Checking the validity of truncating the cumulant hierarchy description of a small system

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We analyze the behavior of the first few cumulant in an array with a small number of coupled identical particles. Desai and Zwanzig (J. Stat. Phys., 19, 1 (1978), p. 1) studied noisy arrays of nonlinear units with global coupling and derived an infinite hierarchy of differential equations for the cumulant moments. They focused on the behavior of infinite size systems using a strategy based on truncating the hierarchy. In this work we explore the reliability of such an approach to describe systems with a small number of elements. We carry out an extensive numerical analysis of the truncated hierarchy as well as numerical simulations of the full set of Langevin equations governing the dynamics. We find that the results provided by the truncated hierarchy for finite systems are at variance with those of the Langevin simulations for large regions of parameter space. The truncation of the hierarchy leads to a dependence on initial conditions and to the coexistence of states which are not consistent with the theoretical expectations based on the multidimensional linear Fokker-Planck equation for finite arrays.
I. INTRODUCTION

The description of nonlinear stochastic systems can hardly be carried out without approximations due to the interplay of noise and nonlinearity. In some problems, the stationary distribution for the relevant variables is available in analytical form, but in general very little information can be obtained without approximations. A convenient way of describing the system dynamics is in terms of cumulant moments satisfying an infinite set of coupled ordinary differential equations. For all practical purposes, this infinite hierarchy needs to be truncated in order to obtain a finite set of closed equations. A very much used approximation consists in truncating the infinite hierarchy at the Gaussian level by neglecting cumulants of order three and higher. For a stochastic variable $Y(t)$, Marcinkiewicz indicated that the characteristic function $\Gamma(\lambda) = \langle \exp(i\lambda Y(t)) \rangle$ can be expressed as $\Gamma(\lambda) = \exp(P(\lambda, t))$ where $P(\lambda, t)$ is a polynomial of first or second degree in $\lambda$. Consequently, as pointed out by Hänggi and Talkner, the truncation of the hierarchy at levels higher than two is problematic, although, as these authors emphasize, it is not an empty concept. In their own words "it only means that the neglect of cumulants beyond a given order cannot be justified a priori".

In this work we consider the statistical mechanical description of a stochastic array containing a small finite number $N$ of coupled identical elements. The dynamics will be given by a set of $N$ coupled nonlinear stochastic differential equations for the degrees of freedom characterizing the elements of the array. Equivalently, we can describe the system in terms of an $N$-dimensional joint probability distribution. We will assume that this joint probability distribution satisfies an $N$-dimensional linear Fokker-Planck equation (FPE).

Obtaining dynamical information from the FPE is plagued with difficulties due to the nonlinear character of the dynamics. As mentioned above, a way of dealing with them is to consider the cumulant moments satisfying an infinite hierarchy of ordinary differential equations. In the case of the arrays studied in this work, Desai and Zwanzig derived from the FPE such an infinite hierarchy. Two types of cumulants appear: diagonal cumulant moments associated to a single degree of freedom, $M_i(t)$, and cross cumulant moments, $\mu_{ijk...}(t)$ involving two or more variables. For an infinite system, the off-diagonal cumulant moments are negligible if they were zero at the initial preparation (see). In other words, off-diagonal cumulant moments are not generated by dynamical evolution in the case of infinitely large systems. But even then, for all practical purposes, the hierarchy has to be approximated by truncating it at a certain level. The results of truncating at different levels the hierarchy of diagonal cumulant moments in the $N \to \infty$ limit was already
discussed by Desai and Zwanzig. As also indicated in the, the cumulant truncation is a successful strategy in that limit.

By contrast with the previous work of Desai and Zwanzig, the present work focuses on systems with a small number \( N \) of elements. In this case, both the diagonal and off-diagonal cumulant moments have to be taken into account. It is then an open question whether truncating the infinite hierarchy is an adequate approximation strategy. It is not possible to solve analytically the truncated set of equations at any level. So we will rely on a numerical treatment of the set. Our goal is to elucidate whether truncation of the infinite hierarchy of cumulant moments at different levels provides a reliable approximation for small finite arrays. To this end, we will compare the results for the first few cumulant moments obtained from the truncated hierarchy with those obtained by numerically solving the set of the \( N \) coupled Langevin equations. Besides the numerical simulations of the Langevin dynamics, the results of the truncated hierarchy will also be contrasted with the exact results expected from the stationary solution of the \( N \)-dimensional Fokker-Planck equation, as well as the global stability H-theorem. We will see that the simulation results agree with the exact known information, while the truncation strategy might lead to results incompatible with the exact results.

