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Coupled Fractal Nanosystem: Trap – Quasi-two-dimensional Structure

O.P. Abramova * and S.V. Abramov

Donetsk National University, 24 University st., Donetsk, 83001, Ukraine

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Abstract: For a model nanosystem various types of quasi-two-dimensional fractal structures are obtained. To this end the theory of fractional calculus and the concept of fractal are used. Various types of fractal nanotraps based on quasi-two-dimensional fractal structures are obtained by the method of sections. It is shown that the behavior of the deformation field for the coupled state of the fractal nanosystem is essentially different from the behavior of the deformation field for the uncoupled state. It is proposed to use fractal nanotraps for trapping individual particles or groups of particles in order to study their physical properties.

Keywords: *quasi-two-dimensional fractal structures; fractional calculus; nanosystem; nanotraps; numerical modeling.*

Mathematics Subject Classification (2010): 93A10, 93A30.

1 Introduction

Investigating the fundamental properties of nanosystems and nanomaterials of a new generation [9–11, 14] is actual for the modern areas of nanotechnology, structural and nonlinear mechanics [8]. The active nanostructural elements in real nanomaterials are clusters, pores, quantum dots, wells, two-dimensional quantum billiards (quantum corrals) [17]. These elements can find their application in quantum information science, nanomechanics, quantum optics, and for the quantum computers, molecular spin memory devices [14]. The theoretical description of the chaotic states in the structural mechanics, analysis of nonlinear dynamical models of attractors and the chaotic simulation are discussed in the books [8, 16–18].

Quasi-two-dimensional fractal structures such as fractal linear, elliptic and hyperbolic dislocations, fractal quantum dots (particles or groups of particles) [3–6] may occur in

* Corresponding author: mailto:oabramova@ua.fm

model nanosystems. The location of the singular points (attractors) of the deformation field in the core of fractal structures is typical for linear dislocation, real ellipse, hyperbola or an imaginary ellipse. In the general case the behavior of the deformation field near these singular points is stochastic and has unusual quantum statistical properties [3–6], there is the presence of quantum chaos [17].

For theoretical description of fractal objects it is proposed to use the theory of fractional calculus [15], the Hamilton operators [1, 2] and the concept of fractal [12]. For experimental investigations of physical properties of individual atoms (electrons, photons) and quantum measurement it is needed to create special traps: nanosystems are represented by a trapped particle (or a group of particles) in the trap. W. Paul [13] considered the electromagnetic traps for charged and neutral particles (having a dipole moment). In [17] the traps (quantum corrals) constructed experimentally from individual atoms (molecules) are considered. Physical properties of the particles placed in such traps qualitatively differ from those of free particles. If we have single atom in the trap, it is possible to observe the interaction of the atom with the radiation field and the statistical behavior of a single atom in a pure form. Using the variety of external actions (acoustic, electromagnetic, mechanical excitation, laser cooling, etc.), we can change the state of the atoms in the trap [11, 14, 17]. In papers [9, 10] the experimental methods that made it possible to measure and govern individual quantum systems are proposed.

The purpose of this paper is to investigate the possibility of constructing fractal nanotraps based on quasi-two-dimensional fractal structures and governing the behavior of coupled systems: fractal trap – fractal structure.

2 Fractal Structures and Fractal Traps

We consider a model nanosystem [3–6]: volumetric discrete lattice $N_1 \times N_2 \times N_3$, whose nodes are given by integers n, m, j, $(n = \overline{1, N_1}$; $m = \overline{1, N_2}$; $j = \overline{1, N_3})$. The dimensionless variable displacement u of lattice nodes in a fractal trap is described by analogy with [3 - 6], but with a changed value Q

$$u = (1 - \alpha)(1 - 2sn^2(u - u_0, k))/Q. \tag{1}$$

Here α is the fractal dimension of the deformation field u along the Oz-axis ($\alpha \in [0, 1]$); u_0 is the constant (critical) displacement; k is the modulus of the elliptic sine.

