ENERGY STRUCTURE OF LOCALIZATION

V. BERDICHEVSKII[1] and L.TRUSKINOVSKII[2]
[1]The Faculty of Mathematics and Mechanics, Moscow State University, 119899 Moscow, GSP-3 (USSR)
[2]Vernadskii Institute of Geochemistry, the Academy of Sciences, Moscow (USSR)

ABSTRACT

It is shown that a great number of physical objects with localized energy are described by theories with the same mathematical structure: the energy is the sum of two terms - one is a nonconvex functional of field variables and other is a quadratic functional in their gradients. The following examples are considered: bending of rods, dimples in shells, vapor bubbles in a liquid, necking, solitary waves, elementary particles, dislocations.

INTRODUCTION

There is a great number of physical objects in nature with which it is possible to associate energy, localized in space - solitary waves, elementary particles, dislocations in crystal lattice, vapor bubbles in liquid, domen walls in magnetics etc. There arises a question: what is the mathematical structure of the theory which makes it possible to describe such localized congigurations in a natural way as regions of high field gradients. It is clear that such a theory should be nonlinear. This question is deeply connected with the problem of nonlinear generalization of Maxwell's electrodynamics, where charges perform as localized states with a finite energy (cf.[1]). We know a number of theories of localized states (for solitons [2], particle-like solutions in field theory [3], different interfacial boundaries [4-6], dimples on shells [7], dislocations [8]). The aim of the present paper is to draw attention to the fact that all theories suggested have common energy structure: energy is the sum of a nonconvex functional of field variables and a quadratic functional in their gradients. Usually, the density of the energy contains two terms: nonconvex function of field variable and a quadratic form in their derivatives. Some examples

are considered here: rod bending, shell buckling, vapor bubbles, necking, solitons, dislocations, elementary particles.

Although almost all the above (excluding rod bending) have already been considered before such a unification and common outlook throw additional light upon the subject. In particular, we discover deep analogy between the dimple edge energy and the energy of interfacial tension.

ENERGETICAL STRUCTURE OF LOCALIZATION

In this paragraph we deal with the main conception in a simplified one-dimensional situation.

Let us consider a scalar field $u(x)$, x changes in the segment $[-l, l]$. The energy of the field $u(x)$ has the form

$$E = \int_{-\ell}^{\ell} F(u)dx \qquad (1)$$

where $F(u)$ is the energy density. If $F(u)$ is strictly convex, the energy E achieves its minimum on the singular minimizing element.

If $F(u)$ is nonconvex, the number of minimizing elements can be infinite.

For example function $F(u) = Au^2(u-1)^2$ has two local minimums $u = 0$ and $u = 1$ with the same values of the energy density $F = 0$. Then, all the minimizing elements have the next structure: the segment $[-1,1]$ is devided on several intervals and, at each of them, the function $u(x)$ has a constant value: 0 or 1.

Let us add the term $\frac{1}{2}\varepsilon^2(du/dx)^2$ to the energy density. Then the jumps become energetically unprofitable because the energy connected with a jump is infinite. Therefore all the jumps are smoothed and so changed by continuous transition.

In this connection it is interesting to investigate the structure of the stationary points of the energy functional considered.

In order to exclude the influence of boundary points we put $\ell = \infty$

$$E = \int_{-\infty}^{\infty} (F(u) + \frac{1}{2}\varepsilon^2 (\frac{du}{dx})^2)dx . \qquad (2)$$

We'll denote the limit values of function $u(x)$ for $x = +\infty$ and $x = -\infty$ by u_- and u_+ respectively. For definiteness,

we now suppose that $u_- \leq u_+$.

Stationary points of the functional E (2) are the solutions of the equation

$$\frac{\partial F}{\partial u} - \varepsilon^2 \frac{d^2u}{dx^2} = 0 \tag{3}$$

As $d^2u/dx^2 \to 0$ for $|x| \to \infty$ from the equation (3) it follows that the limit values u_- and u_+ of the function $u(x)$ are stationary points of the function $F(u)$:

$$\frac{\partial F}{\partial u} = 0, \text{for } u = u_+, \quad u = u_- \tag{4}$$

Further we shall use the terminology of the theory of phase transitions, so we shall say that the system "is in phase state" u_* if $u(x) \equiv u_*$ and u_* - is the stationary point of $F(u)$. So, one can say with some degree of liberty, that in $x = -\infty$ the system is in u_--phase state and in $x = +\infty$ the system is in u_+ phase state, so the function $u(x)$ describes two-phase state - the continuous transition from u_- phase state to u_+ state (interfacial region).

Let us lower the order of the equation (3), multiplying it by $\frac{du}{dx}$ and integrating on x. We obtain

$$F(u) - \frac{1}{2} \varepsilon^2 \left(\frac{du}{dx}\right)^2 = h \tag{5}$$

where h is a constant.

As $\frac{du}{dx} \to 0$ when $|x| \to \infty$ from the equation (5) it is seen that the values of F in the points u_- and u_+ are equal to h; so, they are identical

$$F(u_-) = F(u_+) \tag{6}$$

The equality (6) is highly notable. It shows that "coexsistance" is possible only between phases with equal values of energy. As it will be shown below, the equality (6) appears to be an analogy of the Gibbs condition [9] of chemical potentials equality in thermodynamic equilibrium (in the theory of phase transitions the role of energy density $F(u)$ is played by a chemical potential).

Let us consider the structure of solutions for the functions

F(u), represented in Fig. 1 a,b,c

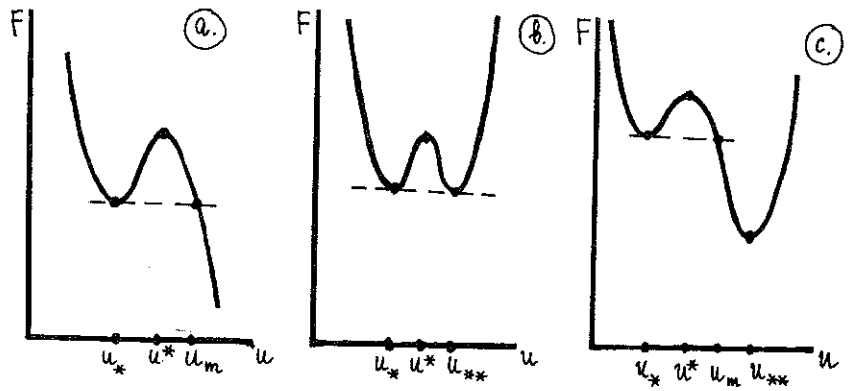

Fig. 1

Functions F(u) 1a, and 1b are particular cases and F(u) 1c is a common one. Function F(u) 1a is a result of drawing the second local minimum of F(u) 1c down in $-\infty$. Function F(u) 1b corresponds to the case of equal values of function F(u) 1c in points of local minimum.

Let us consider only nontrivial solutions, i.e. solutions with $u(x) \neq$ Const.

We shall begin with case 1a, when function F(u) has a local minimum in the point $u = u_*$ and a local maximum in the point $u = u^*$. From the equality (4) and the accepted condition $u_- \leq u_+$, it follows that alternatively $u_- = u_*$ and $u_+ = u_*$ or $u_- = u^*$ and $u_+ = u^*$, or $u_- = u^*$ and $u_+ = u^*$. The second variant is impossible because of (6). The third one is also impossible: according to (5) $h = F(u_+)$, so we have the inequality $F(u) - h = F(u) - F(u_+) \leq 0$, which is in contradition with the inequality $\frac{1}{2}\varepsilon^2(\frac{du}{dx})^2 = F(u) - h \geq 0$. The first variant can be realized and the type of the solution is presented in Fig. 2a.

The solution u(x) increases from the value $u_- = u_*$ up to the value u_m, which is defined by the equation $F(u_*) = F(u_m)$, and then descreases to the value $u_+ = u_*$. This solution has the following physical meaning - the system as a whole is in u_* - phase state which corresponds to the local minimum of the energy. The existance of the minimum lying nearby which is deeper (in our case it is equal to $-\infty$) "gains over" part of the system into the phase state with $u \neq u_*$; the last one is localized in space.

