Particle-like solutions in nonequilibrium 3D media.

A. S. Lomov and M. I. Rabinovich
Institute of Applied Physics, Academy of Sciences of the USSR

(Submitted 9 November 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **48**, No. 11, 598–602 (10 December 1988)

A model of a two-component nonlinear field is proposed for describing the self-focusing of stable, localized 3D structures. A numerical simulation has revealed the simplest such structures: the "elementary particles." Bound states of these particles are used to form arbitrary stable localized solutions.

1. Although attempts to find particle-like solutions for nonlinear fields have been pursued actively for a fairly long time now, the effort has so far been rewarded with only a few examples of stable localized solutions. Fundamental progress in this direction stemmed from the discovery of solitons. Stable static solitons, however, occur only in a 1D situation. Long-lived 2D and 3D solitons are usually time-varying.[1,2] One might expect that solitary 3D static solutions should exist stably according to the nonlinear field equations which describe the processes that occur in nonequilibrium dissipative media. Self-focusing stable spatial lattices are known to be observed in such media. These may be lattices with square cells, honeycombs, etc.[3-5] The appearance and establishment of such lattices are usually described by gradient field equations of the type $(\partial u_j/\partial t) = -(\delta F/\delta u_j)(\delta F/\delta u_j$ is a variational derivative, and the functional F has the meaning of a free energy). Since we are interested in equations which allow the establishment of localized static structures, equations of this sort would also naturally be sought in the class of gradient field equations (or of the related equations which have been perturbed in such a way that the localization mechanism which results from the perturbation does not disrupt the aperiodic time evolution of the field).

As generating equations it is meaningful to use gradient equations of fields which are characterized by a corresponding length scale (which also determines the lattice constant). The existence of such a scale is usually associated with a pronounced spatial dispersion, which is manifested in the structure of F by the appearance of spatial derivatives of various orders. One of the simplest functionals of this type might be a free-energy functional in the Swift-Hönberg form,

$$F_1 = \int \left(\frac{\alpha}{2} u_1^2 - \frac{\beta}{3} u_1^3 + \frac{1}{4} u_1^4 + \frac{1}{2} [(q^2 + \nabla^2) u_1]^2 \right) d\mathbf{r}. \quad (1)$$

The terms ∇^2 and ∇^4 describe diffusion of various orders; their joint effect determines the length scale of the lattice which arises in the nonequilibrium medium. An individual cell of such a lattice may serve as a prototype of a localized static structure, but only if it becomes independent of the other cells. Such a situation is possible if the field outside the cell is suppressed by some other field; i.e., the medium must not be a single-componemt medium.

Let us assume that in addition to the field u_1 we have a field u_2, which is described by a functional

$$F_2 = \int \left(-\frac{1}{2} u_2^2 + \frac{\gamma}{4} u_2^4 + \frac{1}{2} D \nabla^2 u_2^2\right) d\mathbf{r}. \tag{2}$$

The equations which we are seeking are then written in the form $(\zeta, \xi > 0)$

$$\frac{\partial u_1}{\partial t} = -\frac{\delta F}{\delta u_1} + \zeta \Phi_1(u_1, u_2), \qquad F = F_1 + F_2 \frac{1}{\mu}, \tag{3}$$

$$\frac{\partial u_2}{\partial t} = -\frac{\delta F}{\delta u_2} + \xi' \Phi_2(u_1, u_2).$$

The perturbations $\Phi_1(u_1,u_2)$ and $\Phi_2(u_1,u_2)$ describe the interaction between u_1 and u_2. We choose these functions in the form $\Phi_1 = u_1 u_2$, $\Phi_2 = u_1$. We then have a clear physical interpretation: In that part of the space in which u_1 is negative, the field u_2 also goes negative, and it suppresses u_1 in the immediate vicinity. As a result, we find the system of equations

$$\frac{\partial u_1}{\partial t} = [(\zeta u_2 - \alpha) - (q^2 + \nabla^2)^2] u_1 + \beta u_1^2 - u_1^3, \tag{4}$$

