Topological soliton dynamics in a stochastic ϕ^4 model

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Received 19 June 1990; revised manuscript received 20 September 1990; accepted for publication 30 October 1990
Communicated by A.R. Bishop

We study the propagation of topological solitons in a stochastically perturbed ϕ^4 model, by means of numerical simulations tested on exact predictions for this system. We establish the regimes of weak and strong noises, describe how solitons are affected and find an empirical law for energy evolution.

Nonlinear models have proved themselves a very powerful tool in a number of physical problems throughout the last two decades [1]. A class of them that have deserved increasingly attention during this period is that of nonlinear Klein–Gordon models, mainly the sine-Gordon and ϕ^4 ones. Both of them are very often related to problems in condensed matter physics (see, e.g., ref. [2] for a review). The ϕ^4 model, which we concern ourselves with in this Letter, has been used to study, for instance, structural phase transitions in ferroelectric or ferromagnetic materials [3–6], or topological excitations in quasi-one-dimensional systems (biological macromolecules [7], polymer chains [8–10]). It is usually defined by the following dimensionless Hamiltonian,

$$H=\sum_{n=1}^{N}\left[\frac{1}{2}\left(\frac{\mathrm{d}\phi_n}{\mathrm{d}t}\right)^2+\frac{\epsilon_0}{4}(1-\phi_n^2)^2\right]+\sum_{n=1}^{N-1}\tfrac{1}{2}(\phi_{n+1}-\phi_n)^2\,, \tag{1}$$

where ϕ_n stands for the nth-particle displacement from its equilibrium position na, a being the lattice constant. From (1) we can derive the equations of motion for each particle, which turn out to be

$$\frac{\mathrm{d}^2\phi_n}{\mathrm{d}t}-(\phi_{n+1}-2\phi_n+\phi_{n-1})-\epsilon_0(\phi_n-\phi_n^3)=0\,. \tag{2}$$

The model is named after the ϕ_n^4 term that appears in the second part of the Hamiltonian, i.e., in $\epsilon_0(1-\phi_n^2)^2/4$. This represents an on-site, double well potential acting on each particle of the chain. Physically, it can be originated from a heavy ion sublattice in the case of displacive systems [3,4] or hydrogen-bonded compounds [7], or from the π-electronic cloud in polymers [8–10]. The ϕ^4 model reproduces fairly well the phenomenology of these and related systems provided that the structure responsible for the regular arrangement of double well potentials is rigidly *fixed*. However, this assumption might not be satisfied in real physical situations, because the lattice that gives rise to the potentials could *fluctuate* due to thermal excitation, interaction with noisy external fields, etc., modifying its parameters (barrier height, minima positions) or, in extreme cases, its shape. Besides, inclusion of thermal and quantum fluctuations in the ϕ^4 chain leads also to changes in the potential barrier [11]. In this work we address ourselves to the study of kink propagation in one of these extensions of the ϕ^4 model, namely the following: the barrier height is allowed to vary randomly in time by setting $\epsilon_0\equiv 1+\xi(t)$, $\xi(t)$ being a Gaussian white noise with mean value $\langle\xi(t)\rangle=0$ and correlation $\langle\xi(t)\xi(t')\rangle=2D\delta(t-t')$. This particular choice for ϵ_0 is intended to represent rapid changes of the on-site potential in a large (compared to soliton width) spatial scale, as a first step that should be comprehended before considering more realistic fluctuating (and perhaps spatially inhomogeneous) models.

Apart from physical motivations, our research has to do with the general effort about the study of stochastic perturbations, not only in the ϕ^4 model [12], but in almost all of the most important nonlinear models (see ref. [13] for a review). A large part of this effort has been devoted to the sine-Gordon model (see ref. [13] and references therein), because the integrability of the unperturbed model permits the use of sophisticated perturbative techniques, like those based on the inverse scattering transform [13,14], to obtain many interesting results. The ϕ^4 model is not integrable and these procedures are not available to treat it: however, other approaches have been developed for that purpose. Such perturbative results hold up to a certain time that depends on the strength of the fluctuations and, after that moment, numerical simulations are the only known tool to achieve information on these systems. Some computational work has been carried out [12,15,16] on stochastically perturbed ϕ^4 and sine-Gordon models, for additive noises or multiplicative noises coupled *linearly* to the field ϕ, i.e. terms of the form $\epsilon_0\phi$, with ϕ_0 defined as above. Hence, this Letter is aimed to complete those works (in what respects to the ϕ^4 model) with the study of a *nonlinearly* multiplicative stochastic perturbation.