The changed value Q considers both the interaction of the nodes in the main plane of rectangular discrete lattice and the interplanar interactions by an angular parameter $\varphi(j)$. This allows to fulfill a stochastic (due to changes in the internal parameters, the process of self-organization) governing of the alteration of these structures. The initial expression for Q in the coordinate system nOm has the form

$$Q = p'_0 + q_1 + q_2; \quad q_1 = p'_1 n + p'_2 m; \quad q_2 = -(p_{11}n^2 - 2p_{12}nm + p_{22}m^2). \tag{2}$$

Here the functions q_1, q_2 are linear quadratic forms with respect to the independent variables n, m. The expression (2) has six parameters. The parameter p'_0 is independent of the variables n, m; parameters p'_1, p'_2 are included in the linear form; parameters p_{11}, p_{12}, p_{22} determine the behavior of the quadratic form.

The rotation operation of the coordinate axes by angle $\varphi > 0$ is used to go from the coordinate system nOm to the coordinate system $n'Om'$ according to the formulas

$$n' = n\cos\varphi - m\sin\varphi; \quad m' = n\sin\varphi + m\cos\varphi. \tag{3}$$

Doing the operation of parallel translation of the coordinate system we obtain an expression for Q

$$Q = p_0 - b_1(n' - n_0)^2/n_c^2 - b_2(m' - m_0)^2/m_c^2. \tag{4}$$

Here, the previous parameters are related with the new parameters by expressions

$$\begin{gathered} p_0' = p_0 - b_1 n_0^2/n_c^2 - b_2 m_0^2/m_c^2; \quad p_1' = 2n_0 b_1 \cos\varphi/n_c^2 + 2m_0 b_2 \sin\varphi/m_c^2; \\ p_2' = 2m_0 b_2 \cos\varphi/m_c^2 - 2n_0 b_1 \sin\varphi/n_c^2; \quad p_{11} = b_1 \cos^2\varphi/n_c^2 + b_2 \sin^2\varphi/m_c^2; \\ p_{22} = b_1 \sin^2\varphi/n_c^2 + b_2 \cos^2\varphi/m_c^2; \quad p_{12} = (b_1/n_c^2 - b_2/m_c^2)\sin\varphi\cos\varphi. \end{gathered} \tag{5}$$

Parameters $(n_c')^2 = p_0 n_c^2/b_1$, $(m_c')^2 = p_0 m_c^2/b_2$ play the role of semi-axes of quasi-two-dimensional structures of the type of elliptical or hyperbolic dislocation in a coordinate system $n'Om'$. To classify the type of fractal structures, we introduce a row-vector $b = (b_1, b_2, p_0)$.

When $b = b_{11} = (1, 1, p_{01})$, $p_{01} > 0$ a fractal elliptical dislocation at state 1 (ED1) is obtained. When $b = b_{12} = (-1, -1, -p_{01})$ a fractal elliptical dislocation in state 2 (ED2) is obtained.

For fractal hyperbolic dislocation we have four states HD1, HD2, HD3, HD4 with $b = b_{21} = (1, -1, p_{02})$, $b = b_{22} = (1, -1, -p_{02})$, $b = b_{23} = (-1, 1, p_{02})$, $b = b_{24} = (-1, 1, -p_{02})$, respectively, where $p_{02} > 0$.

The fractal quantum dot in the two states QD1, QD2 is obtained at $b = b_{31} = (1, 1, -p_{03})$, $b = b_{32} = (-1, -1, p_{03})$, respectively, where $p_{03} > 0$.

The set of fractal quantum dots (the imaginary line dislocations) can be in four states SQD1, SQD2, SQD3, SQD4 with $b = b_{41} = (1, 0, -p_{04})$, $b = b_{42} = (0, 1, -p_{04})$, $b = b_{43} = (-1, 0, p_{04})$, $b = b_{44} = (0, -1, p_{04})$, respectively, where $p_{04} > 0$.

Fractal linear split dislocation can be in four states LSD1, LSD2, LSD3, LSD4 with $b = b_{51} = (1, 0, p_{05})$, $b = b_{52} = (0, 1, p_{05})$, $b = b_{53} = (-1, 0, -p_{05})$, $b = b_{54} = (0, -1, -p_{05})$, respectively, where $p_{05} > 0$.