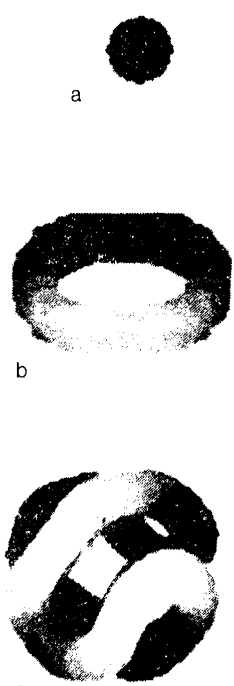

FIG. 1. The elementary particles which are described by Eqs. (4) and (5). a: Sphere. b: Torus. c: Spherical lattice. The parameter values are $\alpha = 0.3$, $\beta = 1$, $\zeta = 1$, $\mu = 0.05$, $\gamma = 4$, and $D = 0.1$ (here and in the other figures, the spatial distribution of the surface $u_1 = \text{const} = 0.4$ is shown; the parameter values are held constant).

$$\mu \frac{\partial u_2}{\partial t} = u_2 - \gamma u_2^3 + \xi u_1 + D\nabla^2 u_2 , \qquad \xi = \xi' \mu \ . \tag{5}$$

The variables u_1 and u_2 in this system can be interpreted as (for example) the deviations of the concentration of a substance (u_1) and of the temperature (u_2) from the equilibrium values in the medium in which an exothermic reaction is occurring.

Since different spatial lattices (including lattices with different defects) are typically established for a field described by functional (1), depending on the initial conditions, i.e., since there is a multistability, we might expect that different localized structures would also be realized in our model at identical values of the parameters but under different initial conditions. It thus seems important not only to establish the fact that stable particle-like solutions exist in system (4), (5) but also to identify the elementary particles which are formed in the interaction of various bound states.

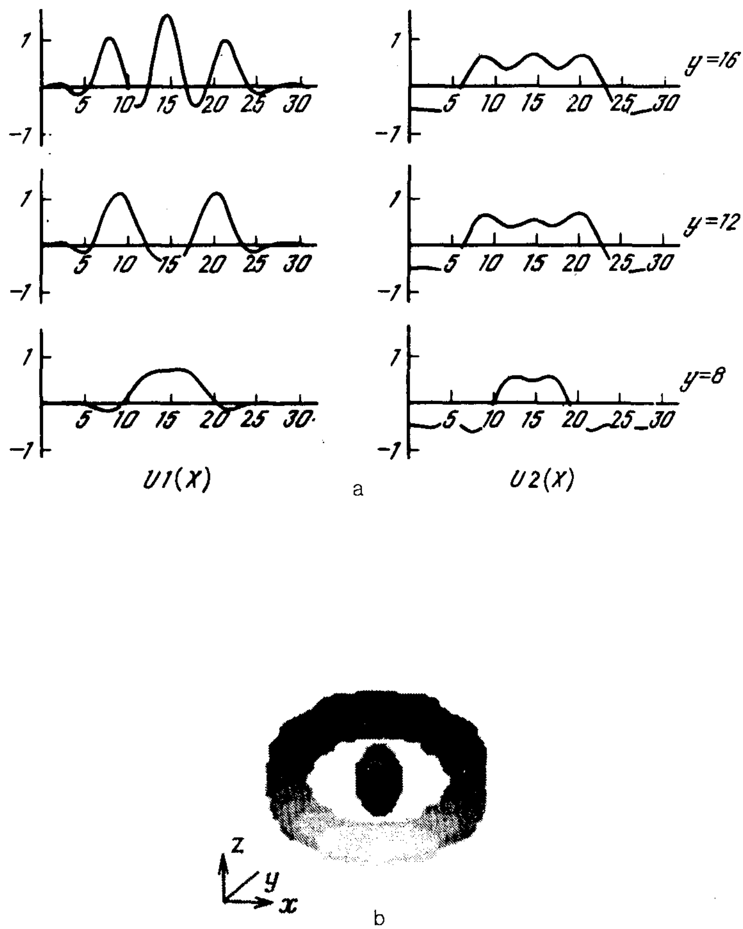

FIG. 2. a—Distribution of the fields u_1 and u_2 for the torus-sphere bound state shown in part b.

2. Numerical simulations have shown that model (4), (5) does indeed describe a self-nucleation and a stable existence of particle-like 3D solutions of various topologies. Three elementary particles have been observed: a sphere, a torus, and a spherical lattice (Fig. 1). Their length scales are $\sim q$. With appropriate initial conditions, stable solutions in the form of bound states of these elementary particles (identical or different) have been realized (see Figs. 2 and 3).

