Application of group theory methods to describe the evolution of the order parameter of multiferroics

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The talks is based on Barchelor's qualifying work
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Description of the tasks:

- To find analytic 2-component solutions of the Ginzburg–Landau–Devonshire equation for the polydomain 180° domain structure of a multiaxial multiferroic film using the group-theoretic Ovsyannikov–Lie method.

- To obtain analytic expressions for the free energy of the system and analyze its dependence on the thickness of the film and the boundary conditions on its surface.

Introduction

The structure of the 180° rotating uncharged domain wall was studied using *Landau–Ginzburg–Devonshire approach*.

We find an exact analytic solution for corresponding stationary equation describing polydomain structure in a multiaxial ferroic film.

We used this solution to obtain free energy and analyze its dependence on the film thickness.

Lie - Ovsyannikov symmetry method

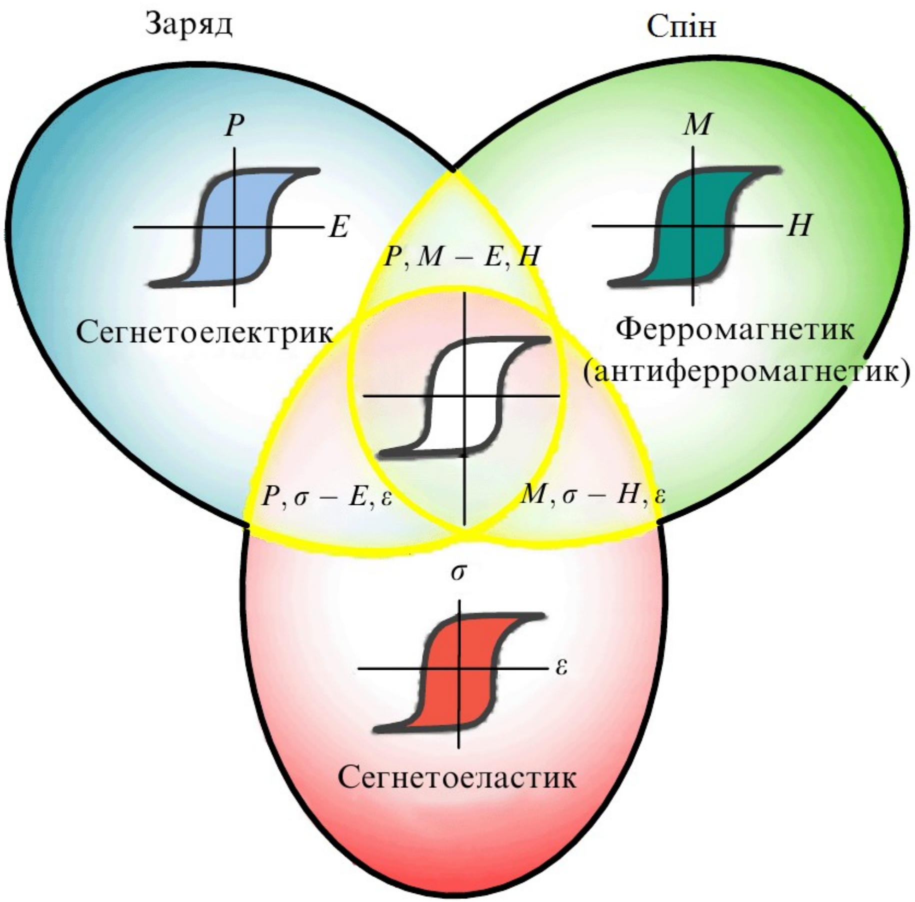
Lie - Ovsyannikov symmetry method was used to obtain analytic solutions.

The method is based on the using of continuous groups of equation’s symmetries and corresponding algebra of invariance of the equation.

For each subalgebra of the algebra there corresponds a special ansatz for solution which reduces number of independent variables.

The method allows to find not just one solution, but a whole family of them!

Multiferroics



There are three classes of ferroics: ferromagnetic, ferroelectric, and ferroelastic.
Materials in which at least two types are present are called multiferroics.

In multiferroics, it is actually possible to observe the **magnetoelectric effect**.