II. THE MODEL

We consider a global coupling model that can be viewed as a set of nonlinear “oscillators”, each of them described by a “coordinate” \( x_i \). The dynamics of the system is given by the set of coupled Langevin equations (in dimensionless form)

\[
\dot{x}_i = x_i - x_i^3 + \frac{\theta}{N} \sum_{j=1}^{N} (x_j - x_i) + \xi_i(t),
\]

where \( \theta \) is the strength of the global coupling term. This parameter will be taken to be either positive or negative. The terms \( \xi_i(t), \ i = 1, 2, \ldots N \) represent \( N \) uncorrelated Gaussian white noises with zero averages and \( \langle \xi_i(t_1) \xi_j(t_2) \rangle = 2D\delta_{ij}\delta(t_1 - t_2) \). This model was introduced by Kometani and Shimizu\(^5\) as a model for muscle contractions, and it was later on analyzed by Desai and Zwanzig\(^4\) from a Statistical Mechanics perspective. The model describes \( N \) degrees of freedom each of them globally coupled to all the other ones. Each degree of freedom has an intrinsic nonlinear dynamics. The nonlinearity and the presence of the noise terms render the behavior of the system far from trivial.

An alternative formulation of the dynamics is in terms of the linear Fokker-Planck equation for
the joint probability density $f_N(x_1, x_2, \ldots, x_N, t)$,
\[
\frac{\partial f_N}{\partial t} = \sum_i \frac{\partial}{\partial x_i} \left( \frac{\partial U}{\partial x_i} f_N \right) + D \sum_i \frac{\partial^2 f_N}{\partial x_i^2},
\]
\[\text{(2)}\]
where $U$ is the potential energy relief,
\[
U = \sum_{i=1}^{N} V(x_i) + \frac{\theta}{4N} \sum_{i=1}^{N} \sum_{j=1}^{N} (x_j - x_i)^2,
\]
\[\text{(3)}\]
with the single particle potential,
\[
V(x_i) = \frac{x_i^4}{4} - \frac{x_i^2}{2}.
\]
\[\text{(4)}\]

The term $V(x_i)$ describes a symmetrical potential with two wells of equal depths separated by a hump at $x_i = 0$. The interaction part of the full potential modifies it in such a way that for $\theta > 1$ the two wells blend into a single minimum at $x_i = 0$. For $\theta < 1$, the two wells exist, but their locations and the barrier height depend on $\theta$. Note that for $\theta > 0$, the interaction energy contribution to the full potential favors that any pair $x_i$ and $x_j$ should have the same sign (both either positive or negative), while for $\theta < 0$, the opposite happens and the interaction tends to favor configurations with positive and negative values of the variable.

The only explicit solution of Eq. (2) is its long time stationary one, given by
\[
f_{st}^N(x_1, x_2, \ldots, x_N) = \frac{1}{Z} \exp \left( -\frac{U}{D} \right)
\]
where $Z$ is a normalization function. This solution is independent of the initial condition, and the system will necessarily relax to it, although the time it takes to do it might be, depending on the system parameters, extremely large. It should be noted that we keep the finite number of particles $N$ fixed, while we take the long time limit. Had we have taken the limit $N \to \infty$ first, as done in the infinite size limit studies, and afterwards the long time limit, the result would differ.

As mentioned above, Desai and Zwanzig\textsuperscript{4} derived an infinite hierarchy of ordinary differential equations for the cumulant moments. Neglecting the cumulant moments of order five and higher one gets a set of 11 equations for the first four order (diagonal and off-diagonal) cumulant moments (see the Appendix in\textsuperscript{4}). For asymptotically large systems ($N \to \infty$), Desai and Zwanzig found that, for some regions of parameter space, zero is the only stationary value for the first cumulant moment. For other regions of parameter values, there are two stable nonzero stationary values, while the zero value becomes unstable. The regions are separated by a transition line whose shape depends on whether $\theta > 1$ or $0 < \theta < 1$. As we will see in the next section, the truncated hierarchy of cumulants for small systems might yield several stable stationary moments depending
upon the initial preparation, as obtained within the \( N \to \infty \) limit. Nonetheless, those results are incompatible with the unicity of the solution of a multidimensional linear FPE and with the independence from initial condition of the long-time results, required by the H-theorem.

