Nucleation theory, the escaping processes, and nonlinear stability

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We study the solutions describing the critical ''germs'' in nucleation theory, escaping processes, and fractures. We present systems with exact solutions in $D=1,2,3$ dimensions. We show that when there exist connections between the particles in more than one dimension, the stability is much more increased. In systems where the potential well is a degenerate point, the critical germ solution has a power-law behavior. For $D=3$ there can exist a continuum of stationary states where all the points of the order parameter take values that are out of the stability zone (i.e., the potential well) leading to effective marginal stability. We discuss the relevance of these results for different physical systems and its connections with recently intensively studied phenomena like sand-pile dynamics, self-organized criticality, noise-induced synchronization in extended systems, and quantum tunneling in the framework of field theory. [S0163-1829(99)01906-2]

I. INTRODUCTION

The problem of describing the stability of a system is one of the basic question of the dynamics. In the study of many physical phenomena, such as fragmentation, phase transition, and chemical reaction, it becomes necessary to estimate if a given instability will die or grow, driving the system to a new ''phase.'' The main portrait of those processes is that of nucleation,[1,3] where drops grow or disappear depending on their Gibbs energies.

Many of those physical phenomena[2–27] can be described by the equation

$$\frac{\partial^2 \varphi}{\partial t^2}+\gamma\frac{\partial \varphi}{\partial t}=\nabla^2\varphi+F(\varphi)+g(\mathbf{x},t), \qquad (1)$$

where $F(\varphi)=-\partial U(\varphi)/\partial\varphi$, the potential $U(\varphi)$ (see Fig. 1) possesses at least two (asymmetrical) wells (minima) at the points φ_1 and φ_3 separated by a barrier (a maximum) at the point φ_2 ($\varphi_1<\varphi_2<\varphi_3$). [We will assume $U(\varphi_3)<U(\varphi_1)$]. The function $g(\mathbf{x},t)$ is an external force that can be stochastic. Problems related to Eq. (1) appear in Physics, Chemistry, Engineering, Biology, etc. Let us just mention some scientific areas: phase-transition theory[2,14,15,18,23] chemical reactions,[19] escaping processes,[19,24,26] stability of engineering structures,[24,26] fractures,[27] quantum tunneling,[12,14,19] field theory,[12,17] etc.

For some problems it is sufficient to consider one well and a barrier. This is obtained in the formulation of Eq. (1) making $U(\varphi_3)=-\infty$. In other problems we can have a well between two symmetric barriers.[24,26]

We are interested in the transition from the metastable state φ_1 to state φ_3. Equation (1) (with space-independent φ)[19,24,26,29,30] is used as an approximate model for chemical reactions, fractures, and the stability of engineering structures. Hence, a unique particle moving in the potential $U(\varphi)$ is considered. In this case, in the absence of the force $g(\mathbf{x},t)$, the point φ_2 is the limit for the stability of the particle. However, both experiments,[28] and simulations[27,31] show a considerable extension of the elongation φ before the instability occurs. In the case of metals under stress, this phenomenon was labeled delayed fracture.[28] Recently, some space-time models have been investigated.[27,29] It has been shown that the elongations can take considerably greater values.

In phase-transition theory,[10,12] it is a common place to consider the existence of a critical ''germ'' for the transition. Field configuration $\varphi(\mathbf{x},t)$ with a radius greater than that of the critical germ should develop the instability in order to produce the transition to the state φ_3. Recently Gorokhov and Blatter[13] worked on some similar problem on stability.

The present work will be dedicated to the study of the solutions describing the critical germs. These solutions have been studied in a large number of papers, e.g., Refs. 10, 18, and 23. However, due to the great mathematical difficulties that are presented in Eq. (1) (especially for dimensions $D>1$), in most of the works the authors use approximations and/or numerical methods. Therefore, many interesting phenomena have been overlooked. We will present systems with exact solutions. This will permit us to analyze with deeper understanding some surprising phenomena that can occur for $D>1$.