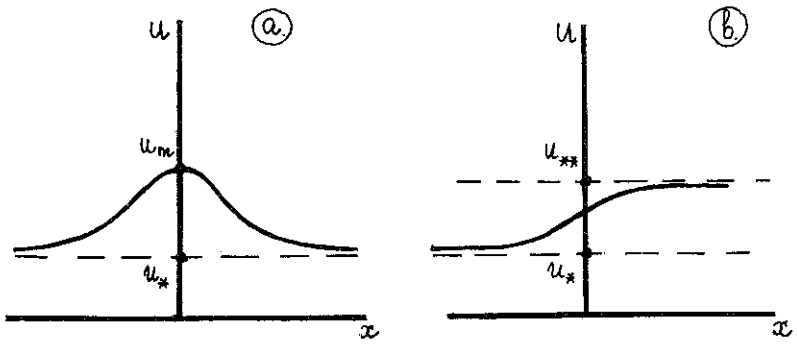

Fig. 2

Function $u(x)$ can be found from (5) by quadrature. In particular, for the function $F(u) = \frac{u^2}{2} - \frac{u^3}{6}$ the solution $u(x)$ is expressed through elementary functions

$$u = 3\,\mathrm{sech}^2\frac{x}{2\varepsilon} \qquad (7)$$

We see from (7) that localized state has the width of order ε. This also follows from (2), because the solution does not depend on ε after the change of veriables $x \to x/\varepsilon$

Let us turn now to case 1b. For the same reason as in case 1a there are no solutions joining the state u_* with u^* and u_{**} with u^*; there is a nontrivial solution with $u_- = u_*$, $u_+ = u_{**}$, and its qualitative structure is presented in Fig 2b. This solution describes the following physical situation: at $-\infty$ the system is in the phase state u_*, at $+\infty$ the system is in another phase state u_{**} and the function $u(x)$ describes gradual transition from one phase to another - the structure of interfacial boundary. The width of the boundary is of order ε. The investigated solution $u(x)$ can be expressed in terms of elementary functions for $F(u) = \frac{u^4}{4} - \frac{u^2}{2}$.

$$u = \mathrm{th}\frac{x}{\sqrt{2}\,\varepsilon}$$

In case 1c there is only one nontrivial solution: $u_- = u_*$, $u_+ = u_*$, $\max u(x) = u_m$. It looks just the same as in case 1a. It is worth mentioning that the solution analysed does not depend on the depth of the minimim in point u_{**}: the only important

thing is that the value of F in point u_{**} should be less than in point u_*.

The solutions considered will have finite energy if we regularize the energy functional (2) by subtracting the constant h from the energy density F ($F(u_-) = F(u_+) = h$).

Thus, we have obtained two solutions: one of them is monotone and the other is not. The first is usually called kink and the second is known as a solitary wave. It can be demostrated [3] that the first is stable in the sense that it corresponds to the minimum of the functional, but the second is unstable and corresponds to the saddle point. Nevertheless the solitary wave solutions are of considerable interest, because they make it possible to calculate the minimal energy of the fluctuation, transforming the system from one phase state to another.

Until now we investigated one-dimensional case which of couse is a model one. In situations of physical interest the energy usually depends on a number of functions and the solution is seldom expressed in quadratures. Nevertheless the main conception may be used for constructing a qualitative solution in multidimensional case as well.

ROD BENDING

The energy structure which we have described - nonconvex function + higher derivatives can be observed in the theory of rods and shells. First we shall analize the theory of rods.

Let us consider the rod which is straight in the nondeformed state, and let us load it axially. We assume that the rod is deforming in one plane and that the symmetry of the cross-section is such that no torsion occurs. Hence, the kinematics of the rod can be described with two functions - the components of the displacement vector. We denote the longitudinal displacement by $u(x)$, the transverse displacement by $w(x)$; x is the length of the axis line in nondeformed state (Fig. 3a).

The measure of rod extension γ and the measure of rod bending ϱ are given by the formulas

$$\gamma = \frac{du}{dx} + \frac{1}{2}\left(\frac{dw}{dx}\right)^2, \qquad \varrho = \frac{d^2w}{dx^2} \tag{8}$$

We do not mention restrictions here which make the use of (8) possible.

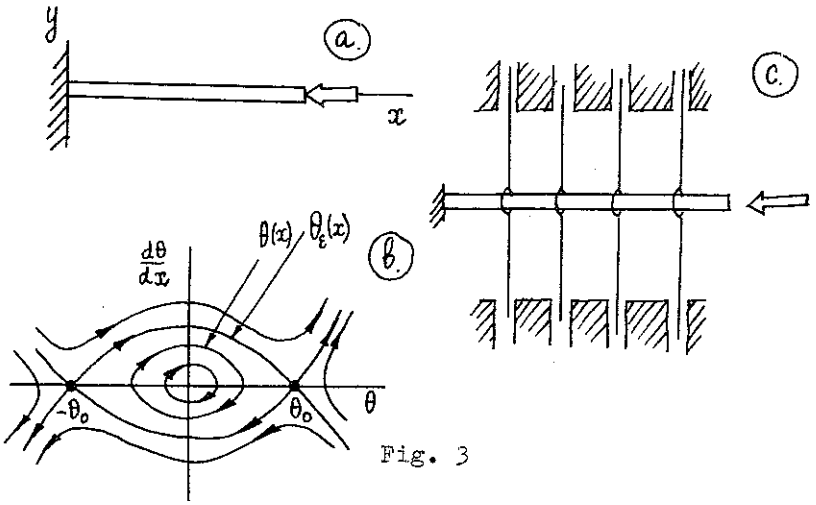

Fig. 3

The density of the rod elastic energy Φ can be expressed as a sum of the strain and bending energy:

$$2\Phi = ES\gamma^2 + EI\varsigma^2 \qquad (9)$$

Here E is Young's modulus, S and I are the area and the inertia moment of a cross-section.

Let us introduce parameter ε through the equality

$$\varepsilon^2 = I/S$$

Parameter ε has the dimension of length. Now we can rewrite the expression for the energy density in the next form:

$$2\Phi/ES = \left(\frac{du}{dx} + \frac{1}{2}\left(\frac{dw}{dx}\right)^2\right)^2 + \varepsilon^2\left(\frac{d^2w}{dx^2}\right)^2 \qquad (10)$$

Let us assume that the boundary points of the rod are not fixed. Then the finding of energy stationary points relative to $w(x)$ is equivalent to the same problem relative to $\theta(x) = dw/dx$; the energy depends on W through θ and $d\theta/dx$ only and we can construct admissible function $w(x)$, if we know $\theta(x)$.

So, we get

$$2\Phi/ES = \left(\frac{du}{dx} + \frac{1}{2}\theta^2\right)^2 + \varepsilon^2\left(\frac{d\theta}{dx}\right)^2$$

Now consider the rod under axial load with a fixed linear longitudinal displacement $u = ax$, a is a fixed negative constant (the rod is compressed). Let us mention, that transverse displacement is free. We introduce new constant θ_o by the formula $a = -\frac{1}{2}\theta_o^2$ and write down the energy density of the system + constraint in the form

$$2\Phi/ES = F(\theta) + \varepsilon^2(\frac{d\theta}{dx})^2, \quad F(\theta) = \frac{1}{4}(\theta^2-\theta_o^2)^2 \tag{11}$$

We see that the energy density contains two terms: nonconvex function $F(\theta)$ *), possesing two local minimums with equal values of F and the square of the first derivative of $\theta(x)$.

The structure of solution on infinite interval has been investigated above. We consider now the case of finite interval.

The equilibrium rod configurations are the stationary points of the functional

$$\int_0^\ell \Phi\, dx + M_o\theta(0) - M_1\theta(\ell) \tag{12}$$

where M_o and M_1 are the moments applied to the rod ends. Note that M_o and M_1 should not be equal. From (11) and (12) we find

$$F(\theta) = \varepsilon^2(\frac{d\theta}{dx})^2 + h, \quad ES\,\varepsilon^2\frac{d\theta}{dx}\Big|_{x=o,l} = M_{o,l}$$

It is obvious, that for zero moments the solution can be written down in the form (Fig. 2b)

$$x(\theta) = 2\varepsilon\int_{-\sqrt{\theta_o^2-h_o^2}}^{\theta}\left[(\theta'^2-\theta_o^2)^2-h_o^4\right]^{-\frac{1}{2}}d\theta'$$

The constant $h_o = \sqrt[4]{4h}$ can be obtained from the condition $x(\sqrt{\theta_o^2-h_o^2}) = l$. If the rod is thin enough, that means $\varepsilon/\ell \ll 1$, the integration limits in (12) can be referred to infinity. Then the solution has the form

$$\theta_\varepsilon = \theta_o \operatorname{th}\frac{\theta_o x}{2\varepsilon}$$

*) It should be noted that for $a>0$ the function $F(\theta) = (a+\frac{1}{2}\theta^2)^2$ is convex and the effect of localization is absent.

This solution describes the structure of the fin. When ε tends to zero, the continuous solutions θ_ε a.e. uniformly converge to the discontinuous solution with the jump

$$\theta = \begin{cases} -\theta_0, & x < 0 \\ \theta_0, & x > 0 \end{cases}$$

If we calculate the energy we obtain $\frac{2}{3} ES\varepsilon\theta_0^2$.
It is obvious that all the energy is concentrated in the fin, because in the region with zero curvature the strain energy is also equal to zero.

The kinematic constraint for the function $u(x)$, introduced before, can be realized with the help of a simple physical model. Let us fasten to the points of the rod (with the help of hinges) a great number of rigid fibres and, after the rod is compressed, we introduce fibres inside cylinders as is shown in Fig. 3c. The fibres slide inside cylinders without friction. If the number of fibres is big enough, we can describe such a situation using the theory considered.

