. Further increase in the confinement parameter $\kappa$ eventually leads to the occurrence of a very large cluster, with near all the grains, located at the center of the symmetrical potential. In this situation, only two types of jumps are likely to occur, either the particle performs a small jump near the border or it travels all the way from one side to the other side of the system. As a result, a pronounced peak for $s/N \sim 1$ becomes evident in the avalanche size distribution.

To obtain the probability $P(s)$ for an avalanche of size $s$, we can identify

$$P(s) = \sum_{i=\infty}^{\infty} \left( \prod_{k=i}^{i+s-1} \rho(k|i) \right) (1 - \rho(i + s|s)) \Theta_{i+s,i},$$ \hspace{1cm} \(11\)

where $\Theta_{i+s,i} = \min(1, e^{-\beta(\phi_{i+s} - \phi_{i})})$, and, considering the symmetry, we are summing over avalanches to the right, and $\rho(k|m)$ is defined as the probability of finding the $k$th site occupied, given that the $m$ previous sites have been also found occupied. Note that $\rho(k|m)$ is different from the original particle distribution $\rho_k$, that is, the fact that we know the $m$ previous sites were occupied, changes the probability of finding the next one occupied. One should note that, in the limit where $m = N$; if the previous $N$ sites had a particle, then the next one has to be empty and $\rho(k|N) = 0$, independent of $k$. We can expect $\rho(k|m)$ to follow the Fermi distribution, however, the chemical potential $\mu(k|m)$ has to be determined by a modified normalization constraint:

$$\sum_{i=-\infty}^{k-m-1} (1 + \exp(\phi_i - \mu(k|m)))^{-1} + \sum_{i=k}^{\infty} (1 + \exp(\phi_i - \mu(k|m)))^{-1} = N - m.$$ \hspace{1cm} \(12\)

To obtain $\mu(k|m)$ we do not need to sum over the $m$ sites we know are occupied, and the normalization have to account only for the remaining $N - m$ particles.

Equations (11) and (12) may be used to compute the probability of avalanches for any potential, however, inverting eq. (12) to obtain $\mu$ may not be that simple. In the case of a linear potential, $\phi(x) = \kappa|x|$, this can be done by approximating the sums in eq. (12) to solvable integrals, \(\sum_{i=j}^{j+1} \rho_i \approx 5^{-1} \int_{j-1/2\delta}^{j+1/2\delta} \rho(x)dx\). If the avalanche we are considering does not jump over $x = 0$, that is $k < 0$ or $k - m > 0$, we obtain a cubic equation in $e^{\kappa|k|m|}$:

$$\left(1 + e^{\kappa N} \right)^{-1} \left(1 + e^{\kappa N} \right) e^{\kappa N}\left(1 + e^{-\kappa(k+1/2)}\right) - e^{\kappa N} \left(1 + e^{\kappa N} \right) e^{\kappa N} = 0.$$ \hspace{1cm} \(13\)

Equations (13) and (14) have only one positive real root that can be identified as $e^{\Delta\phi}$, from which we can compute the avalanche size distribution. In fig. 3 we compare the avalanche size distributions obtained in this way with results from numerical simulations of the model. The excellent agreement found confirms the precision of this approach.

From the probability of each possible jump, we can evaluate the energy fluctuation $\langle \Delta\phi^2 \rangle$ as the average squared potential difference in each event. In fig. 4 we show the dependence of $\langle \Delta\phi^2 \rangle$ on the confining parameter $\kappa$ for different number of particles. As one can observe, for each $N$, there is a specific value $\kappa^*$ where $\langle \Delta\phi^2 \rangle$ is maximum. We show in fig. 5 the corresponding avalanche size
distributions for these values of $\kappa^*$. The obtained results can be collapsed onto a single universal curve using the values of $N$ and $\kappa^*(N)$, as shown in the inset of fig. 5. It is precisely at this condition that the avalanche size distribution presents a power-law shape. Moreover, as shown in the inset of fig. 5, the values of $\kappa^*$ can be used to collapse onto a single universal curve all the distributions obtained for different numbers of particles.