II. STATIONARY CRITICAL SOLUTIONS

There exists an unstable stationary critical solution that is a limit for the escaping process and plays the role of a critical germ[10,14,15,18,23] for the development of the instability in the system. Let us concentrate on solutions with radial symmetry. The stationary solutions of Eq. (1) $[g(\mathbf{x},t)=0]$ satisfy the equation

$$\frac{d^2\varphi_s}{dr^2}+\frac{D-1}{r}\frac{d\varphi_s}{dr}+F(\varphi_s)=0, \qquad (2)$$

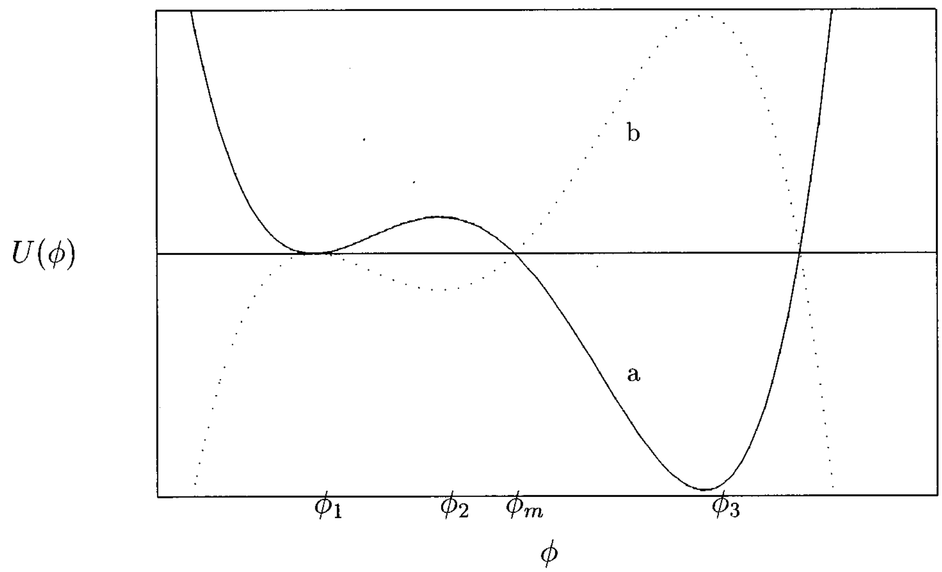

FIG. 1. The potential as a function of the order parameter φ. (a) is the physical potential $U(\varphi)$. (b) is the potential for the fictitious particle $V(\varphi)=-U(\varphi)$.

where D is the space dimension. It is possible to prove that when $U(\varphi)$ possesses a minimum in $\varphi_1=0$, a maximum in φ_2 and it can take negative values for $\varphi>\varphi_m$ $[U(0)=U(\varphi_m)=0]$, there exists a solution with a maximum in $r=0$ and asymptotically it tends to zero for $r\rightarrow\infty$. This solution corresponds to the critical equilibrium state mentioned above. In Fig. 2 we show the phase trajectories for Eq. (2). The curves in Figs. 2(a) and 2(b) belong to the case $D=1$. In this case, the homoclinic orbit Fig. 2(b) corresponds to the critical solution.[27] The trajectories Figs. 2(c) and 2(d) correspond to the critical solutions in the cases $D=2$ and $D=3$, respectively. Another way to ''see'' these solutions is the following.[12] Equation (2) can be analyzed as a Newton's equation for a unitary-mass particle moving in the potential $V(\varphi)=-U(\varphi)$. Here φ plays the role of ''coordinate'' of the ''particle'' and r plays the role of ''time.'' Additionally, we have a ''dissipative force'' $(D-1)/r(d\varphi/dr)$. Our critical solution corresponds to a motion of the fictitious particle from an initial point $\varphi(0)\geqslant\varphi_m$ with $(d\varphi/dr)(0)=0$, that terminates in the maximum $\varphi=0$ of $V(\varphi)$. For the case $D=1$ the maximum of φ situated in $r=0$, coincides with φ_m. (The dissipative force is zero and the ''mechanical energy'' is conserved). However, for $D>1$ the mechanical energy decreases with the motion of the particle. Let us define the mechanical energy of the particle:

$$E=\frac{1}{2}\left(\frac{d\varphi}{dr}\right)^2+V(\varphi). \tag{3}$$

Hence,

$$\frac{dE}{dr}=-\frac{(D-1)}{r}\left(\frac{d\varphi}{dr}\right)^2\leqslant 0. \tag{4}$$