Before entering into the investigation itself, it is important to understand how the perturbation acts on a kink. Since the random term is multiplied by $(1-\phi_n^2)^2$, it is evident that the particles in the kink tails, i.e. those whose relative displacement is $\phi_n \approx \pm 1$ (or, in other words, those lying in the bottom of one of the two potentials wells), do not feel the potential variations, and subsequently behave as if there were no perturbation at all. As a result, only the center of unperturbed kinks, which are the initial condition of our simulations, will suffer the noise effects at early stages of the soliton evolution. Notice that the linearly multiplicative noises studied in refs. [12,15,16] affect the whole kink and *essentially* its tails, and so their effects are far more appreciable than the ones of our choice (we will come back to this topic below). It should be also realized that our perturbation changes the scale of the potential, turning it upside down if ϵ_0 becomes negative, but preserving the shape of the double well and the minima position, while the linearly multiplicative noises can transform it into a single well potential and vice versa.

Let us now start the study of the stochastic ϕ^4 model. Firstly, we are going to carry out a few simple analytical calculations to learn its most important characteristics. We follow the usual procedure taking the continuum limit: if kinks are much wider than the lattice spacing a, the ordinary differential equations (2) can be replaced by the partial differential equations

$$\frac{\partial^2\phi}{\partial t^2} - \frac{\partial^2\phi}{\partial x^2} - [1+\xi(t)](\phi-\phi^3)=0\,, \tag{3}$$

where the role of $\phi_n(t)$ is now played by the displacement field $\phi(x,t)$. Expression (3) with $\xi(t)=0$ is nothing but the celebrated ϕ^4 equation, and its properties are well established (see, for instance, ref. [17]). One of them is that it possesses two conserved quantities, namely the total energy and the total momentum, defined, respectively, as the integrals over the whole space axis of the following densities:

$$e(x,t)=\tfrac{1}{2}(\phi_t^2+\phi_x^2)+\tfrac{1}{4}(\phi^2-1)^2\,,$$
$$p(x,t)=-\phi_t\phi_x\,. \tag{4}$$

These quantities are not conserved anymore when $\xi(t)\neq 0$, and, in fact, we can use their evolution laws, obtained from (3), to get information about the system. For this purpose, we neglect kink distortions (radiation) caused by the perturbation, and suppose that the main effect of the noise is to turn the position and the speed of the kink center into unknown functions of time [18]. In this so-called adiabatic approach, and by means of a kink-like ansatz inserted in the evolution laws for the energy and the center of energy, it is possible to arrive (for details see refs. [12,16], and refs. [13,19] for another derivation) to the following Langevin equations,

$$v'(t)=0,$$
$$z'(t)=v(t)-v(t)[1-v^2(t)]\xi(t)\,, \tag{5}$$

where $z(t)$ represents the center of the kink, $v(t)$ is its speed, and the primes stand for the time derivatives. We can deduce from these equations that this approach is rather drastic, because it turns out that the kink speed evolves in a deterministic way (indeed, it is kept constant), and so it does not seem to suffer the effects of the perturbation. With respect to $z(t)$, having in mind initial conditions $z(0)=0$ and $v(0)=v_0$, it is easy to see that

$$\langle z(t) \rangle = v_0 t ,$$

$$\sigma^2(t) \equiv \langle z^2(t) \rangle - \langle z(t) \rangle^2 = \tfrac{1}{2} D v_0^2 (1 - v_0^2) t . \qquad (6)$$

Hence, this perturbative technique predicts that the effect of noise is mainly the introduction of an uncertainty in the position of the kink center $z(t)$, given by its standard deviation $\sigma(t)$, which grows as the square root of time, as if the kink were a point particle propagating across the medium as usual, to which an extra Brownian-like contribution coming from the stochastic term were added.

Next we pass on to the numerical results. We performed a number of simulations of the system (2) starting with initial conditions given by a ϕ^4 kink with different v_0 values for each noise strength. We used a generalization [12] of the conservative Strauss–Vázquez [20] scheme with time step $\Delta t = 0.025$ and spatial step (equivalently lattice spacing) $\Delta x = 0.05$. The spatial extent of the integration was $[-20, 20]$ (801 particles), and, as only the central 401 were perturbed, boundary effects were negligible up to time $t = 20$ (800 time steps). These parameters set up a scenario in which the continuum and the lattice models are very similar and discreteness effects, like, e.g., soliton pinning [21,22], are absent. Finally, we average over 30 realizations of the noise; we have also computed averages over 60 realizations for some cases, verifying that the results were essentially the same.