The system of equations was solved by a direct difference method under the boundary conditions $u_1|_S = 0, (\partial u_2/\partial n)|_S = 0$ in a region with dimensions of $32\times 32\times 32$. Control calculations were carried out with a time step smaller by a factor

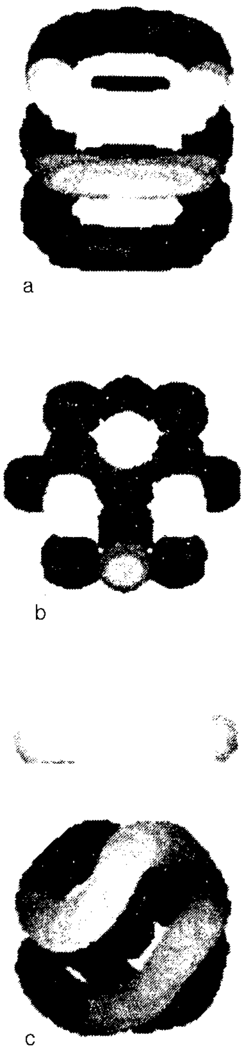

FIG. 3. Examples of stable bound states. a—Three tori; b—cluster of spheres; c—torus and spherical lattice with a sphere inside.

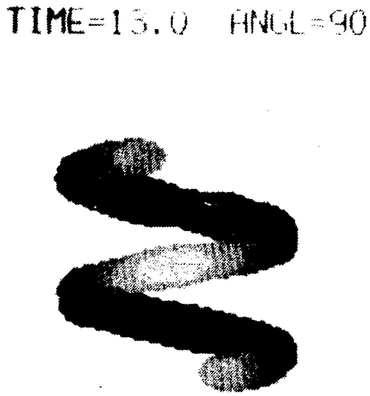

FIG. 4. Metastable structure in the form of a helix.

of four and with a coordinate step smaller by a factor of two. A calculation was pursued until the system reached a steady-state solution; in most cases, no more than 100 time units were required. Some typical parameter values are $\alpha \lesssim 0.5$; $\beta = 1.5$; $0.05 \leqslant \mu \leqslant 0.1$; $\gamma = 4$; $\zeta = 1$; $q = 1$; $\xi = 0.15$; and[1)] $D = 0.1$. It was found that the spatial orientation of the elementary particles is arbitrary: It is determined exclusively by the initial conditions. The topology and dimensions of the particles are universal and do not change when the boundary conditions or the dimensions of the region are changed. We wish to emphasize that in a certain region of imitial conditions nonlinear field (4), (5) allows the formation of a variety of structures, which are not immediate bound states of the elementary particles, e.g., the helix in Fig. 4. However, structures of this type are not attractors (in this case, trivial attractors: equilibrium states) of the system under study, and in the limit $t \to \infty$ they become bound states of elementary particles.

We wish to stress that the physical mechanisms underlying this spontaneous formation of particle-like solutions of a 3D field (associated with the nature of the interaction of the components and the spatial dispersion) are fairly general (see also Refs. 6 and 7) and may operate in a wide variety of nonequilibrium media.

All the calculations were carried out at the multiprocessor complex of the Institute of Space Research, Academy of Sciences of the USSR.

We are indebted to I. S. Aranson, A. V. Gaponov-Grekhov, K. A. Gorshkov, M. M. Sushchik, and E. L. Feinberg for useful discussions.

[1)]At larger values of D and at the given values of the other parameters, the localized structures spread out. At $0 < D < D_0$, the spontaneous formation of any localized solutions is determined by the development of finite-dimensional perturbations.

[1]P. Christiansen, P. Lomdahl, and N. Zabusky, Appl. Phys. Lett. **39**, 170 (1981).

[2]V. G. Makhan'kov, Fiz. Elem. Chastits At. Yadra **14**, 123 (1983) [Sov. J. Part. Nucl. **14**, 50 (1983)].
[3]C. Normand, Y. Pomeu, and M. C. Velarde, Rev. Mod. Phys. **49**, 591 (1977).
[4]J. E. Wesfreid and S. Zaleski (editors), Cellular Structures in Instabilities, Lecture Notes in Physics, Springer, New York, 1984.
[5]A. B. Ezerskiĭ, P. I. Korotin, and M. I. Rabinovich, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 129 (1985) JETP Lett. **41**, 157 (1985)].
[6]A. V. Gaponov-Grekhov, A. S. Lomov, and M. I. Rabinovich, Pis'ma Zh. Eksp. Teor. Fiz. **44**, 224 (1986) [JETP Lett. **44**, 286 (1986)].
[7]A. V. Gaponov-Grekhov, A. S. Lomov, G. V. Osipov, and M. I. Rabinovich, Preprint No. 199, Institute of Applied Physics, Academy of Sciences of the USSR, Gor'kiĭ, 1988.

Translated by Dave Parsons