For $D>1$, the critical solution is produced when $\varphi(0)\equiv\varphi_M>\varphi_m$. If we increase D, the dissipative force will be increased too, and $\varphi_{(0)}$ for the particle should be bigger in order to reach the maximum of $V(\varphi)$ in $\varphi=0$.

The critical solution is unstable.[11,12,15,18,27] Perturbations of the critical solution can lead to a growth of the elongations initiating the escaping process from the well. For the extended system this solution plays the same role of point φ_2 for a single particle moving in the potential $U(\varphi)$. The asymptotic behavior of the critical solutions depends on the behavior of the function $U(\varphi)$ in the neighborhood of the point $\varphi=0$. Suppose that $U(\varphi)$ behaves like

$$U(\varphi)\sim\varphi^n \tag{5}$$

for $\varphi\approx 0$. If $n=2$, for $r\rightarrow\infty\,\varphi_s\,(r)$ decays exponentially. However, for $n>2$ the solution has a power-law behavior for $r\rightarrow\infty$. There exist other potentials $U(\varphi)$ which are continuous but not analytical functions in the point $\varphi=0$. Nevertheless some of these potentials have physical interest. For instance, suppose that $U(\varphi)$ possesses a minimum in $\varphi=0$ [hence $F(0)=0$] but

$$\lim_{\varphi\rightarrow\infty}\left|\frac{\partial^2\varphi}{\partial r^2}\right|=\infty. \tag{6}$$

In this case, function $\varphi_s(r)$ decays faster than a simple exponential. Let us see an example:

$$U(\varphi)\sim\varphi^2\ln\varphi. \tag{7}$$

In this situation, the asymptotic behavior of $\varphi_s(r)$ is Gaussian:

$$\varphi(r)\sim\exp(-\gamma^2). \tag{8}$$

III. SYSTEMS WITH EXACT SOLUTIONS

After a complete investigation of equations of type (2), using the so-called qualitative theory of dynamical systems[31–33] (including topological concepts), and with the additional information about the behavior of solutions in the neighborhood of fixed points, it is possible to construct func-