The kinematic constraint, of course, is significant for the appearance of localized states. It is well known that the Euler's rod has no such states. The reason is that function $u(x)$, which was fixed in considered model, varies and has to be found in the case of Euler's rod. It tunes in order to minimize the energy and "softens" the nonconvexity of the strain energy, making localized states impossible. The classical problem without constraints can be solved in exact way and the energy minimum is realized at the solution

$w = 0, \quad u = -\frac{1}{2}\theta_0^2 x \qquad$ for $\theta_0 < \sqrt{2}\,\frac{\pi\varepsilon}{\ell}$

with the energy $1/8\, ES\theta_0^4 \ell$ and $w = 4\left(\frac{\theta_0^2\ell^2}{2\pi^2} - \varepsilon^2\right)\sin\frac{\pi x}{\ell}$,

$u = -\frac{1}{2}\theta_0^2 x - \frac{\pi}{2\ell}\left(\frac{\theta_0^2\ell^2}{2\pi^2} - \varepsilon^2\right)\sin\frac{2\pi}{\ell}x \qquad$ for $\theta_0 > \sqrt{2}\,\frac{\pi\varepsilon}{\ell}$

with the energy $\frac{1}{2} ES\left(\theta_0^2 - \frac{\pi^2\varepsilon^2}{\ell^2}\right)\frac{\pi^2\varepsilon^2}{\ell}$ and the last one bifurcates from the trivial first one at $\theta_0 = \sqrt{2}\,\frac{\pi\varepsilon}{\ell}$. We see that in both cases the localization is absent. That is also true for the constrained rods with $\varepsilon/l \sim 1$.

In the following example, kinematic constraint has not been put from the "outside", but appears in a natural way from the

geometrical features of the construction.

DIMPLES ON SHELLS

The energy structure, considered above, can be found in shells theory. We show that the strain energy and the bending energy correspond to nonconvex and differential parts of energy, respectively. The suggested analogy introduces the problem of finding the structure of the dimple boundary.

Let us write down the expression for the elastic energy density of a shell. To simplify, we consider a shell which is a sphere with radius R in nondeformed state.

It's section accross a meridian is presented in Fig. 4a. The zero value of the angular meridianal coordinate α corresponds to the vertical direction, α being increased in the clockwise direction.

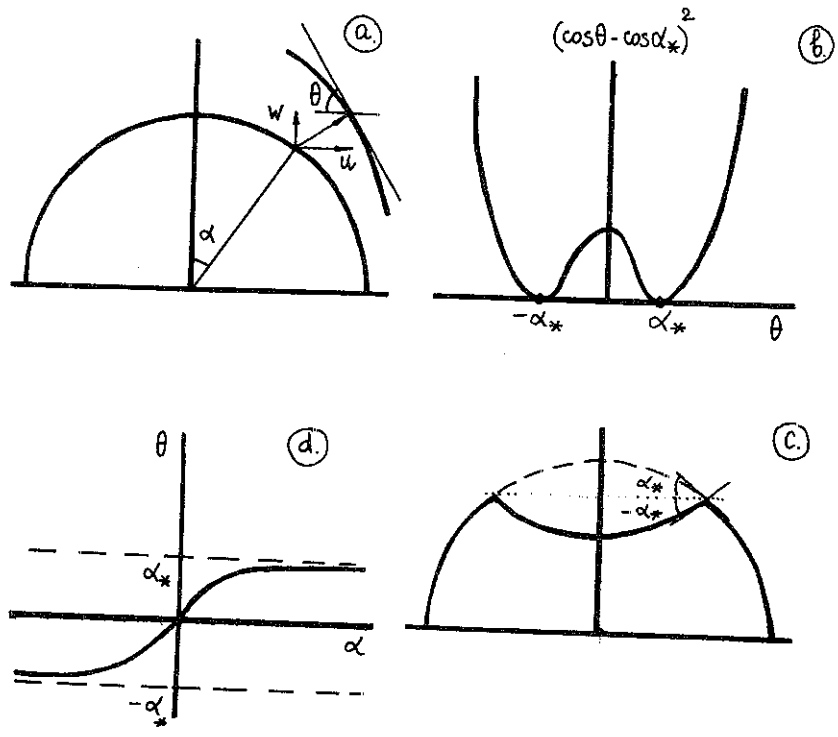

Fig. 4

Let us suppose that the deformation is rotationally symmetric. As a function, characterizing deformed state of the shell, it is convenient to take $\theta(\alpha)$, where θ - is the angle between the

horizontal direction and the tangential direction to the deformed middle surface, α can be used as a Lagrange coordinate of the meridian points (see Fig. 4a). By our condition, the angle θ increases when the tangential line rotates clockwise.

If the meridian deformation is **nonextensional, the function** $\theta(\alpha)$ will be the only characteristic of deformation that we need (up to rigid rotation). If the meridian is subject to extensions we need another function to characterize the deformation; for such function we choose the horisontal component of displacement divided by R, $u(\alpha)$. It is a simple task to calculate the strains γ and γ_1 and the **curvature** variations Δk and Δk_1 of the meridian and of the parallel, respectively, in terms of $\theta(\alpha)$ and $u(\alpha)$:

$$\gamma = \frac{u' - \cos\theta + \cos\alpha}{\cos\theta}\ ; \quad \gamma_1 = \frac{u}{\sin\alpha}$$

$$\Delta k = \frac{1}{R}(\theta' - 1); \qquad k_1 = \frac{1}{R}\,\frac{\sin\theta - \sin\alpha}{\sin\alpha} \tag{13}$$

Prime indicates differentiation with respect to α.

The elastic energy of the shell $\mathcal{E}$ is given by the formula

$$\mathcal{E} = \int \Phi\, d\alpha$$

$$\Phi = \frac{\pi E h R^2}{1-\nu^2}\left[\gamma^2 + \gamma_1^2 + 2\nu\gamma\gamma_1 + \frac{h^2}{12}\left(\Delta K_1^2 + \Delta K^2 + 2\nu\,\Delta K\,\Delta K_1\right)\right]\sin\alpha \tag{14}$$

where h is the shell thickness, ν - is Poisson's ratio, E is Young's modulus.

The limits of integration depend on the shell geometry and their values are not important for us. We assume for simplicity that $-\alpha_0 \le \alpha \le \alpha_0$, $(\alpha_0 \sim 1)$. One can think that the deformation is caused by a consentrated force, applied at the shell's pole.

The expression (14) is far from being simple. Let us try to simplify it. We shall show that for a deformation state localized in the neighbourhood of an angle α_*, the expression (14) can be changed by:

$$\Phi = \pi E h R^2\left[\frac{u^2}{\sin^2\alpha_*} + \varepsilon^2\left(\frac{d\theta}{d\alpha}\right)^2\right]\sin\alpha_* \tag{15}$$

The dimensionless parameter ε is defined by the equality $\varepsilon^2 = h^2/12R^2(1-\nu^2)$. The functions $u(\alpha)$ and $\theta(\alpha)$ satisfy the nonholonomic constraint

$$u' = \cos\theta - \cos\alpha_* \tag{16}$$

If we "remove" the prime in (16), i.e. if we put $u = \cos\theta - \cos\alpha_*$, we obtain the familiar energy with the function $F(\theta)$, shown in Fig. 4b. The derivative in (16) changes to some extent the character of the nonconvexity; however, as it will be seen below, localized states still appear to be possible.

We give now a proof of formulae (15), (16). In the localized state, the functions to be found $u(\alpha)$ and $\theta(\alpha)$ vary at the distance of order ε, hence after the differentiation the large parameter ε^{-1} appears, so we can investigate the functional (15) by the variational-assymptotic method [10].

Let us fix the function $\theta(\alpha)$ and look for the function $u(\alpha)$. In accordance with the general scheme of the variational-assymptotic method, we keep in the energy the main terms, containing $u(\alpha)$, and the main interacting terms between $u(\alpha)$ and $\theta(\alpha)$. As $u' \gg u$, we have

$$= \frac{EhR^2}{1-\nu^2} \quad \frac{1}{\cos^2\theta}\,(u'^2 - 2u'(\cos\theta - \cos\alpha))$$

Varying u', we obtain the equality (16).

Denoting the solution of the equation (16) by u_0, we present $u(\alpha)$ in the form

$$u = u_0 + u_1 \tag{17}$$

where $u_1 \ll u_0$. Substituting the expression (17) into (14) and keeping the main terms, containing u_1, and the main interacting terms, we get

$$\Phi = \frac{EhR^2}{1-\nu^2}\left[\frac{1}{\cos^2\theta}\,u_1'^2 + \frac{2u_0u_1}{\sin^2\alpha_*} + 2\nu\frac{u_1'}{\cos\theta} - \frac{u_0}{\sin\alpha_*}\right] \tag{18}$$

The second term in (18) may be omitted in comparison with the third term, because, $u_1' \gg u_1$. Varying u_1, we find

$$\frac{u'}{\cos\theta} = -\nu\frac{u_0}{\sin\alpha_*} \tag{19}$$

Substituting again (17) into (14), we see that the main term in the strain energy coincides with the first term in (15). The proof is finished by omitting 1 in the expression for Δk (because of $\vartheta' \gg 1$) as well as Δk_1 in comparison with ϑ' (because of $\vartheta' \gg \Delta k$).

Now we turn to the analysis of formulae (15) and (16). We suppose that the width of the localized state is far less than α_*, so the localized state is placed far from the shell's pole. In this case we can consider α as a formal variable, changing at the whole axis: $-\infty < \alpha < \infty$. So we can find the localized states by looking for stationary points of the functional

$$I = \int_{-\infty}^{\infty} \left[\frac{u^2}{\sin^2 \alpha_*} + \varepsilon^2 \left(\frac{d\vartheta}{d\alpha} \right)^2 \right] \sin \alpha_* \, d\alpha \qquad (20)$$

with the functions $u(\alpha)$ and $\vartheta(\alpha)$ subject to the constraint (16).

