Neutron clustering: spatial fluctuations in multiplying systems at the critical point

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Abstract - We investigate the spatial fluctuations of a neutron population close to criticality: the interplay between random births and deaths leads to a spontaneous clustering of the diffusing individuals. By resorting to a statistical mechanics approach, we determine the behaviour of the average neutron neutron density, the pair correlation function and other relevant physical observables. When the individuals are left free to evolve, their ultimate fate is the so-called critical catastrophe, i.e., extinction. When a global constraint is imposed on the total number of individuals, the impact of clustering on diffusion depends on the competition between the time required for a neutron to explore the whole reactor, and the time over which the population has undergone a full generational renewal. In order to illustrate these results, exact formulas and scaling functions are derived for a simple model of nuclear reactor and are compared to Monte Carlo simulations.

I. INTRODUCTION

Self-sustaining chains of neutrons in multiplying assemblies form a prototypical example of a system operating at the critical point [1, 2]. At criticality, which means when births by fission are exactly compensated by losses by capture and leakage, the competition between the fluctuations stemming from birth-death events and those stemming from random displacements subtly affects the spatial distribution of the particles in such systems. This is particularly important during reactor start-up using weak sources: although the population may eventually rise to a level where fluctuations are negligible, yet their effect might persist for long times due to the impact on the initial conditions [2]. The analysis of this statistical behaviour can be carried out by developing the evolution equations for the first few moments of the neutron population, whose foundations were established by Pál and Bell [3, 4], based on earlier pioneering contributions by Kolmogorov and co-workers [5]. For a thorough review, see, e.g., [1, 2].

The physical mechanisms underlying the complex nature of the Pál-Bell equations can be probed by Monte Carlo simulation [6, 7]. In particular, it has been recently shown that at and close to the critical point a collection of neutrons, although spatially uniform at the initial time, may eventually display a highly non-Poisson patchiness, as shown in Fig. 1.

The emergence of such neutron clustering due to the competition between fission, capture and diffusion has been first investigated in [6], based on a formal analogy with the behaviour of ecological communities [8, 9, 10, 11, 12], and later extended to take into account finite-size effects [13], population control [14] and the impact of delayed neutrons [15]. In this work we will revisit the basic findings about neutron clustering and single out the key ingredients that govern the spatial fluctuations.

II. A SIMPLE MODEL OF A MULTIPLYING SYSTEM

In order to illustrate the features of neutron clustering, we will introduce a simplified model of a multiplying system that yet retains all the key physical ingredients. Neutrons will be represented as a collection of particles undergoing random diffusion, reproduction and capture within a homogeneous d-dimensional box of finite volume $V = L^d$, $L$ being the linear size. To simplify the matter, the box will have perfectly reflecting boundaries. The stochastic paths of neutrons are known to follow position and velocity dependent exponential flights [2]. For our model, we approximate these paths by d-dimensional branching Brownian motions with a constant diffusion coefficient $D$ [5]. The diffusing walkers undergo capture at rate $\gamma$ and reproduction at rate $\beta$. In this latter case, the neutron disappears and is replaced by a random number $k$ of descendants, distributed according to a law $p_k$ with average $\nu_1 = \sum_k k p_k$. We are assuming here that all fission neutrons are prompt, so as to keep notation to a minimum: the effects
of precursors will be included later.

At the critical point, we must have \( \gamma = \beta (v_1 - 1) \), i.e., losses compensate births. In this regime, the Galton-Watson theory [5] shows that the ensemble-averaged extinction time \( \mathbb{E}[t_E] \) of the whole population is infinite \(^1\). However, the variance of total number \( N(t) \) of particles in the system grows linearly in time, i.e., \( \sigma^2_t[N] = \mathbb{E}[N^2(t)] - \mathbb{E}^2[N(t)] \propto \beta N t \), whereas the average \( \mathbb{E}[N(t)] = N_0 \) stays constant [5]. This implies that the typical fluctuations of the whole population size, say \( \sigma_t[N] \), will become comparable to the average value \( N_0 \) over a characteristic time \( t = N_0 / \beta \); then, a single fluctuation is capable of killing the entire population [5]. In the context of reactor physics, the extinction of the fission chains at criticality goes under the name of critical catastrophe [2].

In the following, we will show how the interplay between fluctuations on the particle number and diffusion locally affects the spatial distribution of neutrons within the box.

### III. THE PHYSICAL OBSERVABLES

Let us denote by \( n(x, t) \) the instantaneous density of neutrons located at \( x \) at time \( t \). The evolution equations for the statistical moments of \( n(x, t) \) can be derived by resorting to the Pál-Bell equations [1], which can be regarded as a particular case of the more general Feynman-Kac path-integral approach [13]. Both strategies are based on the reciprocity property of random walks [16, 1, 2]; the idea is to write down the equations governing the probability generating functions for \( n(x, t) \), from which the average particle density and the correlations can be obtained by simple derivation (some hints are provided in the Appendix).