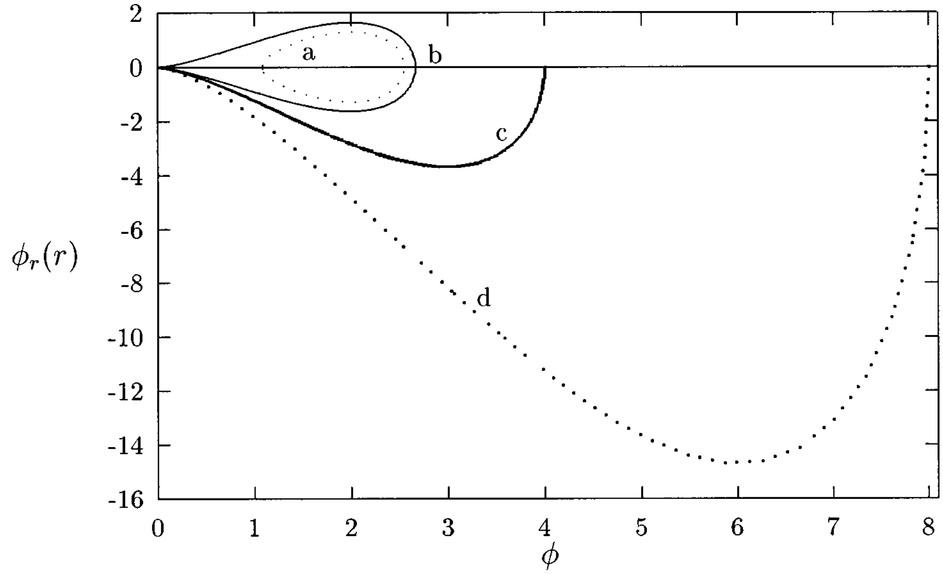

FIG. 2. Phase portraits of Eq. (2), we plot the derivative of φ with respect to r, φ_r, as a function of φ. The orbits (a) and (b) corresponds to the one-dimensional case. The homoclinic orbit (b) is the critical germ solution. The trajectories (c) and (d) correspond to the cases $D=2$ and $D=3$, respectively. They represent the germ solutions for these cases.

tions with all the topological and asymptotic properties of the exact solutions of the given equation. Then, solving an inverse problem, we are able to present systems of type (2) with exact solutions. Later, it is possible to generalize the results for some classes of equations that are topologically equivalent to those obtained for the exact solutions.

Let us see the following particular case:

$$F(\varphi)=a|\varphi|^2-b|\varphi|^3, \tag{9}$$

where $a,b,>0$ are real. In this case, the exact solutions can be obtained:

$$\varphi_s(r)=\frac{Q}{1+Nr^2}, \tag{10}$$

where

$$Q=\frac{4}{4-D}\frac{a}{b}, \tag{11}$$

$$N=\frac{2}{(4-D)^2}\frac{a^2}{b}. \tag{12}$$

From Eq. (9) we have

$$\varphi_2=\frac{a}{b}. \tag{13}$$

The ratio Q/φ_2 increases with the dimension

$$\frac{Q}{\varphi_2}=\frac{4}{4-D}. \tag{14}$$

We should remark that the solution in the form of Eq. (10) is valid only for $D=1,2,3$. From this result we see that the stability of the system increases with the dimension. This generalizes our previous result[27] for one-dimensional chains. This is not a particular result, many others functions $F(\varphi)$ for which analytical results can be obtained show the same kind of behavior.

IV. MARGINAL STABILITY: MULTIPLICITY OF STATIONARY STATES

Before we start to look for the multiplicity of stationary states, we wish to show an equation whose exact solutions will be useful later. Let

$$\frac{d^2\varphi}{dr^2}+\frac{D-1}{r}\frac{d\varphi}{dr}+a\varphi^{m+1}+b^{2m+1}=0. \tag{15}$$

It is straightforward to prove (by direct substitution) that the function

$$\varphi=Q(1+Nr^2)^{-1/m} \tag{16}$$

is an exact solution of Eq. (15) when

$$Q^D=\frac{2(m+1)}{[Dm-2(m+1)]}\frac{a}{b}, \tag{17}$$

and

$$N=\frac{m^2(m+1)}{[Dm-2(m+1)]^2}\frac{a^2}{b}. \tag{18}$$

Note that solution (10) is a particular case of Eq. (16). Using Eqs. (16)–(18) it follows that if