Physically, it is an appearance of *an electric polarization in the presence of magnetic field*

$$M_i = \frac{\alpha_{ij}}{4\pi} E_j$$

And *spontaneous magnetization proportional to the electric field* can occur (**reverse magnetoelectric effect**)

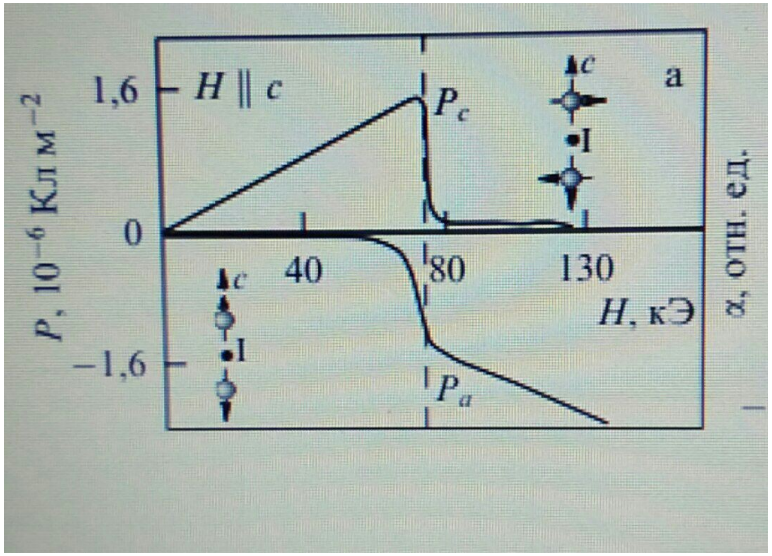
$$P_i = \frac{\alpha_{ji}}{4\pi} H_j$$

From these formulas we see that they connect vectors with different properties with respect to transformations of both space and time (namely, polar and axial vectors). For example, the electric field vector is polar, and therefore its sign changes with space inversion, and remains unchanged with time inversion. Conversely, the magnetization vector is axial, and therefore it is P-even, and T-odd. Hence one can try to obtain a condition for the symmetry of matter, under which the magnetoelectric effect becomes possible

Since the magnetoelectric effect formulas relate vectors with different P, T parity, they can be valid only while combined **PT parity preserves** (in this case, P and T parity separately can be violated).

There are few substances that can have similar properties. For example, they can be exhibited by chromium oxide crystals Cr_2O_3. For them, the electric polarization is induced by a magnetic field, and this **effect is longitudinal**, that is, the vectors P and M are parallel. In strong magnetic fields, phase transitions can occur in which spins, directed along some axis, can tip over into a plane perpendicular to it (**transverse magnetoelectric effect**).

The exchange structure of this material in both orientational states is arranged in such a way that the inversion center transfers chromium ions belonging to one of the antiferomagnetic lattices to another (centroantisymmetric). Thus, the **magnetoelectric effect in a substance is possible** when the **central symmetry is violated**

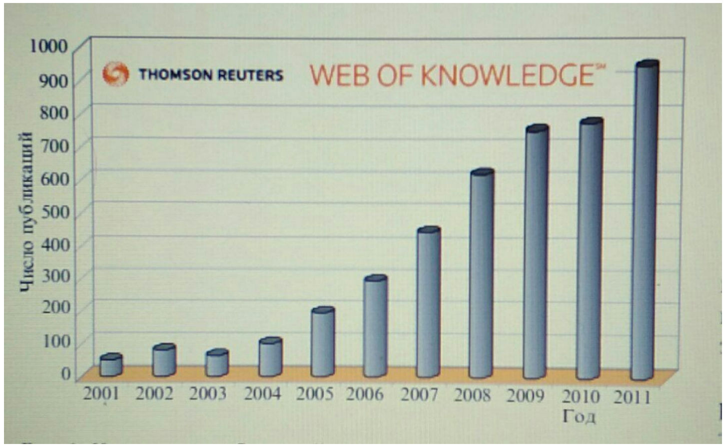


Motivation for the study of multiferroics

The study of multiferroics can be interesting from a purely theoretical point of view, since it is related to the fundamental problem of the relationship between electrical and magnetic phenomena.