The stochastic state of the whole lattice can be realized in two states SSL1, SSL2 with $b = b_{61} = (0, 0, p_{06})$, $b = b_{62} = (0, 0, -p_{06})$, respectively, where $p_{06} > 0$.

The initial fractal quasi-two-dimensional structures are obtained by using the iterative method to solve the equation (1) with Q in the form (2) for the angular parameter $\varphi = 0$, for the values of other constant parameters $\alpha = 0.5$, $k = 0.5$, $u_0 = 29.537$, $n_0 = 14.3267$, $n_c = 9.4793$, $m_0 = 19.1471$, $m_c = 14.7295$, $N_1 = 30$, $N_2 = 40$.

Using the method of sections of original fractal structures (Fig. 1) other sectioned fractal structures (Fig. 2) can be obtained.The original structures are shown in Fig. 1: structure SSL1 for parameter $p_{06} = 0.1523$ (Fig. 1 (a)); structure ED1 for parameter $p_{01} = 1.0123$ (Fig. 1 (b)); structure QD2 for parameter $p_{03} = -3.457 \cdot 10^{-11}$ (Fig. 1 (c)).

Sectioned fractal structures can be used as fractal traps for trapping or capturing other fractal quasi-two-dimensional structures (particles or groups of particles) in order to investigate their physical properties. The deformation field of fractal traps is essentially stochastic both in the area core and inside the fractal structure (Figs. 1, 2). The state of fractal trap at the transition from one node plane to another ($j = \overline{1, N_3}$) can be changed by using the parameter $\varphi(j)$. Sectioned fractal traps (Fig. 2) allow to obtain porous traps: the pores can be on the boundary nodal planes and inside the bulk nanosystem.

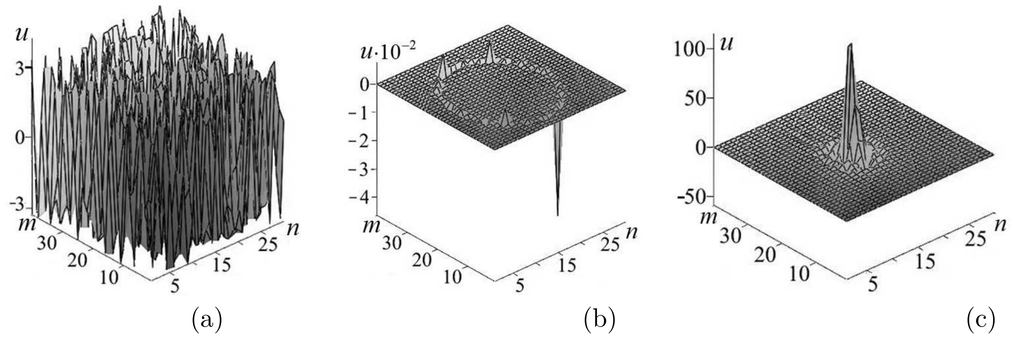

Figure 1: The behavior of the functions u of the original fractal structures on n, m for $\varphi = 0$: SSL1, $p_{06} = 0.1523$ (a); ED1, $p_{01} = 1.0123$ (b); QD1, $p_{03} = -3.457 \cdot 10^{-11}$ (c).