For unperturbed ϕ^4 systems, it has been shown [23] that the Strauss–Vázquez scheme is convergent and stable using the fact that it conserves a discrete energy, but when the perturbation is present, the scheme becomes stochastic and nothing is known about those desirable features. However, it can be rigorously proved [24] that the mean total energy of the system evolves according to

$$\frac{\mathrm{d}\langle E \rangle}{\mathrm{d}t} = 2D \int_{-\infty}^{\infty} \mathrm{d}x \, \langle (-\phi + \phi^3)^2 \rangle . \qquad (7)$$

We have checked whether this formula is verified in our calculations, computing $\langle E \rangle$ both from its definition and by integrating this differential equation. We always found a fair agreement between the two methods over the whole studied range of noise values ($10^{-3} < 2D < 1$), with discrepancies never higher than 3% at the end of the running time ($t = 20$). Three typical examples are shown in fig. 1. Although this is not at all a proof of the stochastic stability and convergence of the scheme, it is at least an indication of consistency, which, along with the reproduction of analytical predictions for weak noises, allows us to be confident that our simulations have actually to do with the underlying system. To our knowledge, this is the first time that such a property is found in numerical schemes to solve stochastic partial differential equations.

Let us summarize the main results of our simulations. The first general outcome was that all the features of kink propagation crucially depend on the kink speed. We observed that *for each noise strength*, slow kinks (here slow means those of simulations with initial speed $v_0 = 0$, 0.025, 0.05, 0.1, 0.2 and 0.5) were always clearly more affected by the perturbation than fast or relativistic ones ($v_0 = 0.8$, 0.9 and 0.99). Henceforth, in all the considerations we report below, we distinguish between different solitons, referring to them as *slow* and *fast*, respectively. However, we must say that the simulations do not support the existence of a critical speed separating both regimes; rather, everything takes place as if the effects of noise continuously depend on the kink speed, in such a way that ultrarelativistic kinks (namely $v_0 = 0.99$) happen to be almost unchanged by the perturbation, while the behavior of slow kinks is quite similar for all their speeds. A perturbative analysis of the problem leads to the same conclusion:

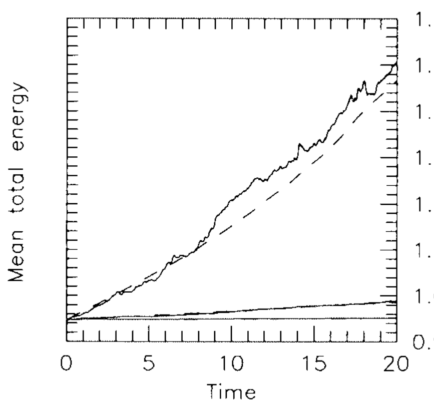

Fig. 1. Energy evolution for a kink when $v_0 = 0.1$ and $2D = 10^{-1}$ (upper curve), $2D = 10^{-2}$ (middle) and $2D = 10^{-3}$ (down). The solid lines are obtained from the energy definition, and the dashed ones from integration of the evolution law.

in ref. [25] it will be shown that the above mentioned smooth dependence comes from factors like $1-v^2$ or powers of it taking part in the first order correction (this kind of terms usually arises when studying stochastic perturbations, see, e.g., ref. [13]), so we must discard a sharp transition between these two kinds of evolution.