The finitness of the functional I involve the conditions $\vartheta' \to 0$, $u \to 0$ when $|\alpha| \to \infty$. So, according to (16), $\cos\vartheta|_{\alpha = \pm\infty} = \cos\alpha_*$ and we have $\vartheta|_{\alpha=\pm\infty} = \pm\alpha_*$. This means, that the localized state has the form of a circular edge (Fig. 4c) and can be considered in the first approximation as an isometric deformation of the sphere: the upper spherical segment is reflected with regards to the horizontal plane. This fully coincides with the theory of shell dimples due to A.Pogorelov[7]

A qualitative form of the dependance of ϑ upon α is presented in Fig. 4d.

In order to obtain the edge energy as function of the parameters ε and α_*, it is convenient to make a change of variables $u \to \bar{u}$, $\vartheta \to \bar{\vartheta}$, $\alpha \to x$ using the formulae $u = a\bar{u}$, $\vartheta = \alpha_* \bar{\vartheta}$, $\alpha = bx$. The values of the constants a and b are choosen in a special way to make the integrand of (20) independent on ε and α_* and the constraint (16) independent on ε and α_* in the limit of small α_*. It is easy to find that we have to set

$$a = b\alpha_*^2 \cos\alpha_*, \quad b = \sqrt{\frac{\varepsilon \operatorname{tg}\alpha_*}{\alpha_*}}$$

Under this choice of the values of the constants the minimal value $\underline{I}$ of the functional I will be equal to

$$\underline{I} = \varepsilon^{3/2} \alpha_*^{5/2} \sqrt{\operatorname{tg}\alpha_*} \cos\alpha_* \; \underline{I}_1(\alpha_*) \tag{21}$$

where $\underline{I}_1(\alpha_*)$ is the minimal value of the functional

$$I_1 = \int_{-\infty}^{+\infty} (\bar{u}^2 + (\frac{d\theta}{dx})^2)dx \tag{22}$$

subject to the constraint

$$\frac{d\bar{u}}{dx} = \frac{1}{\alpha_*^2}(\frac{\cos\alpha_*\bar{\theta}}{\cos\alpha_*} - 1) \tag{23}$$

The constraint (23) in the limit $\alpha_* \to 0$, corresponding to shallow shells, takes the form, independent of α_*

$$\frac{d\bar{u}}{dx} = \frac{1}{2}(1 - \bar{\theta}^2) \tag{24}$$

Tending also α_* to zero in (21) and taking into consideration (14), (15), we obtain the final expression for the edge energy:

$$\mathcal{E} = \pi \, Eh R^2 \, \varepsilon^{3/2} \alpha_*^3 \, \underline{I}_1(0)$$

The equivalent expression was obtained in other terms in the pioneer work by A.Pogorelov [7].

The width of the localization region has in terms of the angle variables the order of $\sqrt{\varepsilon} \sim \frac{h}{R}$. In the terms of arc lenth of the meridian the corresponding order is $R\sqrt{\varepsilon} \sim \sqrt{hR}$.

This analysis makes it possible to get the next corrections for the energy with respect to α_* . To perform this we have to calculate the lower limit of the functional (22), when the constraint contains the first correction term with respect to α_*

$$\frac{d\bar{u}}{dx} = \frac{1}{2}(1 - \bar{\theta}^2) + \frac{5}{24}\alpha_*^2 \; (1 - \bar{\theta}^2) \tag{25}$$

Let us find the order of magnitude of the energy correction term. Presenting the solution in the form $u = u_0 + u_1$, where u_0, u_1 - the solution of our problem for $\alpha_* = 0$, and $u_1 \ll u_0$, $\theta_1 \ll \theta_0$ we get

$$I_1 = \underline{I}_1(0) + \int_{-\infty}^{+\infty} 2(u_0 u_1 + \frac{d\theta_0}{dx}\frac{d\theta_1}{dx})dx + \int_{-\infty}^{+\infty} (u_1^2 + (\frac{d\theta_1}{dx})^2)dx \to \inf_{u_1, \theta_1} \tag{26}$$

where u_1 and θ_1 satisfy the linearized restrictions (25)

$$\frac{du_1}{dx} = -\theta_0\theta_1 + \frac{5}{24}\alpha_*^2(1-\theta_0^2) \tag{27}$$

The Euler's equations for the variational problem (22), (24) have the form

$$2u_0 = \frac{d\lambda}{dx}, \quad \lambda\theta_0 - 2\frac{d^2\theta}{dx^2} = 0 \tag{28}$$

Here λ is a Lagrangean multiplier for the constraint (24). Because of (28), the first integral in (26) does not depend upon u_1 and θ_1:

$$\int_{-\infty}^{\infty} 2\left(u_0u_1 + \frac{d\theta_0}{dx}\frac{d\theta_1}{dx}\right)dx = -\int_{-\infty}^{\infty}\lambda\left(u_{1x} + \theta_0\theta_1\right)dx =$$
$$= -\int_{-\infty}^{\infty}\lambda\frac{5}{24}\alpha_*^2(1-\theta_0^2)dx = c\,\alpha_*^2 \tag{29}$$

Therefore the problem of finding u_1 and θ_1 comes to the minimization of the second integral in (26) subject to the constraint (27). It is convenient to make the change of variables: $u_1 = \alpha_*^2 u_2$, $\theta_1 = \alpha_*^2\theta_2$. Then there appears the multiplier α_*^4 in front of the second integral in (26), though in the constraint (27) parameter α_* disappears. Hence the problem of determining u_2 and θ_2 does not contain the small parameter and the second integral in (26) has the order α_*^4. Thus, when α_* is sufficiently small the function $\underline{I}_1(\alpha_*)$ has the asymptotic form

$$\underline{I}_1(\alpha_*) = \underline{I}_1(0) + c\alpha_*^2$$

According to (29) the constant c can be found after we solve the problem (22), (24), corresponding to case $\alpha_* = 0$.

Let us estimate the error of the expression $\varepsilon^2\theta'^2$ for bending energy. Because of $\theta' = \frac{\alpha_*}{6}d\bar{\theta}/dx$, $6 \sim \sqrt{\varepsilon}$, the replacement of $(\theta'-1)^2$ by θ' brings us to error of order $\varepsilon\alpha_*^{-2}$ in comparison with unity (we note that the integral of the term, linear on θ', vanishes). The same error is due to omitting the bending energy of the parallel $(\Delta k_1)^2$. The quantity $\varepsilon\alpha_*^{-2}$ has the order of hR/r^2, where r is the distance between the fin and the shell axis. So, our expression is admissible if $r \gg hR$.

The position of the localized state (of the fin) can be determined by the procedure, suggested by Pogorelov [7]: we have to

equalize the variation of the fin energy with respect to free parameter α_* to the corresponding work of external forces.

If $r \sim \sqrt{hR}$ we can't replace the expression (14) by (15), though it is possible to make other simplifications which are due to the fact that the deformed region is localized in the vecinity of the pole, so we can take α and θ to be small enough in the boundary-layer which appears. For the measures of strain and bending we have simplified expressions

$$\gamma = u' + \frac{1}{2}\left(\theta^2 - \alpha^2\right), \gamma_1 = \frac{u}{\alpha}, \quad \Delta k = \frac{1}{R}\left(\theta' - 1\right), \quad \Delta k_1 = \frac{1}{R}\frac{\theta - \alpha}{\alpha}$$

For the integral it is possible to take again the infinity limits. It is convenient to introduce function φ instead of $\theta(\alpha)$: $\theta = \alpha + \varphi$. Therefore the energy is given by the formula

$$\mathcal{E} = \pi E h R^2 \int_{-\infty}^{\infty} \left[\alpha\left(u' + \varphi\left(\alpha + \varphi\right)\right)^2 + \frac{u^2}{\alpha} + \varepsilon^2\left(\alpha\varphi'^2 + \frac{\varphi^2}{\alpha}\right)\right] d\alpha$$

Here ε is determined by $\varepsilon^2 = h^2/12R^2$; we have also put $\nu = 0$ for simplicity. Calculation of the energy comes now to the solving of the system of two ordinary differential equations for $u(\alpha)$ and $\varphi(\alpha)$

Now we consider the case of spherical shell subjected to a uniformly distributed normal load p. The potential energy due to the load p is given by

$$A = \pi p R^3 \int_0^{\alpha_0} \sin^2\alpha \, \sin\theta \, d\alpha$$

For simplicity we limit ourselves with the case of shallow shell ($\alpha_0 \ll 1$).