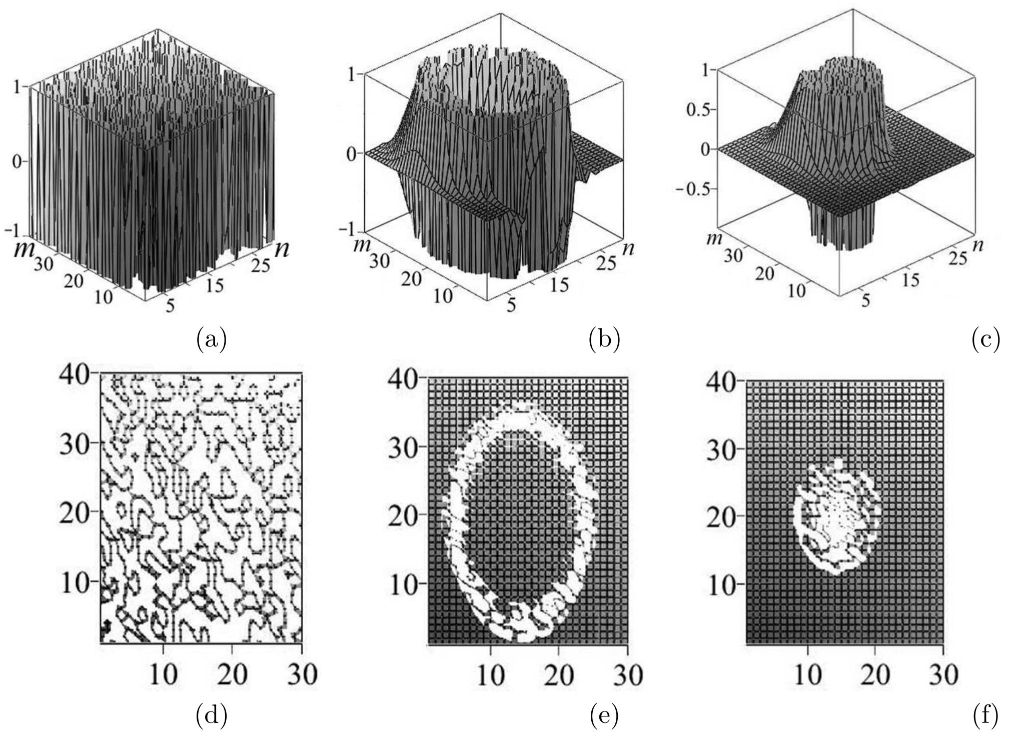

Figure 2: The behavior of the functions u of sectioned structures (a, b, c) and their cuts (d, e, f) $u \in [-1, 1]$ (top view) on n, m for $\varphi = 0$: SSL1 (a, d); ED1 (b, e); QD1 (c, f).

3 Coupled Systems: Fractal Trap - Fractal Structure

We investigate the state of the system: the fractal trap – fractal structure (Figs. 3, 4). The state of such a system is significantly different depending on the choice of the type of the iteration process when solving the basic non-linear equations.

As fractal traps the fractal structures SSL1 (Fig. 1 (a)), ED1 (Fig. 1 (b)) are used. As fractal structures the structures QD1 (Fig. 1 (c)); SQD1 with $p_{04} = 3.457 \cdot 10^{-11}$ are chosen.