$$m=\frac{2}{D-2}, \tag{19}$$

then it is possible to obtain a family of solutions for the equation

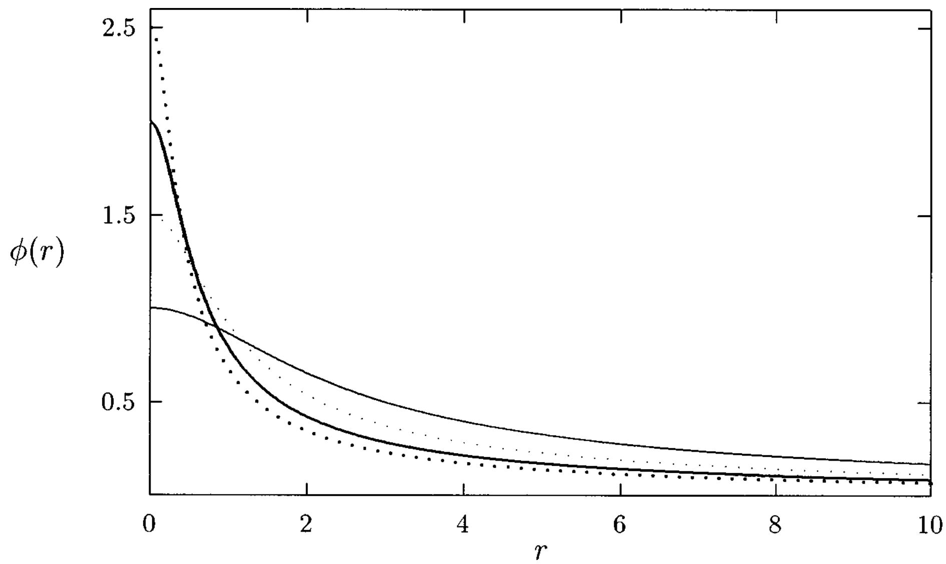

FIG. 3. Marginal stability solutions $\varphi(r)$ with different amplitudes. Note that the solutions decay faster for great amplitudes.

$$\frac{d^2\varphi}{dr^2}+\frac{D-1}{r}\frac{d\varphi}{dr}+b\varphi^{2m+1}=0. \tag{20}$$

These solutions will be expressed by the function

$$\varphi=\frac{Q}{(1+Nr^2)^{1/m}}\equiv\frac{Q}{(1+Nr^2)^{D/2-1}}, \tag{21}$$

where Q and N must fulfill the relation

$$N=\frac{m^2 b}{4(m+1)}Q^{2m}. \tag{22}$$

As a particular case of Eq. (20) we have

$$\frac{d^2\varphi}{dr^2}+\frac{2}{r}\frac{d\varphi}{dr}+b\varphi^5=0, \tag{23}$$

for which we get the family of solutions

$$\varphi=\frac{Q}{[1+(b/3)Q^4r^2]^{1/2}}. \tag{24}$$

Let us return to the auxiliary mechanical system consisting of a fictitious particle moving in the potential

$$V(\varphi)=-U(\varphi).$$

A particle that starts its movement in the point $\varphi(0)=\varphi_m$ should pass the point $\varphi=\varphi_2$ in order to reach the point $\varphi=0$. We can expect that in a vicinity of point φ_2 the particle makes oscillations. This is true for $D=1$.[15] In order to facilitate our analysis, we will momentarily make the affine transformation $\psi=\varphi-\varphi_2$ in such a way that the maximum of potential $U(\varphi)$ [local minimum $V(\varphi)$] will be in $\psi=0$. It is also supposed that in the neighborhood of $\psi=0$, the potential $U(\varphi)$ behaves as

$$U(\psi)\sim\psi^{2n}, \tag{25}$$

For $n=1$, $D=1$, the point $\psi=0$ is a focus: the particle will make damped oscillations in the vicinity of $\psi=0$. Nevertheless, for $n>1$ when we increase D, a very interesting bifurcation can occur, if

$$D>\frac{(2n-1)}{n-1}. \tag{26}$$

This condition is obtained when we investigated the behavior of the solution in a neighborhood of a point $\psi=0$. Only for $D>(2n-1)/(n-1)$ we have solutions tending to the point $\psi=0$ when r tends to infinity. For instance, the solution (16)–(18) is possible only for $Dm-2(m+1)>0$. But in this case $2n=m+1$. So, this solution exists for $D>(2n-1)/(n-1)$. The focus becomes a node. If the particle starts its movement in a vicinity of the point $\psi=0$ [with $\psi(0)>0$], then it will make an overdamped movement that will end in the point $\psi=0$ (for $r\to\infty$). The particle will not visit the negative values of ψ. This means that Eq. (1) will have stationary solutions for which all the points are on the right-hand side of the maximum $\varphi=\varphi_2$ of potential $U(\varphi)$. An initial state with this configuration not necessarily and immediately will fall down to the right of the maximum $\varphi=\varphi_2$ of potential $U(\varphi)$.