Let us denote by \( G_t(x; x_0) \) the Green’s function satisfying the backward equation

\[
\frac{\partial}{\partial t} G_t(x; x_0) = L^*_t G_t(x; x_0),
\]

where

\[
L^*_t = D \nabla^2 x_0 + \beta (v_1 - 1) - \gamma,
\]

with the boundary conditions of the problem at hand and the initial condition \( G_0(x; x_0) = \delta(x - x_0) \). Intuitively, the Green function physically represents the average number of particles appearing at \( x \) at time \( t \) for a single particle started at \( x_0 \) at \( t = 0 \), or equivalently the average number of particles originally present at \( x_0 \) at \( t = 0 \) for a single particle detected at \( x \) at time \( t \), by the reciprocity theorem [16]. The average neutron density \( \psi_t(x) \) at a point \( x \) can be expressed as

\[
\psi_t(x) = \mathbb{E}[n(x, t)] = N \int dx_0 q(x_0) G_t(x; x_0), \tag{4}
\]

where \( N \) is the number of individuals composing the initial neutron population, and \( q \) is the spatial probability distribution function of each neutron at time \( t = 0 \) (assuming independence) [13]. For a critical reactor, \( \beta (v_1 - 1) = \gamma \) and we thus have \( L^*_t = D \nabla^2 x_0 \). In order to simplify the forthcoming discussion, it is convenient to require that the initial spatial distribution in the box is uniform, namely, \( q = 1/V \). This corresponds to taking the population at equilibrium compatibly with the assigned mass-preserving boundary conditions at \( t = 0 \). Then, from Eq. (4) we would therefore have a flat average density \( \psi_t(x) = N/V = \psi_0 \) at any time, insensitive to local fluctuations.

The analysis of the spatial inhomogeneities shown in Fig. 1 can be carried out by resorting to the two-point correlation function \( h_t(x, y) = \mathbb{E}[n(x, t)n(y, t)] \), which is proportional to the joint probability density for particle pairs simultaneously occupying positions \( x \) and \( y \) [1, 2]. The correlation length can be extracted from the shape of the function \( h \); if \( h \) is almost flat in space, then the correlations will have the same relevance at any spatial site; on the contrary, spatial clustering will be mirrored in a peak at \( x = y \), i.e., an increased probability of finding particles lying at short distances [13, 14]. The overall intensity of the correlations is simply provided by the amplitude of \( h \).

The function \( h_t(x, y) \) can be generally written as \( h_t = h_t^{id} + h_t \), where \( h_t^{id} \) is the contribution from independent trajectories, and \( h_t \) is the contribution of the trajectories correlated via a fission event. For the former, we have

\[
h_t^{id}(x, y) = c_N \psi_0(x) \psi_t(y) + \psi_t(x) \delta(x - y), \tag{5}
\]

including self-correlations, where \( c_N = (N - 1)/N \approx 1 \) for large \( N \gg 1 \) [13]. For the latter, we have

\[
h_t(x, y) = \int_0^t dt' \int dx \mathcal{P}_t(x, t'; y) \mathcal{G}_{t'-t}(x; x') \mathcal{G}_{t'-t}(y; y'), \tag{6}
\]

where \( \mathcal{P}_t(x, t) = \beta v_2 \psi_t(x) \) is the average rate of appearance of particle pairs at position \( x \) and time \( t \), the coefficient \( v_2 = \sum_k k(k - 1) p_k \) being the mean number of pairs created at each fission [13]. For an exactly critical system, assuming again \( q = 1/V \), we have \( \mathcal{P}_t(x, t) = \beta v_2 \psi_0 \), and the pair correlation function thus yields

\[
h_t(x, y) = h_t^{id}(x, y) + \beta v_2 \psi_0 \int_0^t dt' \mathcal{G}_{t'}(x; y), \tag{7}
\]

where we have used the Markov property of the Green’s functions, namely,

\[
\int dx' \mathcal{G}_t(x; x') \mathcal{G}_t(y; y') = \mathcal{G}_t(x; y). \tag{8}
\]

Actually, it is customary to introduce the (dimensionless) normalized and centered pair correlation function \( g \) [12], namely,

\[
g_t(x, y) = \frac{h_t(x, y) - h_t^{id}(x, y)}{\psi_t(x) \psi_0(t)}. \tag{9}
\]

When particles trajectories are very weakly correlated, \( h_t(x, y) \sim h_t^{id}(x, y) \) and thus \( g_t \approx 0 \); we will therefore have Poisson fluctuations. When \( g_t \approx 1 \), the typical local fluctuations will be comparable to the average local density \( \psi_t \). From Eqs. (7) and (9), for an exactly critical system we have

\[
g_t(x, y) = \frac{\beta v_2}{\psi_0} \int_0^t dt' \mathcal{G}_{t'}(x; y). \tag{10}
\]

The amplitude of \( g_t \) decreases with increasing particle density \( \psi_0 \) and with decreasing fission rate \( \beta \), as expected on physical grounds.
IV. INCLUDING DELAYED NEUTRONS

The coupled stochastic evolution of neutrons and precursors can be modelled as a multi-type Galton-Watson reproduction process [2, 5]: the parent neutron disappears and is replaced by a random number \(k_p\) of prompt neutrons, behaving as the parent particle, and a random number \(k_d\) of precursors, with joint probability \(p_{k_p,k_d}\) [1, 2]. We will denote by \(\lambda\) the rate at which a precursor decays to a delayed neutron. When delayed neutrons are considered, the system is critical if \(\beta_v (v_p + v_d - 1) = \gamma\), where \(v_p = \sum_{k_p} k_p p_{k_p,k_d}\) is the average number of prompt neutrons emitted per fission, and \(v_d = \sum_{k_d} k_d p_{k_p,k_d}\) is the average number of precursors created per fission.