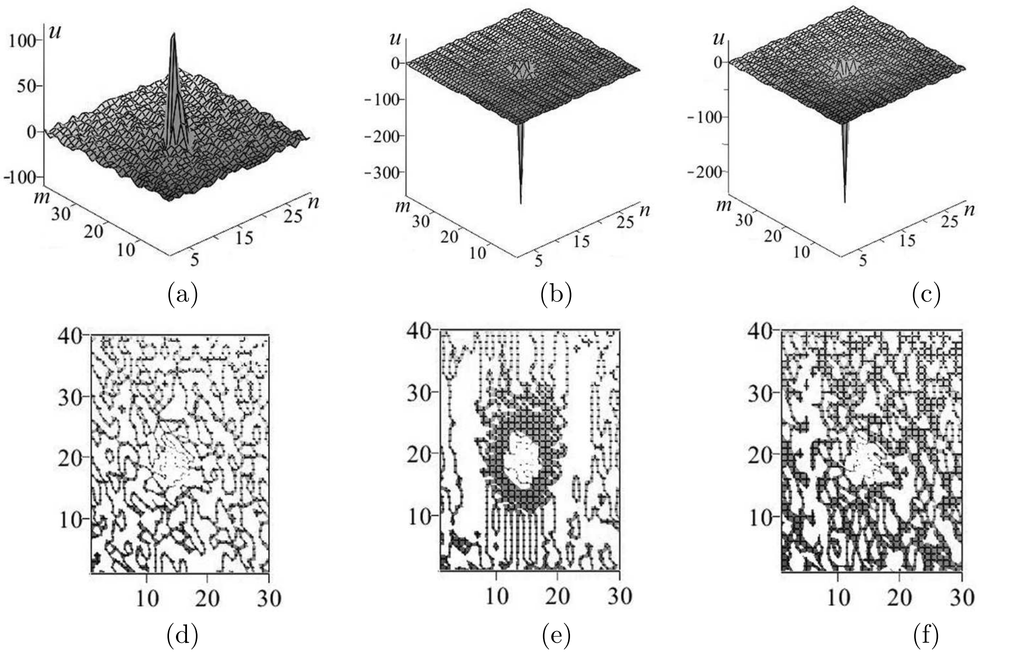

Figure 3: The behavior of u of structure SSL1-QD1 (a, b, c) and cuts (d, e, f) $u \in [-1, 1]$ on n, m for $\varphi = 0$: uncoupled state A (a, d); coupled state B (b, e); deviation δ (c, f).

We investigate the states of the following systems: SSL1-QD1; ED1-QD1; SSL1-SQD1; ED1-SQD1. Independent displacement functions for trap u_1 and structure u_2 are determined by using the iteration method with its values Q_1 and Q_2 structures for selected higher structures by the solution of independent nonlinear equations, respectively

$$u_1 = (1 - \alpha)(1 - 2sn^2(u_1 - u_0, k))/Q_1; \tag{6}$$

$$u_2 = (1 - \alpha)(1 - 2sn^2(u_2 - u_0, k))/Q_2. \tag{7}$$

In this case, the displacement function of the system is given by $u_A = u_1 + u_2$ (uncoupled state A). For the coupled system the nonlinear equation for the displacement function u (coupled state B) is given in the form

$$u = (1 - \alpha)(1 - 2sn^2(u - u_0, k))/Q_1 + (1 - \alpha)(1 - 2sn^2(u - u_0, k))/Q_2; \quad u_B = u. \tag{8}$$

The deviation of the displacement system (state B from state A) is described by the function

$$\delta = (u_B - u_A)/2. \tag{9}$$

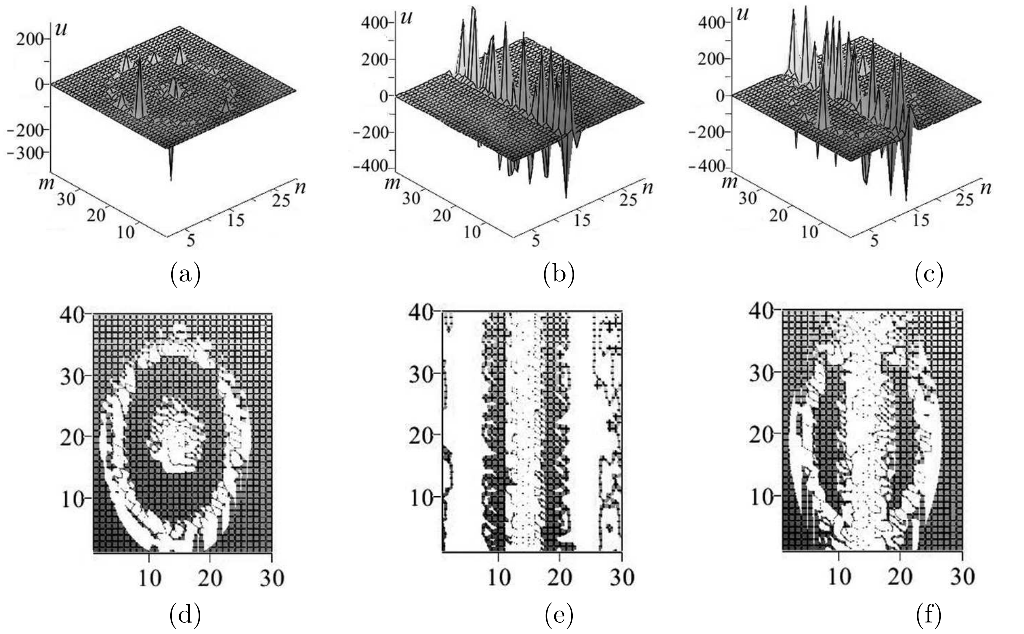

Figure 4: The behavior of the functions u of structures ED1-QD1 (a); SSL1-SQD1 (b); ED1-SQD1 (c) and cuts (d, e, f) $u \in [-1, 1]$ (top view) on n, m for $\varphi = 0$ in state B.