We now discuss what is the threshold range for the noise strength, beginning with the results related to the kink shape (remember that the main assumption of the adiabatic approach was that it was not modified). Noises with strength $2D \leqslant 10^{-2}$ did not produce visible effects on the shape of kinks independently of their initial speed. Noises with $2D=10^{-1}$ acting on slow kinks originated radiation that appeared mainly behind them, while fast ones emitted a much less amount of linear waves and still verified the adiabatic hypothesis for practical purposes. Finally, when $2D=1$, slow kinks rapidly altered, maintaining their integrity up to a certain moment in which the chain seemed to arrive at a highly unstable situation; at that moment, energy (always increasing, cf. eq. (7)), reached a value about twice or three times its initial one, and then crossed over to a quite faster growth. Shortly afterwards, this evolution ended in a blow-up of the solution (even in this extreme situation, it must be stressed that the scheme verifies quite well the energy evolution law up to the blow up time). On the other hand, fast kinks were severely distorted and radiated largely, but they did not suffer the same blow up in the time reached in our simulations. We carried out some test runnings for $2D=0.5$ and we found the same general picture of energy growing and kink instability, the main difference being that kinks survive for a longer time; the blow up was again found to be correlated to the energy crossover. In fig. 2 we show a typical example of final kink shape to illustrate the effect of intermediate (strong but not catastrophic) noises. We want to mention that this result must be compared to those in refs. [12,16], where it was established that the effect of *linearly* multiplicative perturbations becomes important over a threshold much smaller than ours, namely $2D \geqslant 2.5 \times 10^{-4}$. We believe that this is a consequence of the fact that linear perturbations influence the whole chain while the one we study here affects only the kink structure and the particles that

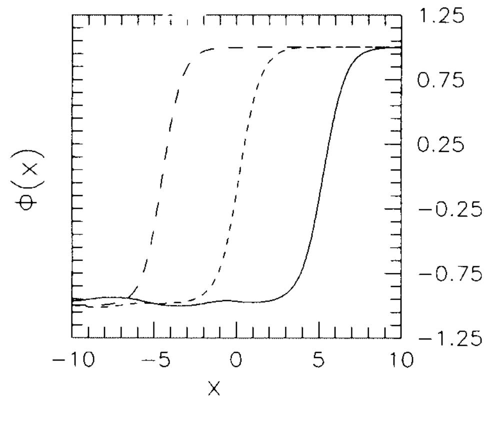

Fig. 2. A kink with $v_0=0.5$ rightwards ($2D=10^{-1}$) at $t=1$, $t=10$ and $t=20$. Radiation travelling to the left is clearly seen.

progressively move out of the minima of the double well potential.

The conclusion that we have drawn in the previous paragraph that $2D=0.1$ is some sort of a threshold (not strictly but in a wide sense, because it is not at all like a critical point) between weak and strong noises is also confirmed by checking whether eqs. (6) are recovered or not from the simulations. The first one of these formulae is never exactly verified, but we have found that when $2D \leqslant 10^{-2}$ it holds in a fairly approximate way. This is shown in fig. 3, where we have plotted the mean relative center deviation, which we define as $\Delta z \equiv [v_0 t_{\text{final}} - \langle z(t_{\text{final}}) \rangle]/v_0 t_{\text{final}}$ versus noise strength, t_{final} being the final time reached in the simulations (t = 20 time units as we mentioned above) and $\langle z(t_{\text{final}}) \rangle$ the mean position reached by the kink at that time. It can be seen from that plot that when noise strength is equal or less than 10^{-2}, Δz is less than 3%. Notice that for each noise strength there are several points, each one of them corresponding to a different initial speed. We have always observed that the greater the initial speed was, the less Δz became for each value of noise, although Δz had almost the same value for all the slow kinks. The values of Δz began to be large for noises of strength $2D=0.1$ (cf. fig. 3) except for fast kinks (notice the lower point at $2D=0.1$, outside the error bars, in fig. 3; it corresponds to $v_0=0.8$). Finally, for $2D=1$ we have already reported that slow kinks suffered a blow up; in spite of this, we have plotted in fig. 3 the same quantity Δz,

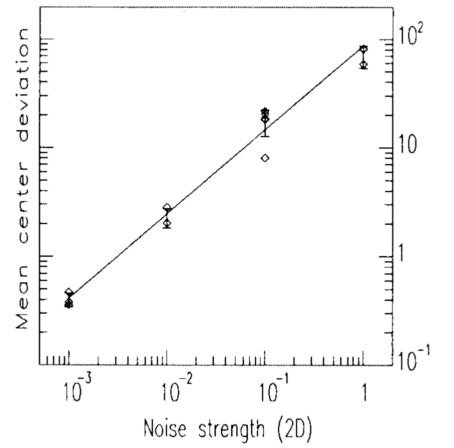

Fig. 3. Log-plot of $\Delta z \equiv [v_0 t_{final} - \langle z(t_{final}) \rangle]/v_0 t_{final}$ versus $2D$. Δz is expressed in the ordinate axis as a percentage. Points for each noise value correspond to different v_0, while error bars indicate the standard sample deviation of such sets of values. The line is a fit to all the points given by $y=399.47 \times (2D)^{0.997}$. Ultrarelativistic results are not shown.