Next we extend our results to two-dimensional systems. In this case, a grain at position $\mathbf{r}_i = (x_i, y_i)$ moves in a randomly selected direction until it finds the nearest empty site. The transition is then accepted or not following the same Metropolis algorithm previously described for the 1D case, but now with a confining parabolic potential of the form, $\phi(\mathbf{r}_i) = \kappa(x_i^2 + y_i^2)$. Figure 6 shows the radial profile of the average occupancy, $\rho(r)$, for two-state two-dimensional sandpiles confined by a parabolic potential. The number of particles is $N = 100000$ and different curves correspond to distinct values of the potential strength $\kappa$. The solid lines correspond to the Fermi distribution obtained without fitting parameters, calculated for different values of $\kappa$ and $\beta = 1$. In all simulations, we use $\delta = 1/\sqrt{N}$.

The qualitative behavior of the system is the same as in 1D, namely, the stronger the confining potential, the narrower the profile with the maximum occupancy at the center of the potential approaching unit. Further increasing $\kappa$, the occupancy saturates at $\rho \sim 1$ and the profile becomes broader, resembling a step function. Also shown in fig. 6 are typical snapshots of the grain positions for the same values of $\kappa$, colored according to the size of the clusters they belong to. If the confinement is weak, all sizes of clusters are present, with larger clusters located at the center of the potential. As $\kappa$ increases, larger and more compact clusters are favored at the center of the potential, tending to a limit where most of the grains belong to a single, compact cluster with an irregular surface.

As for the one-dimensional case, the results in fig. 6 computed for distinct confinement strengths show that the average radial profiles of occupancy in 2D are perfectly consistent with the Fermi-Dirac distribution, but now subjected to the normalization condition, $\int_0^\infty \frac{\rho(r)\rho^\kappa}{\kappa\rho^\kappa}dr = N \Rightarrow \mu = \frac{1}{\beta} \ln(e^{\beta \frac{\kappa}{2} \chi^2} - 1)$. This excellent agreement between simulations and the Fermi-Dirac distribution suggests that in two-dimensions the system satisfies the generalization of the FPE (3) to higher dimensions, which is of the form

$$\frac{\partial \rho}{\partial t} = \nabla \cdot [\Omega(\rho)\nabla \rho] - \nabla \cdot [A(\mathbf{r})\Psi(\rho)], \quad (15)$$

where $A(\mathbf{r}) = -\nabla \phi(\mathbf{r})$, with the condition (4) still valid in 2D. As shown in fig. 7, the avalanche size distribution for the two-dimensional system also presents non-trivial properties, with an exponential decay for a weak confining potential. In the case of a strong confining potential, a peak also appears corresponding to avalanches of the order of the system size. Likewise the 1D case, the confining potential, at a specific condition, leads to an avalanche size distribution that follows a power law.

**Conclusions.**—In summary, here we studied the effect of a confining potential on the behavior of a two-state sandpile model in one and two dimensions. A continuum nonlinear diffusion equation could be derived from the microdynamical description of the model that is shown to be perfectly consistent with the transport of grains observed from numerical simulations. This equation, besides displaying singularities in both the diffusion and drift terms, has a stationary-state solution for the spatial profiles of average occupancy of grains that maximizes the Fermi-Dirac entropy. Moreover, our results show that...
the introduction of a confining potential to the two-state sandpile model, if properly tuned, can lead to power-law behavior in the distribution of grain-jump sizes. These results are rather surprising since 1D systems usually do not display non-trivial critical states nor power-law behavior. They can be explained in terms of the non-homogeneity introduced by the confining potential and the complex fluctuations due to the singular-diffusion dynamics. The extension to two-dimensions reveals that the strongly non-linear features of the system together with the intrinsic exclusion mechanism present in the model also lead to the Fermi-Dirac distribution for the occupancy profiles. Power-law distributions of avalanches sizes are also observed in 2D at specific values of the intensity of the confining potential.

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