The fractal trap SSL1 (Fig. 1 (a)) and the fractal structure QD1 (Fig. 1 (c)) are selected to investigate the displacement function u of system SSL1-QD1 (Fig. 3). For the uncoupled state A (Figs. 3 (a, d)) the behavior of the displacement function is significantly different from that of the displacement function for the coupled state B (Figs. 3 (b, e)). This changes the direction and the amplitude of the main peak and the behavior of the deformation field in the whole area $N_1 \times N_2$ of the nodal plane of the lattice. The dependency of the deviation δ for these states from n, m is given in Figs. 3 (c, f). Some other types of coupled structures (in state B) are shown in Fig. 4.

For these structures the behavior of the displacement functions for coupled state B is also essentially different from that of the displacement function for the uncoupled state A. In this case, the fractal structure QD1 can play the role of a single particle, and the fractal structure SQD1 - the role set of particles.

4 The Influence of Translation and Rotation on the State of the Coupled System

We investigate the influence of the angular parameters $\varphi = \varphi_{61}$ (for the traps SSL1), and $\varphi = \varphi_{31}$ (for the fractal structure QD1) on the state of the coupled system SSL1-QD1.

The initial state of this coupled system for $\varphi_{61} = 0$ and $\varphi_{31} = 0$ is given in Figs. 3 (b, e). Fractal trap SSL1 remains in the initial state with $\varphi = \varphi_{61} = 0$, then from (2), (5) for Q_1 we obtain

$$Q_1 = p_{06}; \quad p'_0 = p_{06}; \quad p'_1 = p'_2 = p_{11} = p_{22} = p_{12} = 0. \tag{10}$$

For the structure QD1 being captured at $\varphi = \varphi_{31} \neq 0$ from (2), (5) we find the expression for Q_2

$$Q_2 = p'_0 + p'_1 n + p'_2 m - p_{11} n^2 + 2p_{12} nm - p_{22} m^2; \tag{11}$$

$$p'_0 = -p_{03} - n_0^2/n_c^2 - m_0^2/m_c^2; \quad p'_1 = 2n_0 \cos\varphi_{31}/n_c^2 + 2m_0 \sin\varphi_{31}/m_c^2;$$

$$p'_2 = 2m_0 \cos\varphi_{31}/m_c^2 - 2n_0 \sin\varphi_{31}/n_c^2; \quad p_{11} = \cos^2\varphi_{31}/n_c^2 + \sin^2\varphi_{31}/m_c^2; \tag{12}$$

$$p_{22} = \sin^2\varphi_{31}/n_c^2 + \cos^2\varphi_{31}/m_c^2; \quad p_{12} = (1/n_c^2 - 1/m_c^2)\sin\varphi_{31}\cos\varphi_{31}.$$

The displacement function $u_B = u$ of the coupled system SSL1-QD1 (Fig. 5) is determined when solving the nonlinear equation (8) with the values for Q_1 from (10) and Q_2 from (11)-(12) for the angular parameter $\varphi_{31} = \pi/8$ (right polarization) and $\varphi_{31} = -\pi/8$ (left polarization).