An example of those solutions are the functions Eq. (25). More explicitly: the equation

$$\frac{\partial^2\psi}{\partial t^2}+\gamma\frac{\partial\psi}{\partial t}=\nabla^2\psi+b\psi^5, \tag{27}$$

whose potential $U(\psi)$ possesses only one maximum situated in the point $\psi=0$, will have a continuous set of stationary solutions [see formula (24) and Fig. 3] for which the values of $\psi(r)$ (for all r, $0\leqslant r<\infty$), will be ''out'' of the equilibrium position $\psi=0$. One will expect that an initial condition $\psi(x,y,z,0)$ with the structure of Eq. (24) would develop the instability of the maximum $\psi=0$, and will lead to a dynamics such that

$$\psi(0,t)\to\infty. \tag{28}$$

This is not the case in our example. Any equation of type Eq. (1) with a maximum in the point $\varphi=\varphi_2$ which holds the conditions Eqs. (25) and (26) will have a continuous set of solutions with the properties discussed above. We should stress the difference between these stationary solutions and the critical solutions in one dimension. The critical solutions have unique amplitude and shape. The smallest perturbation will cause the instability, which will lead to any of the stable minima of $U(\varphi)$.

Nonetheless, when the conditions Eqs. (25) and (26) are fulfilled we have a continuum of stationary solutions. These solutions are not asymptotically stable. After a small perturbation, the system does not return to the same state. In general, if the perturbation is small enough, the system will remain balanced in another stationary solution (taken from these solutions that belong to the continuous set). This is a situation similar to that when we move a particle on a flat surface $[U(\varphi)=\text{const}]$, which is an ''indifferent'' equilibrium state. Just note that here the true potential $U(\varphi)$ is not a constant and what is moving is not a single particle but a space-dependent structure, and finally, we are in the presence of a spatiotemporal system. So, we are presented with a set of infinite indifferent equilibrium states with marginal stability. This is something that resembles in some way the sand pile. The sand pile possesses infinite metastable stationary states. In both systems (the sand pile and ours) we observe self-organized criticality and power-law behaviors. The physical meaning of marginal stability in our models is the existence of an infinity of metastable stationary states. A perturbation can produce different outcomes between a single shift and an avalanche, depending on where the perturbation is applied and how strong it is. As a result of marginal stability and self-organized criticality, the system will produce critical structures of states which are barely stable.[21,22]

When the potential $U(\varphi)$ has two finite minima such that $U(\varphi_3)<U(\varphi_1)$, we still will have a continuous set of stationary solutions but the maximal amplitude is limited. Systems with nonparabolic extrema have been used as models in reaction-rate theory.[19,20] However, the real systems do not need to be degenerate in order to present the phenomena here discussed. For sufficiently flat extrema we will observe similar effects. For instance, since the real systems are finite, the power laws can be observable even if they do not extend to infinity.

V. CONCLUSIONS

Previously, we have seen[27] that the function φ can take considerably greater values without the development of the instability in a chain of linked particles, rather than for the system of a single particle. Moreover, when there exist connections between the particles in more than one dimension, the stability is much more increased.

For some systems, more specifically for fractures, a discrete model has important characteristics.[29,30] A very important point as well is the existence of fractal surfaces or fringes formation in diffusion limited aggregation.[37,38] However, even in those cases a simple radial-symmetric approach may give us a good idea of the instability evolution.

In systems where the well (minimum of the potential) is a degenerate point, the critical limit state has a power-law behavior. Thus, Gaussian distributions of perturbations have more difficulties in creating the conditions for the escape. That is, these systems are more stable than Morse systems. Perturbations with long-range correlations would be more effective in generating the instability than, e.g., a white noise.