Similarly as done for prompt neutrons alone, we will assume that the neutron and precursor populations are at equilibrium within the box at \(t = 0\). The analysis of the statistical moments of the neutron population in the presence of precursors can be again carried out by resorting to the backward approach based on probability generating functions. However, the multi-type branching process will give rise to a system of two coupled equations to be solved simultaneously (see the Appendix), and the resulting expressions for the moments are particularly cumbersome in their general form. Some simplifications can nonetheless be obtained by observing that the rate \(\beta_v\) at which precursors are created and the rate \(\lambda\) at which precursors are converted to delayed neutrons are actually strongly separated. Setting \(\theta = \lambda/ (\beta_v d)\), for typical nuclear systems we have \(\theta = 10^{-3}\) [1, 2]. This leads to the possibility of introducing singular perturbation techniques, which are amenable to easily understandable results [17].

In particular, it is possible to show that for the average neutron density we have [15]

\[
\psi_t(x) \approx \psi^p_{\theta t}(x),
\]

(11)

where \(\psi^p_{\theta t}(x)\) is the average neutron density for a reactor that was to be run based on prompt neutrons alone (i.e., Eq. (4)). This means that in the presence of precursors the time evolution of \(\psi\) is slowed down by a factor \(\theta\). This behaviour is coherent with the classical findings in reactor control theory.

As for the correlation function, for a critical system the precursors induce a stronger effect [15], namely,

\[
g_t(x,y) \approx \theta g^p_{\theta t}(x,y)
\]

(12)

where \(g^p\) is the correlation function for a reactor that were to be run based on prompt neutrons alone (i.e., Eq. (10)). Precursors are therefore extremely effective in quenching the spatial clustering of the neutrons: the spatial correlation function of the neutron population has a much slower evolution in time \((t \to \theta t)\), and its amplitude is further rescaled by a factor \(\theta\). A rigorous derivation can be found in [15]. Equations (11) and (12) allow transposing the results obtained for \(\psi^p\) and \(g^p\) to the case of systems run with both neutrons and precursors.

V. THE THERMODYNAMIC LIMIT

The so-called thermodynamic limit is attained by considering a large number \(N \to \infty\) of particles in a large volume \(V \to \infty\) [12, 13]. Suppose that the individuals are uniformly distributed in \(V\) at time \(t = 0\), and impose that the limit average particle density \(\psi_0 = N/V\) is finite. At criticality, the Green’s function for a \(d\)-dimensional infinite system without delayed neutrons is the Gaussian density

\[
G_r(x; x_0) = \frac{e^{-x^2}}{(4\pi Dt)^{d/2}},
\]

(13)

which spatially depends only on the relative particle distance \(r = |x - x_0|\). The average particle density is stationary, namely, \(\psi_t(x) = \psi_0\) when starting from a flat initial condition \(q = 1/V\). As for the pair correlation function, from Eq. (10) we get

\[
g_r(r) = \frac{\beta V_v}{8\pi^{d/2} D \psi_0}\, r^{2-d} \Gamma_{d/2-1}\left(\frac{r^2}{8Dt}\right),
\]

(14)

where \(\Gamma_\alpha(z) = \int_0^\infty e^{-u}u^{\alpha-1}du\) is the incomplete Gamma function [12]. The asymptotic time behaviour of Eq. (14) strongly depends on the dimension \(d\): it is known that \(g_r(r) \sim \sqrt{r}\) for \(d = 1\), \(g_r(r) \sim \log(r)\) for \(d = 2\), and \(g_r(r) \sim g_2(r)\) for \(d > 2\),

\[
g_d(r) = \frac{\beta V_v (\frac{d}{2} - 1)}{8\pi^{d/2} D \psi_0} r^{2-d}
\]

(15)

being an asymptotic stationary spatial shape [12, 13]. This means that in low dimension \(d \leq 2\) a critical multiplying system will eventually display clustering \((g_r\textit{ diverges})\), irrespective of the average particle density \(\psi_0\). For \(d \geq 3\), the amplitude of \(g_d(r)\) can be reduced by acting on \(\psi_0\), and clustering can thus be quenched. The dimension-dependent behaviour of \(g_r(r)\) is basically a consequence of Polya’s theorem, which states that random walks in unconstrained domains with \(d > 2\) are transient, i.e., very effective (conversely, particles come back to their starting point almost surely for \(d \leq 2\)).

VI. CONFINED GEOMETRIES

We will now focus on particles evolving in a finite-size \(d\)-dimensional box of linear size \(L\). For the sake of simplicity, we will neglect delayed neutrons. By evoking the separation of variables, \(G_r(x; x_0)\) can be expanded in terms of a discrete sum of eigenfunctions \(\varphi_k\) of the operator \(L^d\) [13], in the form

\[
G_r(x; x_0) = \sum_k \varphi_k(x)\varphi^\dagger_k(x_0)e^{ikx},
\]

(16)

where \(\alpha_k\) are the associated eigenvalues. The functions \(\varphi^\dagger_k(x_0)\) can be explicitly derived from the completeness condition

\[
\sum_k \varphi_k(x)\varphi^\dagger_k(x_0) = \delta(x - x_0),
\]

(17)

and imposing normalization. By applying Neumann boundary conditions, for the \(d\)-dimensional box we have

\[
\varphi_k(x) = \prod_{i=1}^d \cos\left(\pi k_i \frac{x_i}{L}\right)
\]

(18)
of the whole population. When the concentration depends on dimension $d$ the extinction time $\tau_E$ is a bounded function for large $\beta / \nu$. The quantity $\psi_0 = N / V$ of individuals in the population is large (and the system is spatially bounded), it is reasonable to assume that $\tau_E > \tau_D$.