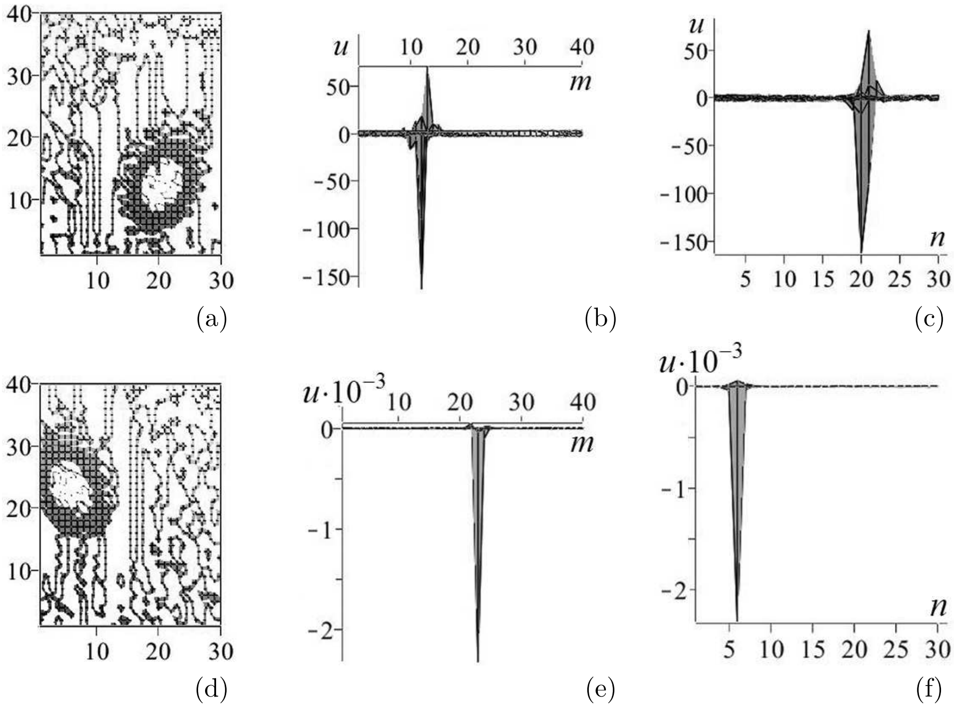

Figure 5: Dependencies of cuts $u \in [-1, 1]$ (a, d) and projections (b, c, e, f) of u on φ_{31} for structure SSL1-QD1 (state B): $\varphi_{31} = \pi/8$ (a, b, c); $\varphi_{31} = -\pi/8$ (d, e, f).

The projections of the displacement function on the planes mOu (Fig. 5 (b, e)), nOu (Fig. 5 (c, f)) allow us to determine the coordinates of the main peak. We introduce the state vector $M = (m, n, u)$. Then for the peak down with right polarization $M = M_1 = (12, 20, -160)$ are found. Then for the peak down with left polarization $M = M_2 = (23, 6, -2300)$ are found. The state vector $M = M_0 = (19, 14, -360)$ of the peak down with $\varphi_{31} = 0$ is found from Fig. 3 (b). We investigate the influence of the angular parameters $\varphi = \varphi_{11}$ (for the trap ED1) and $\varphi = \varphi_{31}$ (for the fractal structure QD1) on the state of the coupled system ED1-QD1.

The initial state of this coupled system for $\varphi_{11} = 0$ and $\varphi_{31} = 0$ is given in Fig. 4 (a, d). Fractal trap ED1 remains in the initial state with $\varphi = \varphi_{11} = 0$, then from (2), (5) for Q_1 we obtain

$$Q_1 = p_0' + p_1'n + p_2'm - p_{11}n^2 + 2p_{12}nm - p_{22}m^2; \quad p_0' = p_{01} - n_0^2/n_c^2 - m_0^2/m_c^2; \quad (13)$$

$$p_1' = 2n_0/n_c^2; \quad p_2' = 2m_0/m_c^2; \quad p_{11} = 1/n_c^2; \quad p_{22} = 1/m_c^2; \quad p_{12} = 0. \quad (14)$$

For the captured structure QD1 at $\varphi = \varphi_{31} \neq 0$ the expressions for $Q2$ (11) - (12) are used. The displacement function $u_B = u$ of the coupled system ED1-QD1 (Fig. 6) is determined when solving the nonlinear equation (8) with the values for Q_1 from (13)-(14) and Q_2 from (11)-(12) for the angular parameter $\varphi_{31} = \pi/8$ (right polarization) and $\varphi_{31} = -\pi/8$ (left polarization).