A surprising phenomenon is that for $D=3$ there can exist stationary states where in all the space points the function ψ takes values that are out of the potential well. A single particle placed out of the maximum of $U(\varphi)$ with $\varphi(t=0)>\varphi_2$ will move irreversibly to the right. Extended systems in one and two space dimensions with a distribution of elongations, such that all the points have values of φ greater than φ_2, will evolve as well to a state far away from the left well. However, as has been shown, in three-dimensional systems there can exist continuous sets of stationary solutions in ''indifferent'' equilibrium with marginal stability. In one-dimensional systems when we consider a kink solution[9,15,18,34–39] the stationary solution contains values that coincide with the unstable equilibrium position of the potential, and besides it contains points that, considered isolated, would not be equilibrium points. Notwithstanding, these ''isolated'' particles are ''sustained'' by the majority of the particles that are inside the wells. In fact, the kink is a very robust solution.

In one and two dimensions, one can have initial conditions where part of the points is out of the well (the rest is inside the well), which do not escape. However, most of these initial configurations are not stationary solutions. A stationary solution can be only one (the critical equilibrium solution), which is openly unstable. The continuum set of marginally stable stationary solutions is possible due to the existence of a qualitatively stronger cooperation between constituent particles in the three-dimensional case. For $D=3$ there occurs a kind of ''bifurcation'' that conducts to an extraordinary effective damping for the particles in their motion on the potential. Suppose now that we have a bistable potential $U(\varphi)$ $[U(\varphi_1)=U(\varphi_3)]$ and the system is perturbed by oscillating forces $g(x,t)$ (deterministic and/or stochastic, including noise). In this case, the complexity of the systems we are studying will manifest itself in a very spectacular fashion. The capacity of the three-dimensional system to support structures, unthinkable in lower dimensions, would be enhanced. We can foresee the existence of fractal dynamics.[30,40,41]

Consider a D-dimensional network of coupled nonlinear oscillators (the mechanical system is by itself an important physical system, however, with this model we can describe many other physical systems, e.g., a D-dimensional array of Josephson junctions). Our results show that the dynamics is dramatically different in $D=3$ in comparison with the dynamics of small dimensions. We will observe the formation of a scale-invariant structure of minimal stable states. Recent studies[42,43,22] indicate the possibility of enhancing the response of a nonlinear oscillator driven by the noise and a periodic signal by coupling it into a one-dimensional chain of identical oscillators. The authors have noted the possibility of using this effect in neural networks, signal processing, and device applications including bioengineering receptors and remote sensing arrays. The output signal-to-noise ratio may be maximized by treating the coupling and noise strength as design parameters. The cooperation between the oscillators is qualitatively stronger than in small dimensions. So, the dimension of the array could be a different design parameter.

The enhancement of synchronization is produced by the collective spatial and temporal motion of the array. We can show that the dynamics of the oscillators can approach metastable states with marginal stability, which in $D<3$ would be completely unstable. The coupling (in three dimensions) in cooperation with the noise and the nonlinear potential will organize the network in space and time in a way unthinkable in $D<3$.

Finally, we would like to address the problem of quantum barrier penetration in field theory.[12,14,19] In this context, our critical equilibrium state (now defined with the radial variable $r=\sqrt{x^2+y^2+z^2+\tau^2}$), where $\tau=it$ in dimension $D+1$,[12,14] is equivalent to the so-called ''bounce'' solution (it is called the instanton solution, too).

If we consider $(3+1)$-dimensional systems with quasirectangular-well potentials as those discussed in Sec. IV, we will see that the action of the instantonic solution is effectively infinite.

The probability Γ of barrier penetration in field theory was calculated by Coleman:[15]

$$\Gamma \sim e^{-\beta/h}, \tag{29}$$

where β is the action corresponding to the instantonic solution. Therefore, we can predict that, in the framework of field theory $(D=3)$, with an inhomogeneous potential $U(\varphi)$ with rectangular wells and barriers, the phenomenon of localization necessary will be present.

It is very important to notice that we have studied here only the critical solutions, and there is still this question: *how long will it take for a system to go from the metastable equilibrium position φ_1 to a stable position φ_3*? Indeed, we have solved this problem[44] only for $D=1$. It remains an open and hard problem for $D>1$. We hope this work could shed some light on this question.

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