The shape of the rescaled $g_t(x, y)$ depends on the interplay of $\tau_D$ and $\tau_E$ [13], as illustrated in Fig. 2. Immediately after the initial time, $g_t(x, y)$ displays a peak at short distances $x \approx y$, which mirrors the effects of local fluctuations responsible for spatial clustering. The amplitude of the peak is proportional to the dimensionless ratio $\xi = \beta \nu L^2 / (ND) \propto \tau_D / \tau_E$, which precisely reflects the competition between migration and reproduction: the amplitude is smaller for larger $D$ and smaller $\beta$ (for fixed $L$ and $N$), and vice-versa. The width of the peak, which is related to the correlation length of the system, is governed by diffusion, and is a growing function of $D$. For times shorter than the mixing time $\tau_D$, the amplitude of the peak grows due to births and deaths dominating over diffusion, whereas its width increases due to diffusion. When $t \gg \tau_D$, the particles have explored the entire volume, and $\mathcal{H}_t(x, y)$ freezes into a tent-like shape

$$\mathcal{H}_\infty(x, y) = \lim_{t \to \infty} \mathcal{H}_t(x, y) = \beta \nu \psi_0 \sum_{k \neq 0} \frac{\varphi_k(x) \varphi_k(y)}{2 |\alpha_k|}.$$  

The total number of neutrons in the reactor also undergoes global fluctuations, $N$ being finite. This progressively lifts upwards the contribution $\mathcal{H}_\infty(x, y)$ by a spatially flat term (associated to the fundamental mode) that diverges linearly in time as $t / \tau_E$. Finally, for times larger than the extinction time $\tau_E$, $g_t(x, y) > 1$ everywhere. This physically means that, no matter how dense the population is at $t = 0$, neutrons are eventually doomed to extinction within $t \approx \tau_E$: in this respect, statistical equilibrium at the critical point is "a mathematical fiction", as argued in [18]. Including delayed neutrons would not qualitatively change these findings. However, the extinction time $\tau_E \approx \tau_E^p / \theta^2$ would be much longer than $\tau_E^p = N / (\beta \nu)$ corresponding to prompt neutrons alone [15].
VII. FLUCTUATIONS CLOSE TO CRITICALITY

Let us assume that the system is initially at equilibrium with respect to the spatial distribution, with \( q = 1/V \), but criticality is not ensured, i.e., \( \gamma \neq \beta (\nu_1 - 1) \). From Eq. (4) we have thus

\[
\psi_t(x) = \psi_0 e^{\alpha t}.
\]  

(23)

The sign of the fundamental eigenvalue \( \alpha_0 = \beta (\nu_1 - 1) - \gamma \) determines the asymptotic behaviour of the average particle density: when \( \alpha_0 > 0 \) the system is super-critical and the population diverges in time; when \( \alpha_0 < 0 \) the system is sub-critical and the population shrinks to zero. As for the pair correlation function, from Eq. (9) assuming again \( q = 1/V \) we obtain

\[
g_t(x, y) = \frac{\beta v_2}{\psi_0} e^{-\alpha t} \int_0^\infty dt' e^{-\alpha t'} G_{2\nu}(x; y),
\]  

(24)

The ultimate fate of the pair correlation function at long times depends on the rate \( \alpha_0 \) at which the average population is increasing or decreasing. When \( \alpha_0 > 0 \), the pair correlation function for long times asymptotically converges to the constant

\[
g_t(x, y) \rightarrow \frac{\beta v_2}{N \alpha_0},
\]  

(25)

which means that fluctuations will be equally distributed at any spatial scale. The average population is exponentially increasing at a rate \( \alpha_0 \), thus contributing to the mixing of the individuals: for sufficiently large \( N \) one would expect the amplitude of the pair correlation function to be \( g \ll 1 \), and fluctuations to be safely neglected. However, it may still happen that \( g \gg 1 \), when the number of initial particles is \( N \ll \beta v_2 / \alpha_0 \), i.e., basically for small perturbations around criticality, with \( \alpha_0 \approx 0 \). This can be understood as a competition between the growth time constant \( 1/\alpha_0 \) of the average population and the extinction time \( \tau_e = N/(\beta v_2) \): if \( \alpha_0 \) is rather small, strong correlations may have enough time to develop, despite the smoothing effect induced by the appearance of an increasing number of new particles. When \( \alpha_0 < 0 \), the pair correlation function at long times grows unbounded exponentially fast, as \( g_t(x, y) \sim \exp(-\alpha_0 t) \): the average population is rapidly decreasing, which enhances the relative importance of fluctuations due to correlations.