For this case let us introduce the new quantity $\varrho(r)$ by the formulae

$$\sin\theta \simeq \left(\varrho + \frac{r}{R}\right), \text{ so } \cos\theta \simeq 1 - \frac{1}{2}\left(\varrho + \frac{r}{R}\right)^2$$

and also

$$\theta' \simeq \left(\varrho' + \frac{1}{R}\right), \quad \gamma = Ru' + \frac{\varrho^2}{2} + \varrho\frac{r}{R}$$

Here $r(\alpha) = R\sin\alpha \simeq R\alpha$ - is radial cylindrical coordinate, prime denotes differentiation with respect to r. It is clear that $\varrho(r) = -W'(r)$, where $W(r)$ is vertical deplacement of

the shell. The problem of determining equilibrium configuration comes to the finding of the extremum of energy functional

$$I = \frac{Eh}{1-\nu^2}\int_0^r \Big[(\gamma^2 + \frac{u^2}{r^2}R^2 + \frac{2\nu u\gamma}{r}R)r + \frac{h^2}{12}(\varrho'^2 + (\frac{\varrho}{r})^2 + \frac{2\nu\varrho\varrho'}{r})r + \\ + \frac{2(1-\nu^2)}{Eh}\, p\frac{r^2}{2}(\varsigma + \frac{r}{R})\Big]\, dr \qquad (30)$$

where $r_0 = r(\alpha_0)$. The trivial equilibrium state is given by a constant radial and vanishing tangential displacement:

$$u_0 = -\frac{p(1-\nu)}{2Eh}\,\frac{r}{R}, \quad \varsigma_0 = 0$$

To investigate other states of equilibrium it is convenient to put $u = u_0 + \tilde{u}$, $\varsigma = \varsigma_0 + \tilde{\varsigma}$. In terms of new variables $\tilde{u}(r)$, $\tilde{\varkappa}(r) = \tilde{\varsigma}(r)\frac{R}{r}$ the energy can be rewritten in the form:

$$I = \frac{\pi Eh}{1-\nu^2}\Big[\int_0^\infty (\tilde{u}' - \frac{\tilde{u}}{r})^2\,\frac{r\,dr}{R^2} + 2\int_0^\infty (\frac{\tilde{\varkappa}^2}{2} + \tilde{\varkappa})(\tilde{u}' + \nu\frac{\tilde{u}}{r})\frac{r^3}{R}\, dr + \\ + \frac{h^2}{12R^2}\int_0^\infty \tilde{\varkappa}'^2\, r^3 dr + \int_0^\infty \frac{r^5}{R^4}(\frac{\tilde{\varkappa}^2}{2} + \tilde{\varkappa})^2 dr + \frac{p(\nu^2-1)}{2EhR}\int_0^\infty \tilde{\varkappa}^2 r^3 dr \qquad (31)$$

where we have extended the upper integral limit to infinity, assuming that buckling is concentrated near the pole and boundary effects are not essential.

In order to determine the structure of the energy we use the simplifying assumption going back to von Karman and Tsien [11]: the deflection is vertical, i.e. parallel to the axis of symmetry. Such an assumption can be regarded as a kinematic restriction. Karman-Tsien assumption is incorrect, because of doubling the Euler critical load [12]. Nevertheless we think it to be instructive to clarify the energy structure and to obtain at least qualitative results.

Thus, setting $u = 0$ in (31), we find

$$I = \frac{Eh}{1-\nu^2}\int_0^\infty \Big(\Phi(\tilde{\varkappa}, r) + \varepsilon^2 r\,\tilde{\varkappa}'^2\Big)\, dr$$

where $\varepsilon^2 = \frac{h^2}{12R^2}$ is small parameter and

$$\Phi(\tilde{\varkappa}, r) = (\frac{\tilde{\varkappa}^2}{2} + \tilde{\varkappa})^2\,\frac{r^5}{R^4} + \frac{p(\nu^2-1)}{2ERh} r^3\tilde{\varkappa}^2$$

is nonconvex function of $\tilde{\varkappa}$, parametrized with the load p .

It can be seen that the energy has a familiar structure, containing nonconvex algebraic term and quadratic term in derivatives. "Kink"-solution corresponds to a dimple with edge far from the shell axis; the "solitary wave"-solution corresponds to a dimple in the vicinity of the shell pole.

The method of dimple edge energy calculation can be generalized in a natural way for nonspherical shells as well.

INTERFACIAL BOUNDARIES

In the theory of rods and shells the bending energy, which contains second derivatives of field variables, is important in a number of problems, so the necessity of the including it into the energy expression is commonly accepted. Alternatively, the theory of interfacial boundaries, which we are going to consider, seems to be the only example of essential application of the material models with higher derivatives.

In classical theory of heterophase equilibrium surfaces of material characteristics discontinuities deviding the coexisting phases are introduced. It is suggested, that a surface of discontinuity posseses some energy. The surface position in space is considered as an additional independent degree of freedom. Alternative way of reasoning, introduced for the first time by van der Waals [4], considers interfacial boundary as a thin layer of continuous change of parameters. In order to describe such a layer van der Waals used the weakly nonlocal model of continuum with the mass density of free energy of the form:

$$\varrho\,\Phi(\varrho,\nabla\varrho,T)=\varrho\,F(\varrho,T)+\tfrac{1}{2}\varepsilon^2(\nabla\varrho)^2 \qquad (33)$$

where ϱ is the mass density, T is the temperature, ε is a small parameter. For onephase liquids $\varrho F(\varrho,T)$ is a convex function of ϱ , so the second term in (33) appears to be nonessential. If the liquid exists in two different phase states, the function $\varrho F(\varrho,T)$ has 2 convex branches, determined, generaly speaking, on a noninteracting intervals of the ϱ variable. Van der Waals was the first who suggested to use single nonconvex function $\varrho F(\varrho,T)$ on the whole interval of densities. For example, in the case of van der Waals' gas (liquid), $F(\varrho, T)$ has the form

$$F(\varrho, T) = \varphi(T) - a\varrho - RT \ln\left(\frac{1}{\varrho} - b\right) \qquad (34)$$

where a, b, R - are positive constants. Qualitative appearance of the function F (34) - when temperature is sufficiently small - is shown in Fig. 5.

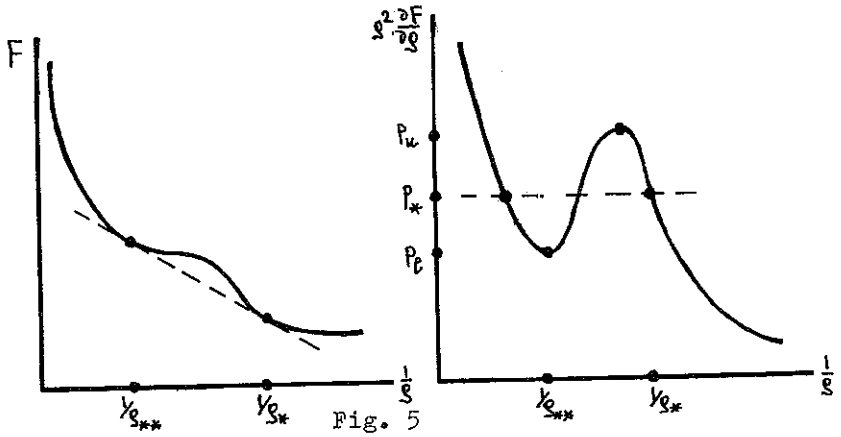

Fig. 5

Van der Waals' theory contains all the ingredients of the class of theories being considered: nonconvexity + high derivatives.

The states of heterophase equilibrium in the domain V under a fixed external pressure p can be found from the equality of variations of free energy and the work of external pressure:

$$\delta \int_V \left(\varrho F(\varrho, T) + \varepsilon^2 (\nabla\varrho)^2 \right) dV = -p\,\delta V \qquad (35)$$

Here it is supposed that the temperature T is also fixed.

It is seen from (35) that equilibrium states are the stationary points of the functional

$$\int_V \left[\varrho F(\varrho, T) + \frac{p}{\varrho} + \frac{1}{2}\varepsilon^2 (\nabla\varrho)^2 \right] dV \qquad (36)$$

We call the function $\mu(\varrho, p, T) = F(\varrho, T) + p/\varrho$ chemical potential*). For a liquid with function $F(\varrho, T)$, shown in

*) This function has meaning of nonequilibrium chemical potential; usually its equilibrium analog: $\mu(p, T) = \min_{\varrho} \mu(\varrho, p, T)$ is named "chemical potential".

Fig. 5, it can be find such $p = p^*$ that the chemical potential $\mu(\varrho, p^*, T)$ would have two local minimums on ϱ with equal values of μ :

$$\mu(\varrho_*, p^*, T) = \mu(\varrho_{**}, p^*, T) = \mu_0$$

It is convinient to change the functional (36), subtracting the constant $\mu_0 M$, where M is the mass, contained in the volume V, $M = \int_V \varrho \, dv$. In the case of unbounded volume $V = R^3$ the integral

$$\int_{R^3} \left[\varrho(\mu(\varrho, p^*, T) - \mu_0) + \frac{1}{2} \varepsilon^2 (\nabla\varrho)^2 \right] dv$$

converges under the condition that the density tends to the values ϱ_* or ϱ_{**} at infinity.