Magnetoelectric phenomena can be interesting as they are not dynamic, that is, they do not occur when charges move or electromagnetic fields change over time: even a static electric field generates a magnetization.

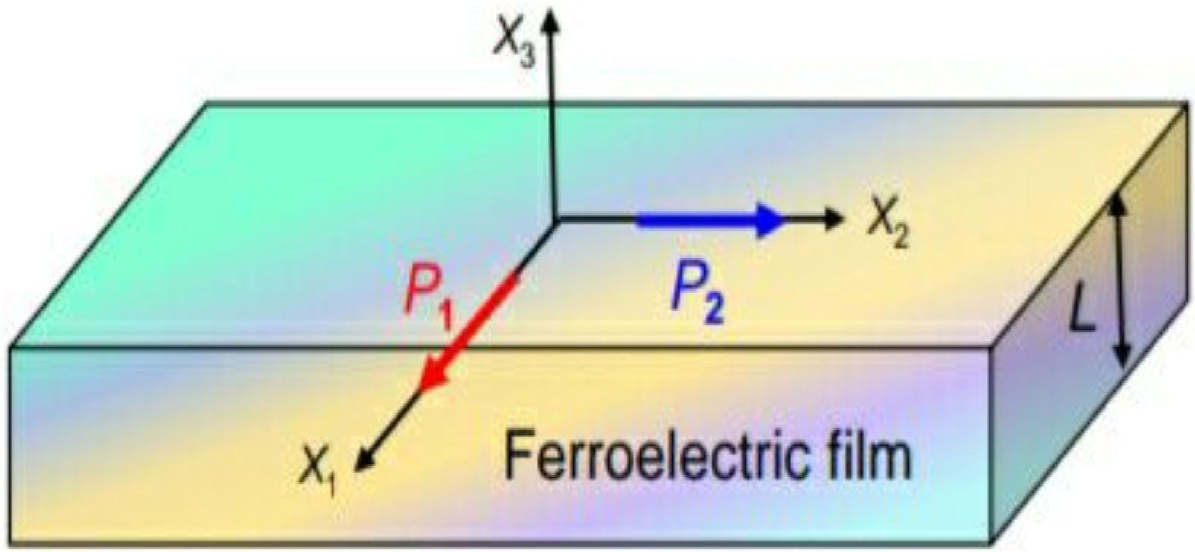
Therefore, there is an interest for application to the theory of materials, as they can help us create magnets that turn on under the influence of a constant electric field, that does not requires energy to maintain itself.



Formulation of the problem

We consider a stress-free multiferroic film with uncharged domain walls.

The film is thick enough.



The geometry of a multiaxial multiferroic film with a polarization vector **P**$(x_3)= (p_1(x_3),p_2(x_3),0)$. We adopted this condition for the reasons of having no depolarization field (or div **P**=0).

Variation of action

If there is no external field, we write down equations that will describe the relaxation of the domain structure.

These equations follow from the variation of the action

$$S = \int_{0}^{\infty} dt \int \left[g_l + g_{grad} - \frac{\rho_i}{2}\left(\frac{\partial P_i}{\partial t}\right)^2 \right] dv$$

This action can be obtained from the energy density

$$G = \int (g_l + g_{grad}) dv + \int g_s ds$$

where $g_L = a_i P_i^2 + a_{ij} P_i^2 P_j^2 - P_i E_i$, $g_{grad} = \frac{g_{ijkl}}{2} \frac{\partial P_i}{\partial x_j} \frac{\partial P_k}{\partial x_l}$, $g_S = \frac{a_i^S}{2} P_i^2$,

are *Landau energies*, *gradient* and *surface energies*, respectively.

Variational action

The system obtained by varying the action S has the form [Landau L. D., Khalatnikov I. M., 1954]

$$2a_1P_1 + 4a_{11}P_1^3 + 2a_{12}P_1P_2^2 - g_{44}\frac{\partial^2 p_1}{\partial x_3^2} = -\rho_1\frac{\partial^2 p_1}{\partial t^2} - \Gamma\frac{\partial p_1}{\partial t},$$

$$2a_1P_2 + 4a_{11}P_2^3 + 2a_{12}P_2P_1^2 - g_{44}\frac{\partial^2 p_2}{\partial x_3^2} = -\rho_1\frac{\partial^2 p_2}{\partial t^2} - \Gamma\frac{\partial p_2}{\partial t},$$

here $\rho_1 > 0$ is a kinetic coefficient and Γ>0 is a Khalatnikov relaxation coefficient.