VIII. THE EFFECTS OF POPULATION CONTROL

Multiplying assemblies are typically subject to physical counter-reactions, such as the Doppler effect, which enforce control mechanisms on the neutron population [2]. The simplest way to model such requirement for an exactly critical system is to impose that the total number \( N \) of neutrons is preserved, by correlating birth and death events [8]: at each fission, a neutron disappears and is replaced by a random number \( k \geq 1 \) of descendants, and \( k - 1 \) other neutrons are simultaneously removed from the collection in order to ensure the conservation of total population. The quantity \( \tau_k = N/(v_2 \beta) \) for a constrained system represents the time over which the system has undergone a full population renewal, and all the individuals descend from a single common ancestor [8].

![Fig. 4. Monte Carlo simulation of the evolution of branching Brownian motions in a two-dimensional box with reflecting boundaries, subject to population control. At \( t = 0 \), particles obey a uniform spatial distribution. In case a), the ratio \( \xi \) is close to unit and clustering phenomena dominate over diffusion (however, since the total particle number is preserved, the population can not go to extinction). In case b), the ratio \( \xi \) is ten times smaller and spatial fluctuations are much milder.](image)

The pair correlation function \( \tilde{h}_t(x, y) \) in the presence of population control can be explicitly computed [14]. The probability for a chosen pair of particles at time \( t \) not to have had a common ancestor is \( U(\tau) = e^{-\gamma \tau} \). The correlated contribution \( \tilde{h}_t \) reads then

\[
\tilde{h}_t(x, y) = \int_0^t d\tau' \int dx' \mathcal{P}_\xi(x', t', t) G_{\nu}(x; x') G_{\nu}(x'; y),
\]  

(26)

where

\[
\mathcal{P}_\xi(x', t', t) = \beta v_2 \psi_0(x) U(t - t')
\]  

(27)

is the average rate of appearance of particle pairs at position \( x \) and time \( t' \) when the system is observed at time \( t \), under the aforementioned constraint on the total population [14]. Imposing a uniform source \( q = 1/V \) therefore yields

\[
\tilde{h}_t(x, y) = \beta v_2 \psi_0 \int_0^t d\tau' U(t') G_{\nu}(x; y).
\]  

(28)

The correlation function can thus be written as

\[
\tilde{h}_t = c_\nu \psi_0(\xi(t)) U(t) + \psi_0(\xi(t)) (\xi(x) - \delta(x - y)) + \tilde{h}'_t,
\]  

(29)

and we finally get \( \tilde{h}'_t = \tilde{h}'_t + \mathcal{H}'_t(x, y) \), where

\[
\mathcal{H}'_t(x, y) = \beta v_2 \psi_0 \sum_{k=0}^\infty \frac{1 - e^{-\beta v_2 \tau_k}}{\beta v_2 \tau_k + 2|\xi_k|} \psi_k(\xi)^2(y)
\]  

(30)

is a bounded function for large \( t \). The diverging term in \( \tilde{h}_t \) has been thus suppressed by population control, which is coherent with the findings in [2] concerning the stabilizing effect induced by counter-reactions on neutron fluctuations.

The rescaled pair correlation function \( g'_t(x, y) \) has two distinct regimes when population control is enforced, as illustrated in Fig. 3. Immediately after the initial time, \( g'_t(x, y) \) displays a peak at short distances \( x \approx y \), which is the signature...
of spatial clustering. The amplitude and the width of the peak have the same behaviour as for the function \( g_1(x, y) \) detailed above. Nonetheless, since the number of particles is preserved, the positive correlations at the center of the box imply negative correlations close to the boundaries. The amplitude of the peak grows and its width increases for times shorter than the mixing time \( \tau_D \), analogously as in the previous case. However, global spatial fluctuations are intrinsically suppressed by \( N \) being fixed due to population control. For times larger than \( \tau_D \), \( H^c(x, y) \) converges to an asymptotic tent-like shape

\[
H^c_\infty(x, y) = \lim_{t \to \infty} H^c_\text{id}(x, y) = \beta v_2 \psi_0 \sum_{k \neq 0} \frac{\varphi_k(x) \varphi_k(y)}{\alpha_k^2} + 2|\alpha_k|.
\]

In this regime, the spatial fluctuations are bounded by

\[
|H^c(x, y)| \leq h^c_\text{id} \left[ 1 + \frac{d}{3} + \frac{h^c}{\beta} \right].
\]

In order for the fluctuations to be small and prevent the emergence of spatial clustering, we must therefore have \( \tau_D \ll \tau_E \), which occurs when the typical spatial separation between particles is thoroughly explored within a single generation (see Fig. 4). In a critical system with population control, spatial clustering can be quenched by simply imposing that \( N \) is sufficiently large, for arbitrary values of the other physical parameters.