If the density depends on the single coordinate $x_1 = x$ the equilibrium configurations are the stationary points of the functional

$$\int_{-\infty}^{\infty} \left[\varrho(\mu(\varrho, p^*, T) - \mu_0) + \frac{1}{2}\left(\frac{d\varrho}{dx}\right)^2 \right] dx \qquad (37)$$

which is just the same as one being considered above. Note, that for the functional (37) conditions (4) and (6) take the form:

$$\varrho \frac{\partial F}{\partial \varrho}\Big|_{\varrho=\varrho_*,\varrho_{**}} = p^*, \quad \left(F + \frac{p^*}{\varrho}\right)\Big|_{\varrho=\varrho_*,\varrho_{**}} = \mu_0$$

and correspond to the equality of pressures and chemical potentials in coexisting phases.

Now we turn to spherical equilibrium configurations, being the stationary points of the functional

$$4\pi \int_0^{\infty} \left[\varrho(\mu(\varrho, p, T) - \mu_0) + \frac{1}{2}\left(\frac{d\varrho}{dr}\right)^2 \right] r^2 dr \qquad (38)$$

For the convergency of the integral (38) we put $\mu_0 = \mu(\varrho_\infty, P, T)$ where $\varrho_\infty = \varrho(\infty)$.

It is interesting to consider the stationary points of the functional (38) for all positive values of external pressure p. There can be defined three singular values of p : lower critical pressure p_l, critical pressure p_* and upper critical pressure p_u, $p_l < p_* < p_u$. They are determined by following

conditions: for $p < p_1$ the function $\mu(\varrho, p, T)$ has the only minimum (at the point ϱ_*), for $p = p_1$ it appears an additional stationary point ϱ_{**} for $p > p_1$ the function $\mu(\varrho, p, T)$ has two local minima at the points ϱ_* and ϱ_{**}, for $p = p_*$ the values of μ at the points ϱ_* and ϱ_{**} are equal, $\mu(\varrho_*) < \mu(\varrho_{**})$ for $p > p_*$, and the local minimum ϱ_* dissappears for $p > p_u$ (Fig. 6a-g).

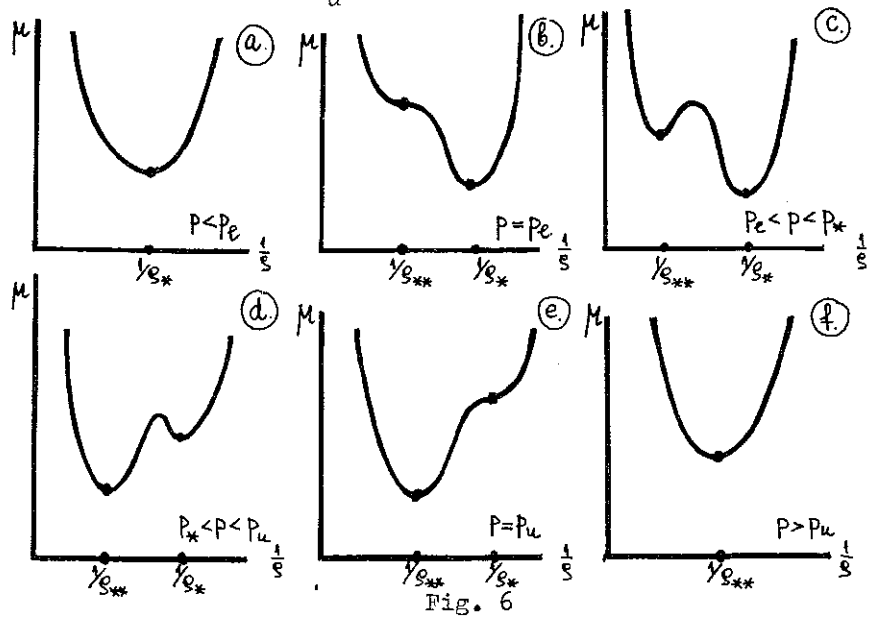

Fig. 6

Although the integrands in (38) and (2) distinguish by the multiplier r^2, the stationary points of (38) and (2) are similar. So, we have:

for $p < p_1$ there is onephase state $\varrho(r) = \varrho_*$

for $p_1 < p < p_*$ there is nontrivial stationary point with $\varrho_\infty = \varrho_{**}, \varrho_0 = \varrho(0) > \varrho_*$ (nucleus of vapour)

for $p_* < p < p_u$ there is nontrivial stationary point with $\varrho_\infty = \varrho_*$, $\varrho_\infty < \varrho_0$ (liquid nucleus)

for $p_* > p_u$ there is onephase state $\varrho(r) = \varrho_{**}$

To show that we need to investigate the equation

$$\frac{\partial}{\partial \varrho}\left[\varrho(\mu - \mu_0)\right] = \varepsilon^2\left(\frac{d^2\varrho}{dr^2} + \frac{2}{r}\frac{d\varrho}{dr}\right) \qquad (39)$$

with the natural boundary conditions $d\varrho/dr\,|_{r=0} = d\varrho/dr\,|_{r=\infty} = 0$. Because $d^2\varrho/dr^2\,|_{\infty} = 0$ as well, the equation (39) yields $\nabla[(\mu(\varrho, p, T) - \mu_0)]/\nabla\varrho = 0$ for $r = \infty$. It can be seen, that this condition connects ϱ_∞ and p:

$$\varrho^2 \frac{\partial F}{\partial \varrho}\Big|_{\varrho_\infty} = P$$

We have to omit the investigation of (39) so as the demonstration of solutions instability because of restricted paper volume; for details see [13, 14]. We note only that integration of (39) gives

$$p(0) - p(\infty) = 2\int_0^\infty \varepsilon^2 \frac{d}{dr}\frac{dr}{r} \tag{40}$$

where $p(r) = \varrho^2 \partial F/\partial\varrho\,|_{\varrho=\varrho(r)}$. For states, localized near $r = R$, the equation (40) is similar to the Laplace formula

$$p(0) - p(\infty) = \frac{2\sigma}{R} \tag{41}$$

From (40) and (41) one can find the expression for interfacial tension

$$\sigma = R\int_0^\infty \varepsilon^2 \frac{d}{dr}\frac{dr}{r}$$

It is obvious that the existence of interfacial surface tension is a manifestation of nonhydrostatic nature of stress tensor. It can be shown that the equation (39) is just an integral of the standard tensor equation of elastic equilibrium [13]. We have to omit the discussion because it needs too much technic of nonlocal continuum mechanics (see [13-16]).

NECKING IN FIBERS

If a long polymeric or metallic fiber is stretched along the axis, a simple homogeneous extension may evolve into a nonhomogeneous state in which the fiber thins down in one or more short regions, i.e. necks appear.

It seems that the formation of the neck can be also described by the theory of energy structure which we are discussing. It is clear that the neck expansion is accompanied by a number of

quite different physical processes, nevertheless we suppose that the first appearence of the neck is due to nonconvexity of the energy.

Let us consider a circular slender cylindrical rod, having radius a and length l in initial nondeformed state. We assume that the deformation can be expressed in terms of the radial displacement $u(x)$ and the displacement $W(x)$ along the axis:

$$\hat{x} = x + W(x), \quad \hat{r} = r(1 + u(x)), \quad \hat{\theta} = \theta$$

Here x, r, θ are cylindrical Lagrangian coordinates in the reference configuration and $\hat{x}$, $\hat{r}$, $\hat{\theta}$ - coordinates of the rod points in deformed state; displacement $u(x)$ appears to be dimensionless.

Components of the strain tensor ε_{ij} depend on r, u, u', W', thus the density of the elastic energy can be thought as a known function of r, u, u', W'. Averaging the energy along the cross-section, we obtain

$$\Phi(u, u', W') = \frac{2\pi}{\pi a^2} \int_0^a V(r, u, u', W') r dr$$

We suppose, that one end of the rod is fastened: $u(0) = 0$, $W(0) = 0$, the other end is loaded with a tensile force P, and the lateral surface is free.

Then the equilibrium configurations are the stationary points of the functional

$$\int_0^l \Phi(u, u', W')dx - PW(1) = \int_0^l \left[\Phi(u, u', W') - PW'\right] dx \qquad (42)$$

It is obvious that in order to find stationary points with respect to W' we have to minimize the integrand in (42) with W'. We denote through $\Phi(u, u')$ the function

$$\Phi(u, u') = \min_{W'} \left(\Phi(u, u', W') - PW' \right)$$

So we need now to find the stationary point of the functional

$$\int_0^l \Phi(u, u')dx$$

with respect to functions $u(x)$, $u(0) = 0$.

It is reasonable to suggest the following approximation for $\Phi(u, u')$

$$\Phi(u, u') = F(u) + \varepsilon^2 u'^2$$

where $F(u) = \Phi(u, 0)$. In linear elasticity

$$\Phi(u, u', W') = \frac{\lambda}{2}(2u + W)^2 + \mu(2u^2 + W'^2) + \frac{a^2}{4}\mu u'^2 \quad (43)$$

Here λ and μ are the Lame's moduli. We see that the function $F(u)$ is convex, so the localization is absent. To obtain the desired effect we need to consider nonlinear elastic material. The situation, studied above is reached, if the energy $V(\varepsilon_{ij})$ and the load P are such that the function $F(u)$ has two local minima. The formation of the "nucleus" of the new phase in a homogeneous state $u(x) \equiv u_{**}$ is possible when the values of F in stationary points u_* and u_{**} are different and $F(u_*) < F(u_{**})$ for $u_* < u_{**}$. Such configurations are characterized by the region of order where the radius of the rod will be less than u_{**}.