We also assume that

Dynamic Ginzburg-Landau-Devonshire equations

Let us introduce the dimensionless coordinate x, film thickness l, polarization components p_1 and p_2, multiferroic anisotropy factor μ, relaxation time τ and kinetic coefficient ρ:

$$x = \frac{x_3}{R_c} \quad l = \frac{L}{R_c} \quad p_1 = \frac{P_1}{P_s} \quad \mu = \frac{a_{12}}{2a_{11}} \quad \tau = -\frac{\Gamma}{a_1} \quad \rho = -\frac{\rho_1}{a_1} \qquad P_s = \left(-\frac{a_1}{2a_{11}}\right)^{\frac{1}{2}} \quad R_c = \left(-\frac{g_{44}}{2a_{11}}\right)^{\frac{1}{2}}$$

Hence the structure of the domain walls in such a film is described by the system of Ginzburg-Landau-Devonshire (GLD) equations:

$$-\rho\frac{\partial^2 p_1}{\partial t^2} - \tau\frac{\partial p_1}{\partial t} = \frac{\partial^2 p_1}{\partial x^2} - p_1 + p_1^3 + \mu p_1 p_2^2$$

$$-\rho\frac{\partial^2 p_2}{\partial t^2} - \tau\frac{\partial p_2}{\partial t} = \frac{\partial^2 p_2}{\partial x^2} - p_2 + p_2^3 + \mu p_2 p_1^2$$

We will solve it using **Lie - Ovsyannikov symmetry method**

How to multiply the solution of a differential equation using its symmetry group

A differential invariant of a group is an invariant of an extended group. Since a differential equation is expressed not only in terms of functions and independent variables, but also in terms of derivatives, we must consider the manifold of the equation

$$E:\ F^{\sigma}\left(x, v, \underset{1}{v}, \dots, \underset{k}{v}\right) = 0, \qquad \sigma = 1..s$$

system of differential equations of the kth order for m sought functions of n independent variables

in the extended space (in addition to independent and dependent variables, there are derivatives).

Then the equation manifold admits a local continuous group of transformations if it is closed under the action of group transformations

$$X_k E\left(x, v, \underset{1}{v}, \dots, \underset{k}{v}\right)|_{E} = 0$$

Theorem (1). If there is a group admitted by the system E, then it automatically acts on the set of solutions of this system (the solutions are invariant with respect to the action of the group).

How to multiply the solution of a differential equation using its symmetry group (an example)

Consider for example the system of equations of motion of an ideal monatomic gas (polytrope exponent 5/3)

$$\frac{d\boldsymbol{u}}{dt} + \frac{1}{\rho}\nabla p = 0 \qquad \frac{d\rho}{dt} + \rho\, div\, \boldsymbol{u} = 0 \qquad \frac{d}{dt}\left(\frac{p}{\rho^{\frac{5}{3}}}\right) = 0$$

This system admits non-trivial projective transformations

$$x'_0 = \frac{x_0}{1 - ax_0}, \quad x'_1 = \frac{x_1}{1 - ax_1}, u' = (1 - at)u + ax_1\, , \rho' = (1 - ax_0)^3 \rho,$$
$$p' = (1 - ax_0)^3 p$$

Using this change of variables and the inverse of them, it can be shown that the system is also satisfied with these functions

$$u(x_0, x_1) = (1 + ax'_0)u'(x'_0, x'_1) - ax'_1 \quad \rho(x'_0, x'_1)$$
$$= (1 + ax'_0)^3 \rho'(x'_0, x'_1), \quad p(x_0, x_1) = \rho'(x'_0, x'_1)$$

Then for a stationary ideal gas (u=0,$\rho_0(x_1) > 0, p_0 > 0$) we will automatically obtain

$$u = -\frac{ax_1}{1 - ax_0}; \qquad \rho = \frac{1}{(1 - ax_0)^3}\rho_0\left(\frac{x_1}{1 - ax_0}\right); \qquad p = \frac{p_0}{(1 - ax_0)^5}$$

We see that each particle of the gas moves with a velocity vector proportional to the initial position vector

.