**IX. SPATIAL CLUSTER DISTRIBUTIONS**

The spatial shape of the particle clusters can be characterized in terms of several moments, namely, the square center of mass

\[
\langle r^2_{\text{com}} \rangle(t) = \left\langle \frac{1}{N} \sum_i r_i(t) \right\rangle^2,
\]

the mean square displacement

\[
\langle r^2 \rangle(t) = \frac{1}{N} \sum_i \langle r_i(t) \rangle^2,
\]

and the mean square distance between pairs of particles

\[
\langle r_p^2 \rangle(t) = \frac{1}{N(N-1)} \sum_{i \neq j} \langle (r_i(t) - r_j(t))^2 \rangle,
\]

where \( r_i(t) \) denotes the position of the \( i \)-th particle in the population. By construction, these three quantities are related to each other by an elegant formula [9]:

\[
\langle r^2_{\text{com}} \rangle(t) + \frac{1}{2} \sum_{i} \langle r^2_i \rangle(t) = \langle r^2 \rangle(t).
\]

The spatial moments can be formally expressed in terms of the average particle density \( \psi(x) \) and of the correlation function \( h(x, y) \). In particular, for the mean square displacement we have

\[
\langle r^2 \rangle(t) = \frac{1}{N} \int |x|^2 \psi(x) dx.
\]
When spatial correlations are weak ($\xi \to 0$), which is obtained for a very large number of particles $N \to \infty$ or a vanishing fission rate $\beta \to 0$, from Eq. (41) we have

$$\langle r_p^2 \rangle_c^\infty \to \frac{d}{6}L^2 = \langle r_p^2 \rangle_{id}$$

and we recover the ideal case corresponding to uncorrelated trajectories. In this case, the center of mass of the population obeys

$$\langle r_{com}^2 \rangle_{id} = \langle r^2 \rangle - \frac{1}{2}N^{-1} \langle r_p^2 \rangle_{id} \approx \frac{1}{N} \langle r^2 \rangle_{id},$$

which basically means that for a collection of independent particles the mean square displacement of the center of mass is equal to the mean square displacement of a single particle of the collection, divided by the number of particles.

When the fission rate $\beta > 0$, we can expand Eq. (41) for a large but finite number of particles $N \gg 1$, which yields

$$\langle r_p^2 \rangle_c^\infty \approx \langle r_p^2 \rangle_{id} \left[ 1 - \frac{\xi}{20} + \cdots \right].$$

This result implies in particular that $\langle r_p^2 \rangle_c^\infty$ will be smaller than in the uncorrelated case because of the effects of spatial clustering. As for the center of mass, we finally get

$$\langle r_{com}^2 \rangle_c^\infty = \langle r_{com}^2 \rangle_{id} \left[ 1 + \frac{\xi}{20} + \cdots \right].$$

Then, $\langle r_{com}^2 \rangle_c^\infty$ will be larger than that of an uncorrelated system.

X. PERTURBING THE INITIAL CONFIGURATION

So far, we have always assumed that the reactor was initially prepared on a spatial distribution proportional to the fundamental eigen-mode, i.e., $q = 1/V$, which was a convenient choice in view of more easily grasping the underlying physical mechanisms. Actually, Eq. (4) for the particle density and Eqs. (7) and (26) for the pair correlation function will hold true for arbitrary initial distributions $q(x_0)$. Instead of considering the full evolution of $\psi_t$ and $h_t$ starting from a given source $q(x_0)$, it is more instructive to address the relaxation to equilibrium starting from a perturbed configuration, for an exactly critical system. Intuitively, the longest-lived perturbation will be obtained when the spatial distribution is proportional to the first excited eigen-mode $\varphi_1$. Let us then assume that the perturbed source is written as

$$q^*(x_0) = \frac{1}{V} [1 + \epsilon \varphi_1(x_0)],$$

where $\epsilon$ is the amplitude of the perturbation, taken so that $q^* \geq 0$. Normalization is trivially satisfied.

Let us now denote the perturbation of the average particle density by $\delta \psi_t(x) = \psi^*(x) - \psi^0(x)$, where $\psi^*_t$ corresponds to the perturbed source $q^*$, and $\psi^0_t$ corresponds to the equilibrium source $q = 1/V$. From Eq. (4), by resorting to the eigen-mode expansion in Eq. (16) and using orthogonality

$$\int d\mathbf{x} \varphi_k(x) \varphi_k^*(x) = \delta_{k,k'},$$

we get

$$\delta \psi_t(x) = \epsilon \varphi_0 \varphi_1(x) e^{\epsilon \tau_D}$$

where for a critical reactor $-\alpha_1 = 1/\tau_D$. This means that the perturbation $\delta \psi_t$ is reabsorbed exponentially fast, with a characteristic time scale equal to the mixing time $\tau_D$: for times $t \gg \tau_D$, the average density asymptotically attains $\psi^*_t \to \psi^0_t$.

As for the pair correlation function, let us similarly denote $\delta h_t = h^*_t - h^{eq}_t$. For a critical system without population control, from Eq. (4), by resorting to the eigen-mode expansion in Eq. (16) and using the orthogonality we get

$$\delta h_t(x,y) \approx \varphi_0 [\delta \psi_t(x) + \delta \psi_t(y)] \left( 1 + \frac{1}{\tau_E} \right)$$

by neglecting terms converging faster. The perturbation $\delta h_t$ is thus also reabsorbed exponentially fast, with a characteristic time scale $\tau_D$. The linear correction is the signature of the diverging term induced by the critical catastrophe. For times $t \gg \tau_D$, the correlation function asymptotically attains $h^*_t \to h^{eq}_t$. When population control in enforced, from Eq. (26) we would get

$$\delta h_t(x,y) \approx \varphi_0 [\delta \psi_t(x) + \delta \psi_t(y)],$$

up to terms converging faster. The rate of convergence is the same as for the previous case, but the linear correction has disappeared. This behaviour is illustrated in Fig. 6 for a critical one-dimensional reactor.
XI. COARSE-GRAINING AND ENTROPY