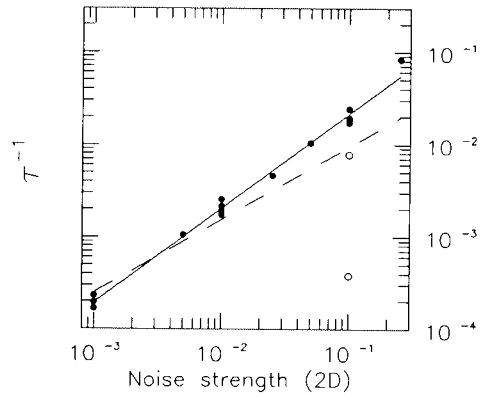

Fig. 4. τ^{-1} versus $2D$. Dashed line ($\tau^{-1}=0.058(2D)^{0.789}$) fits all the points, solid ($\tau^{-1}=0.226(2D)^{1.022}$) all but the two empty circles (upper, $v_0=0.8$; lower, $v_0=0.99$). Points for the same noise correspond to different v_0 as in fig. 3. Error bars are not shown for the sake of plot clarity.

but computed when the energy was twice its initial value, instead of at t_{final}. It can be seen that there is an enormous discrepancy between the adiabatic approach and the numerical results. Another piece of evidence supporting $2D \sim 0.1$ as an approximate threshold comes from $\sigma(t)$. We tested the verification of (6) by fitting power law dependences of the form $\sigma(t) \sim \sigma_0 t^s$ to the numerical results, and we found that for $2D=10^{-3}$ and $2D=10^{-2}$ the so obtained σ_0 and s compare rather well to the theoretical prediction in (6). On the other hand, when noise strength was 0.1, this was not true anymore for slow kinks: σ_0 had nothing to do with the prediction and s reached values around 2. We again stress that there was not a sharp transition but a smooth one; some test experiments with noises between 0.01 and 0.1 showed values of s between 1 and 2, and σ_0 became progressively different from the predicted value. Fast kinks show the same features but, once more, for (about one order of magnitude) stronger noises than slow ones.

The most remarkable outcome of the simulations is that the energy evolution was actually exponential, $E(t) \sim E_0 \exp(t/\tau)$, E_0 being essentially the energy of the initial kink. The exponent τ^{-1} turned out to be roughly linearly dependent on the noise and, for each noise strength, not too strongly dependent on the speed when computed for slow kinks, and quickly decreasing with increasing speed for fast ones. These results are shown in fig. 4, where the dependence on noise strength can be seen, and in fig. 5, where, as an example, we plot the values we obtained for τ^{-1} for different initial speeds at $2D=0.1$. τ has the sense of a stability time, the time for energy to be over twice its initial value, which as we mentioned above, results to be a crossover point to a regime of rapid destruction. This is interesting because τ can be estimated through the empirical law shown in fig. 4, and then we can a priori predict an approximate mean stability time for each kink speed and noise strength. Finally, we complete the description of our findings on the chain energy with a comment concerning its spatial distribution, which exhibits a peculiar be-

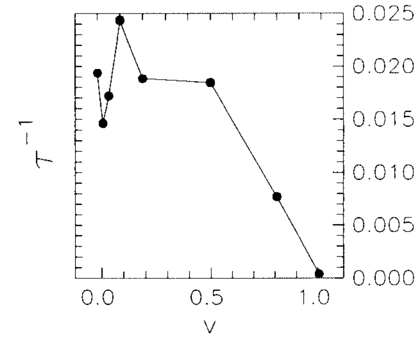

Fig. 5. τ^{-1} versus v for $2D=0.1$. Line is only a guide to the eye.

havior as well. As we have already explained above, it is evident that, initially, the perturbation injects energy in the chain only through the kink structure. We found numerically that more than that energy flows outwards the center in the form of radiation, causing an energy loss in the structure and a global slowing down of the soliton.