III. NUMERICAL SIMULATIONS

We have carried out numerical simulations of the whole set of Langevin equations, Eq. (1). Using the procedure detailed in Ref. 6, we have integrated the Langevin equations for a large number of noise realizations (typically 5000 realizations). Averaging over them, we estimate the first two cumulant moments of a single variable by

\[
M_1(t) = \langle x(t) \rangle \approx \frac{1}{N} \sum_{\alpha=1}^{N} x^{(\alpha)}(t),
\]

and

\[
M_2(t) = \langle x^2(t) \rangle - M_1^2(t) \approx \frac{1}{N} \sum_{\alpha=1}^{N} (x^{(\alpha)})^2(t) - M_1^2(t),
\]

where \( N \) indicates the total number of trajectories and \( x^{(\alpha)}(t) \) indicates the numerically obtained single particle trajectory in the \( \alpha \) noise realization.

Let us first investigate what happens for parameter values such that, in the infinite size limit, Desai and Zwanzig obtained a single stable stationary first moment. In Fig. 1 we depict the behavior of the first four diagonal cumulants obtained from the truncated hierarchy of eleven equations for the cumulants for \( N = 5, D = 1.33, \theta = 2 \) and two sets of initial conditions: \( M_1(0) = 0.3 \) (solid lines) and \( M_1(0) = -0.3 \) (dashed lines). From the numerical simulations of Langevin equations for \( N = 5, D = 1.33, \theta = 2 \) and the same two sets of initial conditions we get the results depicted in Fig. 2. The long-time limit results are independent of the initial preparation and, except for the long time value of \( M_4 \), the truncated hierarchy yields a time evolution of the diagonal moments very much in agreement with those obtained with the Langevin simulations. We have numerically analyzed other set of parameter values and initial conditions and the numerical findings lead us to conclude that, for parameter values such that \( M_{1}^{st} = 0 \) is the only stable stationary solution, the set of eleven equations represents a reliable approximation to the correct behavior for systems of even very modest sizes.

Let us next consider a set of values for the parameters \( \theta \) and \( D \) such that, for infinite systems, Desai and Zwanzig found that truncation of the hierarchy of cumulant moments leads, in the \( N \to \infty \) limit, to two coexisting stable stationary nonzero values for the first moment while \( M_{1}^{st} = 0 \)
FIG. 1. Behavior of the first four diagonal cumulants obtained from the truncated set of eleven equations for the cumulants for $N = 5$, $D = 1.33$, $\theta = 2$ and two different initial conditions: $M_1(0) = 0.3$ (solid lines); $M_1(0) = -0.3$ (dashed lines).

FIG. 2. Behavior of the first four diagonal cumulants obtained from the simulations of Langevin equations for the cumulants for $N = 5$, $D = 1.33$, $\theta = 2$ and two sets of initial conditions: $M_1(0) = 0.3$ (solid lines); $M_1(0) = -0.3$ (dashed lines). $M_3(t)$ and $M_4(t)$ for the two sets of initial conditions are indistinguishable with the graph resolution.

is unstable. In the case of small finite systems, the numerical solution of the truncated hierarchy still leads to three stationary values but $M_1 = 0$ might be stable for a range of initial conditions. This range depends on the system size, the parameter values and the level of truncation. In Fig.
FIG. 3. (Color online) The (black) dots and the (red) squares represent the limiting initial values of \( M_1(0) \) vs. \( N \) separating the region of stability of the long time zero solution of the hierarchy of equations for the cumulants truncated at the fourth order or the second order levels respectively. Note that for \( N < 10 \), \( M_1^{st} = 0 \) for the fourth order truncation regardless of the initial preparation, while for the second order truncation, this fact is true for \( N < 4 \). The initial conditions are \( M_1(0) \neq 0 \) and all the other cumulant are taken to be zero initially. The lines are a guide to the eye. System parameters: \( D = 0.33 \) and \( \theta = 2 \).

We depict the results for \( M_1^{st} \) obtained from the long time solution of the hierarchy of cumulant equations truncated at the fourth order level (black dots) and at the second order level (red squares) with \( M_1(0) \neq 0 \) and all the other cumulant set to zero. For all values of \( N \) considered, we have used \( D = 0.33 \) and \( \theta = 2 \). With the fourth order truncation, the long time solution \( M_1^{st} = 0 \) is stable for \( N < 10 \) regardless of the initial condition. For \( N > 10 \), the stability of the zero solution depends on the initial value \( M_1(0) \). With the second order truncation, the solution \( M_1^{st} = 0 \) is stable for \( N < 4 \), while it becomes unstable for some range of initial conditions as \( N > 4 \). Thus, there is an influence of the level of truncation in the stability diagram of the zero stationary solution.

In Fig. 4 we depict the results for the time evolution of the first four diagonal cumulants obtained from the numerical solution of the truncated hierarchy of equations for \( N = 15, D = 0.33, \theta = 2 \) for two sets of initial conditions \( (M_1(0) = \pm 0.3) \).