So far, we have assessed the behaviour of the average particle density and of the pair correlation function by assuming that these quantities can be measured at any point \( x \) within the box. However, some coarse-graining procedure is introduced by the measurement techniques, which are typically performed over a finite-size detector volume [11, 12]. Suppose then that the \( d \)-dimensional box is partitioned into a regular Cartesian grid having \( M \) meshes, and denote by \( k \), the number of individuals found within a given mesh of index \( i = 1, \cdots, M \). In the absence of branching (\( \beta = 0 \)), the particle trajectories are independent: starting from a source \( q = 1/V \) with \( N \) individuals, we would have

\[
\langle k_i \rangle = \int_{V_i} dx \psi_i(x) = \frac{N}{M} \quad (51)
\]

and

\[
\sigma^2[k_i] = \int_{V_i} dx \int_{V_i} dy \hat{y}^\dagger_i(x, y) - \langle k_i \rangle^2 = \frac{N(M - 1)}{M^2}, \quad (52)
\]

for any index \( i \), where we have used \( V/V_i = M \). When \( M \gg 1 \), \( \sigma^2[k_i] \approx N/M \): independently diffusing particles lead to Poisson fluctuations, as expected. The variance-to-mean ratio \( Y_i = \sigma^2[k_i]/\langle k_i \rangle = 1 \) would not depend on the number of meshes used for coarse-graining [1, 2]. These results could have been equivalently obtained by remarking that at equilibrium the probability of finding \( k \) independently diffusing particles within any given mesh would be given by the Maxwell-Boltzmann distribution \(^2\), namely,

\[
P_{MB}(k|N, M) = \frac{\binom{N}{k}}{k^{(M - 1)^{N-k}}}, \quad (53)
\]

whence the average number of particles per cell

\[
\langle k \rangle = \sum_k kP_{MB}(k|N, M) = \frac{N}{M} \quad (54)
\]

and the variance

\[
\sigma^2[k] = \sum_k k^2P_{MB}(k|N, M) - \langle k \rangle^2 = \frac{N(M - 1)}{M^2}. \quad (55)
\]

In the presence of clustering (\( \beta > 0 \)), the result for the average number of particles would be left unchanged, whereas for the variance there would be position-dependent corrections due to spatial correlations [1, 2]. For the case of an exactly critical reactor without population control, we have

\[
\sigma^2[k_i] = \frac{M - 1}{M} \langle k_i \rangle + \langle k_i \rangle^2 \beta v_2 t + \int_{V_i} dx \int_{V_i} dy \mathcal{H}_i(x, y), \quad (57)
\]

whence an asymptotic variance-to-mean ratio

\[
Y_i = \frac{M - 1}{M} + \frac{\beta v_2}{N} t + \int_{V_i} dx \int_{V_i} dy \mathcal{H}_i(x, y)/\langle k_i \rangle \quad (56)
\]

In the limit of large \( N \) and \( M \), with finite \( \mu = N/M \), \( P_{MB} \) can be approximated by a Poisson distribution with parameter \( \mu \).

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\(^2\)In the limit of large \( N \) and \( M \), with finite \( \mu = N/M \), \( P_{MB} \) can be approximated by a Poisson distribution with parameter \( \mu \).
where \( S_x(n,i) = \frac{1}{n!} \sum_{j=0}^{n} (-1)^j (\binom{n}{j}) (i-j)^n \) are the Stirling numbers of the second kind. This result stems from the particles obeying a Maxwell-Boltzmann distribution for times \( t \gg \tau_D \) when \( \beta = 0 \). In the limit of large \( N \) and \( M \), with finite \( \zeta = M e^{-N/M} \) (which basically means that the number of particles must be larger than the number of meshes, i.e., \( N \gg M \)), the exact distribution in Eq. (60) can be approximated by a Poisson distribution of parameter \( \zeta \). In the presence of fission-induced spatial correlations in a critical reactor, we expect \( s \) to increase with respect to the case of pure diffusion, because of clustering. Without population control, the number of empty cells will eventually saturate to \( s \rightarrow M \) for times \( t \gg \tau_E \), so that the asymptotic distribution will be trivial. When population control is enforced, the distribution \( R(s|N,M) \) will converge to some asymptotic shape at times \( t \gg \tau_D \), with \( (s) \) larger than \( (s)_{id} \). Monte Carlo simulations are displayed in Fig. 8 for a one-dimensional critical multiplying system.

A closely related physical observable is the ensemble-averaged Shannon entropy

\[
\langle S \rangle = -E \left[ \sum_{i=1}^{M} \frac{k_i}{N} \log_2 \left( \frac{k_i}{N} \right) \right],
\]

where we have assumed that the probability of occupation of a cell of index \( i \) is estimated by \( k_i/N \), since all the cells are equally accessible by diffusion. The entropy function \( \langle S \rangle \) is supposed to provide a measure of the phase space exploration [7]. By construction, \( 0 \leq \langle S \rangle \leq \log_2(M) \), where the upper limit would correspond to an ideal repartition of particles uniformly within the box, in the limit of large \( N \). For a purely diffusive system, from Eq. (53) we would obtain

\[
\langle S \rangle_{id} = \log_2(N) - \frac{M}{N} \sum_{k=0}^{N} P_{MB}(k|N,M) k \log_2(k).
\]