It seems to us that the role of the kink structure is fundamental in explaining all the above described phenomena. As we have already mentioned, at least at the first stages of the evolution (i.e. before an important amount of radiation appears), only the particles in the structure will experience the effects of noise. At this point, it is important to observe that the faster the kink is, the narrower it is due to Lorentz contraction: for instance, a kink with speed 0.2 has a width of some 150 particles in our lattice, and the structure of one with speed 0.99 has around 25. Hence, it becomes clear that relativistic kinks have to be less affected. On the other hand, the center of slow kinks spends much more time at the same zone of the chain than that of fast ones; thus, the structure of a kink with constant speed 0.2 would take about 30 time units to cross a certain point, and around 1 time unit if its velocity were 0.99. As the strongly affected particles are those that belong to the soliton center, when a relativistic kink propagates they are not always the same ones, because the soliton rapidly passes over them; instead, when slow kinks are propagating, the same zone of the chain is disturbed for a much longer time, and then the perturbation effects accumulate and become more appreciable. In fact, coming back to our example, our simulations reached $t=20$ time units, and we estimated above the time at which a $v_0=0.2$ kink leaves a certain zone as 30 time units (this time would be even greater taking into account the slowing down of the kink); hence, a group of particles was affected along the entire simulation. In contrast, this was not so in the case of $v_0=0.99$. Lastly, we must also realize that the particles in a relativistic kink structure have far more kinetic energy than those of slow kinks. This property allows them to overcome quite more easily the changes in the barrier height produced by the perturbation, and so the kink propagates with less distortions, and its integrity is preserved under stronger noises than in slow propagation.

The considerations in the preceding paragraph should be sufficient to understand the root of the differences between slow and fast kinks. We believe that the $s>1$ exponents for $\sigma(t)$ and the exponential behavior of the energy might also be qualitatively explained. As energy flows out of the structure, it puts more and more particles away from their equilibrium positions. Thereafter, they begin to be perturbed, moving around the minima in a harmonic-like way (radiation). Their motion is transmitted to their neighbors, and so on. This sort of feed-back process might be the reason for the exponential increasing of the total energy. Since the slow kink structure is much wider than the one of fast kinks, they can initiate this mechanism in a more effective way. Besides, radiation contributes to the uncertainty of the kink center positions, and to the growing of this magnitude, because it generates more waves on its own. This could be the explanation for the anomalous evolution of $\sigma(t)$, and in addition, for the differences between slow and fast solitons.

We finish this Letter with a summary of our main findings. First, we have shown that our procedure to numerically simulate this stochastic model (and maybe other related ones) has some nice consistency properties that make it quite reliable. Second, we have found a general dependence of the results on the initial speed of kinks; though there is not a sharp transition between them, we can loosely speak of slow ($v_0\leqslant 0.5$) and fast ($v_0\geqslant 0.8$) kinks. These two kinds of kinks exhibit the same features but for a different range of noises: while the adiabatic approach holds approximately (though never exactly) for slow kinks under noises with $2D\leqslant 10^{-2}$ and clearly fails when $2D\geqslant 0.1$, fast ones verify the adiabatic assumption even near this last value. Indeed, the higher the initial speed is, the higher the validity limit of the approach becomes. Third, we have described the single kink dynamics in the strong noise regime. Its main characteristics are the slowing down of the kink and the anomalous center standard deviation, which behaves as t^s where s grows with increasing noise strength up to values around 2. Lastly, we have been able to find an empirical law for the energy behavior, that is exponentially increasing, with an exponent dependent mainly on the noise strength and besides being greater for slow kinks than for fast ones. As the kink destruction for very strong noises happens to be correlated with a certain energy value, this gives a predictive usefulness to our study, allowing to estimate a mean stability time for each initial kink. Further research is in progress [25] to completely understand these facts and treat them analytically, as well as to include dissipation and boundaries in the system. In this way the model will be more realistic, contributing to clarify the intrincate relation between fluctuations, disorder and nonlinear phenomena.

We thank the authors of ref. [24] for making available their results to us prior to publication, in particular J.M.R. Parrondo for valuable and illuminating discussions, and R. Brito for a critical reading of the manuscript. We also thank the detailed referee's remarks, which helped us to write a more understandable Letter. We acknowledge the kind allowance of the Centro de Investigaciones Energéticas, Medio Ambientales y Tecnológicas (C.I.E.M.A.T., Spain) to use their IBM 3090 computer. This work has been supported in part by the Dirección General de Investigación Científica y Tecnica (D.G.I.C.yT., Spain) under grant PB86-0005. A.S. was also supported by a fellowship from the program Formación de Personal Investigador of the Ministerio de Educacion y Ciencia (Spain).

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