Let us note, that the considered model predicts the first unstable stage of neck formation, afterwards another physical mechanisms come forward (plasticity for metals), which make such a simplified conservative model inadequate.

The idea of taking into consideration nonconvex functions $F(u)$ is due to Ericksen [18], higher derivatives were introduced recently by Coleman [19]. Autman [20], investigating bifurcations of the trivial solution, obtained an analog of the upper critical load for this problem.

SOLITONS

The analogy between solitons and nuclei of a new phase is not sufficiently complete because the features which characterize solitons are essentially connected with dynamics. Nevertheless in the theory of solitons we meet the same structure of energy. To make this clear, we consider the well-known Korteweg-de Vries equation [2] describing, for instance, surface water waves

$$\eta_t + 6\eta\eta_x + \eta_{xxx} = 0$$

After the change of variables $\eta = \varphi_x$ it obtains the variational structure

$$\varphi_{xt} + 6\varphi_x \varphi_{xx} + \varphi_{xxxx} = 0$$

with the Lagrangian function [21]

$$\Lambda = -\frac{1}{2}\varphi_t \varphi_x - \varphi_x^3 + \frac{1}{2}\varphi_{xx}^2$$

To find the stationary solutions, moving with the constant speed c (we take $c > 0$) $\varphi = V(x - ct)$ we have to solve the equation with the Lagrangian function

$$\Lambda = -V_x^3 + \frac{1}{2}cV_x^2 + \frac{1}{2}V_{xx}^2$$

The last one can be rewritten in terms of $u = V_x$

$$\Lambda = F(u) + \frac{1}{2}u_x^2, \quad F(u) = \frac{1}{2}cu^2 - u^3$$

We see, that Λ has again just the same structure as we have discussed above with the function $F(u)$ presented in Fig. 1a.

DISLOCATIONS

Let us consider the infinite cubic atomic lattice. We can shift atoms of half-space along the crystal plane at a distance b (lattice parameter). It is obvious that the displaced lattice will coincide with itself so our transformation is a symmetry. Assume now that we shift only part of the half-space. Then a dislocation appear - a region of transition from the domain, where displacement takes place to the domain where displacement is absent. We denote by $u(x)$ relative displacement of atoms on both sides of the sliding plane. The elastic energy of distortion of the upper and lower atom rows is due to interaction of both sides along the sliding plane. It is clear that this is a periodic function of displacement $u(x)$ with period b.

The equilibrium distribution of displacement $u(x)$ can be found from the equation, suggested by Peierls [8]:

$$\frac{2\varkappa}{b}\int_{-\infty}^{\infty} \frac{du/d\xi}{\xi - x}d\xi + \frac{2\pi\sigma}{G} = \sin\frac{2\pi u}{b} \qquad (44)$$

where σ is exterior tangential stress along the sliding plane, $\varkappa = \frac{b}{2(1-\nu)}$, G is shear modulus, ν is Poisson's ratio. The integral in the l.h.s. of (44) is due to long-range elastic interaction of a distorted region with the other part of the crystal. The r.h.s. is related with nonlinear interaction of rows of atoms, which is a short range and is localized in the vicinity of the sliding plane.

The analysis of the equation (44) shows that we have again the same energetical structure: algebraic term connected with periodic (nonconvex) interaction energy and elastic energy, represented by nonlocal term. Contrary to the examples examined above, here we meet for the first time a strong nonlocality, therefore Euler's equation appears to be integro-differential.

The simplest nontrivial solution of (44), the kink, (in the case of vanishing load)was given by Peierls [8]:

$$u = \frac{b}{\pi} \operatorname{arctg} \frac{x}{\varkappa}$$

The size of the dislocation core(of the energy localization) is of order $\varkappa$

When $\sigma \neq 0$ there is a familiar nonstable solution of "solitary wave" type [22], which corresponds to the pair of dislocations with opposite signs

$$u = -\frac{b}{\pi}\left(\operatorname{arctg}\frac{x-\eta}{\mu} - \operatorname{arctg}\frac{x+\eta}{\mu}\right) + \frac{b}{2\pi}\beta$$

where $2\eta = \frac{\varkappa G}{\pi\sigma}$ is the distance between dislocations. The parameter β is related with the exterior load $\sin\beta = \frac{2\pi\sigma}{G}$, we have, also, $\mu = \varkappa/\cos\beta$, $\eta = \varkappa/\sin\beta$. The solution collapses if $\cos\beta \to 0$. When $\sigma = G/2\pi$ spontaneous formation of dislocation pair takes place. This stress value correspond to the theoretical shear regidity and appears to be an analog of the upper critical load. We note, that the application of the critical shear stress comes to metastability of the trivial configuration, thus we can interpret this solution as a nucleus of a "new phase".

The equation (44) permits us to describe in a qualitative manner the structure of the dislocation core. Being integrodifferential it is too complicated to analyze. Therefore there have been attempts to restrict to considerations with only weak nonlocality. The most successfull is the model of Frienkel and Kontorova

[23]. In their model the equilibrium configurations are extremals of the functional (for $\gamma = 0$):

$$\int_{-\infty}^{\infty} \left(\frac{du}{dx}\right)^2 - \frac{b^2}{2l^2}\left(1 - \cos\frac{2\pi u}{b}\right) dx$$

where $l = \frac{E}{G(1-\gamma)}^{1/2}$, E is Young's modulus. The Euler's equation coincides with the well-known Sin-Gordon equation. Kink solution in the framework of this model can be expressed through the elementary functions

$$tg\left(\frac{\pi}{4} + \frac{\pi u}{2b}\right) = \exp\left(-\frac{\pi x}{l}\right)$$

This is not the place to discuss the advantages of the considered models of dislocations. We have to point, however, that there is another interpretation of the Frienkel-Kontorova model which is related with the concept of a kink on a dislocation line [24] and, of course, with the analogous behavior of this objects.

ELEMENTARY PARTICLES

It is well-known that the equations of electrostatic scalar field can be obtained from the variational equation

$$\delta \int_V \Lambda \, dV = 0 \qquad (45)$$

where $\Lambda = (\nabla\varphi)^2$, φ is a field variable. Particles are connected with singular solutions: spherical solution of (45) is given by $\varphi \sim 1/r$ where r is radial coordinate. The energy of the considered singular solutions is infinite thus there arise apparent difficulties in physical interpretations of such solutions. One way to overcome this is to add the term $V(\varphi)$ to the Lagrangian. We can't achieve success trying to preserve linear equations, i.e. taking $V = m^2\varphi^2$; the solutions continue to be singular: $\varphi \sim \frac{1}{r}\exp(-mr)$ though "long range" action gives place to "short range" action. To obtain particle-like solutions with finite energy we need to add an essentially nonlinear term, for example, $V = \varphi^2(\varphi - \varphi_0)^2$. As we know "solitary wave" like solutions are unstable, so the problem can not be solved in this way and there have been attempts to construct models of elementary particles in terms of high order tensor fields [3]. Nevertheless the model of scalar field theory with the Lagrangians, similar to

$\Lambda = (\nabla\varphi)^2 + (\varphi^2 - a^2)$, are widely used for qualitative considerations of such phenomena as spontaneous symmetry breaking.

MECHANISM OF PHASE TRANSFORMATION

We have begun with considering of the function $F(u)$ having local minima. However, from the presented examples it is clear that $F(u)$ usually depends on some parameter p and obtains local minima only under special values of p. As a rule, energy functional has the following structure

$$I = \int_a^b F(u)dx + p\int_a^b u dx$$

The function $\mu(u, p) = F(u) + p \cdot u$ has the above property if the condition of the convexity of $F(u)$ is violated and the derivative d^2F/du^2 changes its sign twice *).

The most typical dependence of $\mu(u,p)$ on the parameter p is the following. We have three different intervals on p axis: $p < p_l$, $p_l < p < p_u$, $p > p_u$. When $p < p_l$ the function has the only minimum, at $p = p_l$ there appears the additional stationary point. In the interval $p_l < p < p_u$ the function $\mu(u,p)$ has already two local minima and their depths are equalized at $p=p_*$, where $p_l < p_* < p_u$. When $p > p_u$ we have again only one stationary point, the second vanishes at $p = p_u$. The sequence of transformations of the function $\mu(u,p)$ (Fig. 6) can be characterized in terms of cusp catastrophe. In mechanics the quantities p_l and p_u are called upper and lower critical loads respectively, in thermodynamics they are called spinodal points.

We come to the following physical picture. If $p < p_l$ the system can be found only in the phase state u_*. When $p = p_l$ there appears another phase state u_{**} which is unstable. After $p > p_l$ the newly formed phase becomes stable with respect to infinitesimal disturbances, being unstable with respect to finite disturbances. Such states are called metastable. Absolute minimum is achieved at $u = u_*$ up to the value of $p = p_*$, when the energies of phases become equal. The subsequent increasing of p leads to the shallowing of the minimum, corresponding to $u = u_*$

*) This let us formulate the main conception in the concise form: nonconvexity + higher derivatives.

and it vanishes at $p = p_u$. It is obvious that after $p > p_u$ the only $u = u_{**}$ phase can exist.