When \( N \) is large, \( P_{MB}(k|N,M) \) will be peaked around \( \langle k \rangle = N/M \), and \( \langle S \rangle_{id} \rightarrow \log_2(M) \). In the presence of spatial correlations, the entropy function will be lower than \( \langle S \rangle_{id} \) because of clustering, as illustrated in Fig. 9. Monte Carlo simulations show that the behaviour of \( \langle S \rangle \), when population control is enforced closely follows that of \( \langle r^2 \rangle \), for \( t \gg \tau_D \), \( \langle S \rangle \) will saturate to some asymptotic value \( \langle S \rangle_{\infty} \leq \langle S \rangle_{id} \). Furthermore, we have a scaling \( (\langle S \rangle_{id} - \langle S \rangle_{\infty})/\langle S \rangle_{id} \sim M^{1/2} \) [7].

**XII. CONCLUSIONS**

We have illustrated the physical mechanisms that are responsible for neutron clustering in multiplying systems operated at and close to the critical point. The evolution of the spatial correlations depends crucially on whether population control is enforced. To illustrate this point, exact formulas have been derived for a simple model of nuclear reactor and have been compared to Monte Carlo simulations.

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**APPENDIX: THE BACKWARD EQUATIONS**

Consider a single walker starting from \( x_0 \) at \( t_0 = 0 \). Let \( n(x,t|x_0) \) be the number of particles found in \( dx \) close to \( x \) when the process is observed at \( t > t_0 \). It is convenient to introduce the associated two-volume probability generating
function 
\[ W_t(u, v|x_0) = \mathbb{E}[\mu^{\kappa(x_0)} v^{\lambda(x)}], \]  
(A.1)

It can be shown that \( W_t(u, v|x_0) \) satisfies the backward equation 
\[ \frac{\partial}{\partial t} W_t = D \nabla^2 W_t - (\gamma + \beta) W_t + \gamma + \beta G[W_t], \]  
(A.2)

where \( G[z] = \sum k p_k z^k \) is the probability generating function associated to \( p_k \) \((A.3)\), in the absence of delayed neutrons.

Delayed neutron emission can be included by resorting to multi-type branching processes \([1, 2]\). The probability generating functions \( W^n_t(u, v|x_0) \) for a single neutron starting from \( x_0 \) at \( t_0 = 0 \) and \( W^n_t(u|x_0) \) for a single precursor starting from \( x_0 \) at \( t_0 = 0 \) satisfy the coupled system 
\[ \frac{\partial}{\partial t} W^n_t = D \nabla^2 W^n_t - (\gamma + \beta) W^n_t + \gamma + \beta G^n[W^n_t]G[W^n_t] \]
\[ \frac{\partial}{\partial t} W^n_t = \lambda W^n_t - \lambda W^n_t, \]  
(A.3)

where \( G^n[z] \) and \( G^n[z] \) are the probability generating functions for the number of (prompt) neutrons and precursors at fission events, respectively.

Let us now consider a collection of \( N \) individuals initially located at \( x_0^1, x_0^2, \ldots, x_0^N \) with density \( Q(x_0^1, x_0^2, \ldots, x_0^N) \) at time \( t_0 = 0 \). Assuming that particles evolve independently of each other, the probability generating function satisfies 
\[ W_t(u, v|x_0^1, x_0^2, \ldots, x_0^N) = \prod_{i=1}^N W_t(u, v|x_0^i). \]  
(A.4)

Suppose that the initial positions are independently and identically distributed and obey the factorized density \( Q(x_0^1, x_0^2, \ldots, x_0^N) = \prod_{i=1}^N q(x_0^i) \). The corresponding probability generating function \( W_t(u, v|Q) \) satisfies then \([13]\) 
\[ W_t(u, v|Q) = \left( \int_V dx_0 q(x_0) W_t(u, v|x_0) \right)^N. \]  
(A.5)

The \( m \)-th (factorial) moments of \( n(x) \) and \( n(y) \) can be obtained by derivation of \( W_t(u, v|Q) \) with respect to \( u \) and \( v \), respectively. In particular, the average particle number reads 
\[ \mathbb{E}[n(x, t)] = \frac{\partial}{\partial u} W_t(u, v|Q) \big|_{u=1, v=1}. \]  
(A.6)

For the two-volume correlations we take the mixed derivative, namely, 
\[ \mathbb{E}[n(x, t)n(y, t)] = \frac{\partial^2}{\partial u \partial v} W_t(u, v|Q) \big|_{u=1, v=1}. \]  
(A.7)

In many practical applications, the initial number of particles is itself a random quantity \( K \), with distribution \( Z(K) \). Assuming again independent and identically distributed coordinates \( x_0^k \), \( k = 1, 2, \ldots, K \), Eq. \((A.5)\) can be then generalized as 
\[ W_t(u, v|Z) = \sum_K Z(K) \prod_{k=1}^K \int_V dx_0^k q(x_0^k) W_t(u, v|x_0^k). \]  
(A.8)

Often, the initial configuration is a Poisson point process \([1]\). In this case, the Campbell’s theorem yields \([1]\) 
\[ W_t(u, v|Z) = \exp \left( N \int dx_0 [W_t(u, v|x_0) - 1] q(x_0) \right), \]  
(A.9)

where we have set \( N = \mathbb{E}[K] \) for the average number of source particles.

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