In Fig. 5 we depict the behavior of the first four diagonal cumulants as obtained from numerical simulations of the Langevin equations for a system with \( N = 15, D = 0.33 \) and \( \theta = 2 \) with the two sets of initial conditions. The truncated set of cumulant equations leads to two nonzero first moment stationary values. The discrepancies between the results in Figs. 4 and 5 for the same parameter values are evident. The Langevin simulation results indicate that the long time behavior...
of the cumulants is independent of the initial condition. This fact is consistent with an exact result: according to the H-theorem, the long time equilibrium solution of Eq. (2) is independent of the initial preparation of the system. The first moment, $M_1(t)$, has therefore a single stationary value. Considering the canonical form of the long time solution of Eq. (2) and the symmetry of the potential in Eq. (3) we have that, for any finite system, $M_{st}^1 = 0$, which is the long time value obtained via Langevin simulations. Then, the stability of the nonzero long time solutions and the dependence of the initial preparation seem to be an artifact of the truncation rather than a property of a finite system.

Even for $\theta$ and $D$ values such that multiple steady solutions are possible, the solution $M_{st}^1 = 0$ of the truncated hierarchy is the only stable stationary solution for $N$ sufficiently small ($N < 10$ for the parameter values in Fig. 3). It is worth to compare for these small systems the time evolution of the first few cumulants obtained with the truncated hierarchy with the one provided by Langevin simulations. In Fig. 6 we depict the results of the evolution of the first four diagonal cumulants obtained with the numerical simulations of Eq. (11) for $N = 3$, as well as from the truncated hierarchy of equations for $\theta = 2$, $D = 0.33$. We see that, as expected, for this small system the truncated hierarchy leads to $M_{st}^1 = 0$, in agreement with the results obtained from the Langevin simulations. In contrast, the second and fourth order cumulants steady values obtained from the truncated hierarchy and from the Langevin simulations show large quantitative differences,
FIG. 5. Behavior of the first four diagonal cumulants obtained from the simulations of Langevin equations for the cumulants for $N = 15$, $D = 0.33$, $\theta = 2$ and two sets of initial conditions.

FIG. 6. (Color online) Behavior of the first four diagonal cumulants estimated from the numerical simulations of Eq. (1) for $N = 3$ (solid green lines), as well as from the truncated hierarchy of equations for the cumulant moments (black dashed lines). Other parameter values $D = 0.33$ and $\theta = 2$.

indicating the limitations of the truncated hierarchy.

We now turn our attention to the model with a negative global coupling parameter $\theta < 0$. Figs. 7 and 8 show the results obtained, respectively, with the truncated hierarchy of equations for the cumulant moments, and with the full simulation of the Langevin equations for systems with $N = 10$, $D = 0.5$ and $\theta = -0.5$. We see that the long time limit is independent of the
FIG. 7. Behavior of the first four diagonal cumulants of the truncated hierarchy of equations for $N = 10$, $D = 0.5$, $\theta = -0.5$ for two sets of initial conditions.

initial conditions. There are differences in the long time value for the second and fourth cumulant moments obtained with the hierarchy of equations and the simulations. The relaxation towards the stationary solution is quite fast, although the relaxation time with the full simulation is somewhat longer. Even though the results in Fig. 7 differ quantitatively from the simulations results in Fig. 8, they yield a good qualitative approximation. An extensive numerical analysis of the truncated hierarchy indicates that for $\theta < 0$ there is only a single zero stationary value for the first moment regardless the value of $N$.

IV. CONCLUSION

In conclusion, the work presented here indicates that care must be taken when using an approximation to the dynamical behavior in a chain of interacting identical objects, based on truncating the infinite hierarchy of cumulant moments. Even for very large systems, if the parameter values considered are such that the truncated hierarchy leads to two stable coexisting solutions, the approximation is not correct. The results of the numerical simulations of the Langevin equations and the exact properties of the Fokker-Planck equation for finite systems of any size indicate that the coexistence of two stationary solutions is an artifact of the truncation. On the other hand, when the truncated hierarchy has a single stationary stable solution, it provides a reliable approximation of the system dynamics even for systems of very modest size. Although our conclusions are based on the study of a particular model, we think that they are qualitatively relevant for other cases.
Langevin dynamics with additive noise are good general representations of dynamical systems in contact with a thermal environment. Actually, Langevin dynamics are more realistic than their deterministic limits often used to study dissipative nonlinear systems, where dissipation is included but all fluctuations are neglected. Global interactions are also quite general. The quartic nonlinearity we study here is a particular case. But having a different nonlinearity should not change our qualitative conclusions. The nonlinearity considered includes already the nontrivial effects associated to the dynamical coupling between noise and nonlinearity.

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