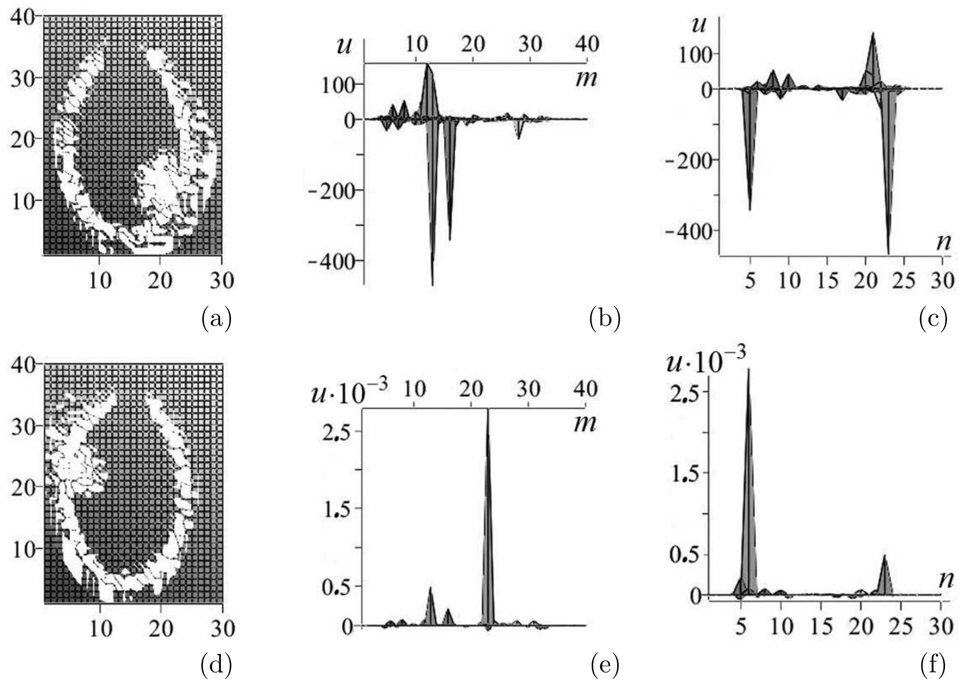

Figure 6: Dependencies of cuts $u \in [-1, 1]$ (a, d) and projections (b, c, e, f) of u on φ_{31} for structure ED1-QD1 (state B): $\varphi_{31} = \pi/8$ (a, b, c); $\varphi_{31} = -\pi/8$ (d, e, f).

The projections of the displacement function on the planes mOu (Fig. 6 (b, e)), nOu (Fig. 6 (c, f)) allow us to determine the coordinates of the main peak. For the main peak down with right polarization $M = M_1 = (13, 23, -440)$ are found. For the peak up with left polarization $M = M_2 = (23, 6, 2800)$ are found. The state vector $M = M_0 = (19, 14, -400)$ of the main peak down with $\varphi_{31} = 0$ is found from Fig. 4 (a).

Changing the angle parameter $\varphi = \varphi_{31}$ for the fractal structure QD1, captured by fractal traps SSL1 with $\varphi_{61} = 0$ or ED1 with $\varphi_{11} = 0$ leads to essential changes of the deformation field, location, amplitudes of the main peaks and the effect of the reorientation of the main peaks of the coupled systems SSL1-QD1 or ED1-QD1.

It is also possible to carry out operations of translation and rotation of the fractal traps only (by changing the angular parameter φ of the trap), leaving a fixed capturing fractal structure or to carry out operations of translation and rotation jointly (both for traps and structures). This offers additional possibilities to govern the coupled systems: fractal trap – fractal structure.

5 Conclusions

The possibility of creating fractal nanotraps based on quasi-two-dimensional fractal structures is shown. By using the method of sections sectioned fractal traps are obtained. The deformation field of fractal traps is essentially stochastic. Sectioned fractal traps allow to obtain porous traps: the pores can be both on the boundary nodal planes and inside the bulk nanosystems. It is proposed to use fractal traps to capture the fractal structures in order to investigate their physical properties in a trap, and also the behavior of the coupled system: fractal trap - fractal structure. It is shown that the behavior of the deformation field for the coupled state of the system (fractal trap – fractal structure) is essentially different from the behaviour of the deformation field for the uncoupled state. By varying the angular parameters it is possible to govern both the states of a separate trap and a captured structure and the state of the whole coupled system.

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