If we increase p, the phase transformation from state u_* to the state u_{**} will occur. We shall consider the process of phase transformation in some detail. Let us assume that the system is in homogeneous state $u \equiv u_*$ when $p < p_1$. After $p > p_1$ it appears additional ability to jump into another phase, though, in the absence of fluctuations the transformation into u_{**} phase can occur only after we go beyond the upper critical load p_u, i.e. after the state u_* becomes unstable (strategy of maximal delay). Classical thermodynamics, assuming fluctuations, accept as a transformation pressure the value $p = p_*$, which corresponds to the equality of phases energies (Maxwell's strategy).

Let us turn now to continuum , characterized by the function u(x). It is obvious that simultaneous transformation of all particles from one state to another is enegretically unfavorable: the necessity to overcome the energetical barrier causes significant energy losses. It seems that this fact was understood for the first time in connection with the investigation of phase transitions, though analogous ideas can be met in the theory of dislocations. The transformation from one phase state to another realizes through the formation of critical nuclei - the localized states of the new phase. Corresponding nonhomogeneous soliton configurations can be modeled by the saddle point of the energy functional.Such solutions of the Euler's equations describe the minimal energy of fluctuation, which transforms the system from metastable state to the stable state. Critical nuclei apparently unstable: the subcritical nuclei have a tendecy to collaps while for the overcritical nuclei the forgoing growth is energetically favorable: such growing nuclei provide the transformation of the system into the new phase state.

Critical nuclei correspond to the localized solutions of "solitary wave" type. It can be shown that by use of suggested analogy we can describe on equal grounds such different processes as the formation of vapour bubbles in overheated liquid, the formation of dimples on shells under pressure, the formation of dislocations in stressed crystal etc. We shall limit ourselves with: a) liquid-vapour transition, b) shells buckling.

In the theory of liquid-vapour transformation the specific volume V corresponds to variable u, F is specific free energy, μ - is specific Gibbs' energy or chemical potential, parameter

p coincides with the exterior pressure. The analysis of the structure of critical nuclei [6, 13] provides the following picture of transformation. When $p < p_1$ only one phase 1 (vapour) is stable and there are no nontrivial solutions of our variational problem. When $p_1 \leq p < p_*$ there appears metastable phase 2 (liquid) and we have nontrivial solutions of "solitary wave" type corresponding to vapour nuclei in liquid phase. Phase 1 stay stable and corresponds to the absolute minimum. When $p = p_*$ the indifferent equilibrium liquid-vapour with flat interfacial boundary (kink solution) is possible thus the transition from the phase 1 to the phase 2 occurs through the formation of the critical nucleus of infinite radious. When $p_* < p < p_u$ phase 2 becomes metastable. In this interval of pressure nontrivial "solitary wave" solutions that model liquid bubbles in vapour are possible. Effective bubble "radious" so as the energy of critical nucleus diminish to zero value when pressure increases from $p = p_*$ to $p = p_u$. The value of pressure $p = p_u$ corresponds to the state of absolute instability of phase 1. After $p > p_u$ only phase 2 is stable and nontrivial solutions are absent.

Thus, phase transformation is possible in the following interval: $p_1 < p < p_u$. Having calculated for all of these pressures the energy of the critical nucleus we can estimate the degree of stability of the equilibrium states.

Let us turn now to the dimple formation on the shell under the compressive exterior pressure p. The dependence of the deflection on the load is presented in Fig. 7. When $p > p_1$ there exists buckled equilibrium state, which differs significantly from homogeneously deformed initial state. When $p = p_*$ both equilibrium states have the same energy and at $p = p_u$ the initial state becomes absolutely unstable.

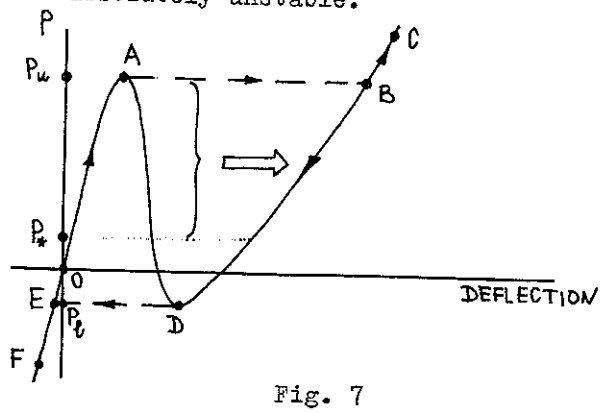

Fig. 7

The pressure p_u is called the upper critical load and it can be calculated in a standard way from the linear theory (see [25]).

In the literature on elastic stability it is usually assumed that, when the load p increases its value, the system evolve to the buckled states through the OABC parth (Fig. 7) and when p decreases - through the CBDEF parth. As we have already seen, the most important are not upper and lower critical loads but rather $p = p_*$: the loss of stability occurs not after $p = p_u$, but after $p = p_*$ (see also [12]).

The estimation of the lower critical load p_1 so as the p_* seems to be one of the most important problems in the theory of shells. The analogy of the buckling phenomena with the process of nuceation makes it possible to suggest the following buckling procedure. The transition to the buckled state is possible when $p_* < p \leq p_u$ and occurs through the formation of the critical uncleus i.e. the dimple, corresponding to the saddle point of the energy functional. The energy of such dimple characterize the energetical level of finite disturbances bringing out of the initial state of equilibrium. If we have $p \sim p_*$ the estimation of the "critical" energy can be made by use of Pogorelov's theory. The equilibrium configurations corresponding to reflection of some spherical segment appear to be unstable, thus dimples with the overcritical radius continue to grow and subcritical dimples vanishes. This coincides with the picture of phase transition in liquid and we obtain analogy between the dimple edge energy and the energy of the interfacial tension. This analogy permits to suggest the new understanding of upper and lower critical loads and to yield the investigation of degree of stability to the problem of saddle points of the energy functional.

CONCLUDING REMARKS

The examples presented above show the identity of the mathematical structure of the energy functional leading to the localization of the energy in quite different physical situations. The main conception concerning energy structure can be repeated in a concise form: nonconvexity + higher derivatives. If the energy of homogeneous states has a number of minima, then the equilibrium configuration is not unique. Regularization can be achieved by the introduction to the functional of additional terms with the derivatives [26]; in all of our examples this was done according to the additional reasons of physical character. The existance of

higher derivatives in the equations equilibrium leads to the appearance of states with localized energy. Thus it can be formulated the following proposal: if a nonconvexity appear, then one mustlook for higher derivatives.

REFERENCES

1 A. Einstein, L.Infeld, B. Hoffman, Ann. Math. 39 (1938) 65-100.
2 D.J. Korteweg, G. de Vries, Philos. Mag. 39 (1895), 422-443.
3 R. Jackiv, Rev. Mod. Phys. 49 (1977) 681-706.
4 J.D. van der Waals, Verhandel. Konink. Akad. Weten., Amsterdam (Sect. 1) 1 (1893).
5 L.D. Landau, E.M. Lifshits, Electrodynamics of Continuum, Nauka, Moscow, 1982 (in Russian).
6 J.W.Cahn, J.E.Hilliard, J. Chem. Phys., 28 (1958) 258-267.
7 A.Pogorelov, Geometrical Methods in Nonlinear Theory of Shells, Nauka, Moscow, 1967 (in Russian).
8 R. Peierls, Proc. Phys. Soc., 52 (1940).
9 J.W. Gibbs, Trans. Connect. Acad., 3 (1876) 108-248; 3 (1878) 343-524.
10 V. Berdichevskii, Variational Principles of Continuum Mechanics, Nauka, Moscow, 1983 (in Russian).
11 T. Karman, H.S. Tsien, J. Aeronaut. Sci. 7 (1939) 43.
12 K.O. Friedrichs, in T. Karman Anniversary Volume, 1941, p.258.
13 L. Truskinovskii, Dokl. AN SSSR, 269 (1983).
14 L. Truskinovskii, Dokl. AN SSSR, 265 (1982).
15 L.I. Sedov, Continuum Mechanics, v. 1, 2, Nauka, Moscow, 1976 (in Russian).
16 R.D. Mindlin, Int. J. Solids and Struct. 1 (1965) 417-436.
17 V. Berdichevskii, J. Appl. Math. and Mech. (PMM) 30 (1966) 510-530.
18 J.L. Ericksen, J. Elast. 5 (1975).
19 B. Coleman, Arch. Rat. Mech. Anal., 83 (1983) 115-137.
20 S.S. Antman, J. Math. Anal. Appl., 44 (1973) 333.
21 J. Whitham, Linear and Nonlinear Waves, 1973.
22 F.R.N. Nabarro, Proc. Phys. Soc. 59 (1947).
23 I.Frienkel, T. Kontorova, JETP (1938) 1340.
24 A. Seeger, D. Schiller, in W.P.Mason (ed.), Physical Acoustics v.3, p.361.
25 R.Joelly, Ueber ein Knickungsproblem an der Kugelschale, Zurich, 1915.
26 J.M. Ball, J.C. Currie, J. Func. Anal., 41 (1981).