Basis of invariants of the Lie group of transformations

In the finite-dimensional case, each Lie group that has a parameters corresponds to an a-dimensional Lie algebra $A_r = \{X_{1,} \dots, X_r\}$

Then we can formulate a criterion for the invariance of a certain expression with respect to the group

Theorem (2) F(x) is an invariant r of the parametric group G if and only if true

$$X_i F = \xi_i^j(x) \frac{\partial F}{\partial x_j} = 0 \quad (i = 1..r)$$

Complete operator system $X_1, .., X_r$

forms a complete system if they are not linearly connected, and there is such a set of functions that

$$[X_\alpha ; X_\beta] = \varphi_{\alpha\beta}^\sigma(x) X_\sigma$$

If we also have $\varphi_{\alpha\beta}^\sigma(x) = 0$ then such a system is called Jacobian

Basis of invariants of the Lie group of transformations

Theorem 3 (about the basis of invariants and the connection between them). A complete system of operators in R^n

$$\{X_{1,} \dots , X_r\}$$

defines n-r invariants that are not related to each other

To obtain invariants, it is convenient to carry out such a change for a given complete system of operators, which makes this system Jacobian

For example, let's choose such coordinates that $(X\varphi_1(x) = 1, \qquad X\varphi_i(x) = 0 \; i \text{ не } 1)$

Then the other operators will take the form

$$X_i = B_i(y)\left(\xi'^{1}_{i}(y)\partial_{y_1} + \xi'^{2}_{i}(y_2, \dots , y_n)\partial_{y_2} + \dots + \xi'^{n}_{i}(y_2, \dots , y_n)\partial_{y_n}\right)$$

But taking into account the factorization of the operators by the multiplier and the independence of the function F from the first variable, we obtain that for i=2..r

$$Y_i = \xi'^{2}_{i}(y_2, \dots , y_n)\partial_{y_2} + \dots + \xi'^{2}_{n}(y_2, \dots , y_n)\partial_{y_n}$$

If we continue this procedure further, then at the next step we get the system

$$B_i = \partial_{\mu^i} \quad i = 1..r)$$

it is clear that it will have n-r invariants $I_1 = \mu^{r+1}(x), \dots , I_{n-r} = \mu^n(x)$

A bit about abstract Lie algebras

The Lie algebra is a structure, the elements of which are representatives of a certain vector space, on which a commutation operation is imposed. Along with this, the properties familiar to us from school must be fulfilled, namely:

$[a_1 X + b_1 Y; z] = a_1 [X; z] + b_1 [Y; z]$ I)

$[X; Y] = -[Y; X]$ ii)

$[X; [Y; Z]] + [Y; [Z; X]] + [Z; [X; Y]]$ Jacobi identity iii)

Let we have a basis $L_r = \{X_1, \dots, X_r\}$

Then the Lie algebra is completely determined by the structure constants

$$[X_i; X_j] = C_{ij}^k X_k$$

Subalgebra $N \subset L$ is called an **ideal**, if $[N; L] \subset N$

We are interested in **non-trivial ideals**, that is, those that are different from the zero element and the entire algebra, which are always ideals. In the future, we will be interested in the maximum dimensional sub-algebra for which the initial set will be an ideal -- **normalizer**

$$N = Nor_L M$$

Obviously, for the ideal, the normalizer will be the whole Lie algebra

A bit about abstract Lie algebras

Lie algebra is **simple**, if it has no proper ideals (different from zero and the whole algebra

One can consider commutators of the algebra with itself.

$$D^{k}M = [D^{k-1}M; D^{k-1}M]$$

Naturally, the question arises whether the sequence can terminate at zero

$$M \supseteq DM \supseteq D^{2}M \supseteq \cdots \supseteq D^{l}M \supseteq \cdots$$

If there exists such k that $D^{k}M = 0$ then M is called **solvable**

If the Lie algebra has no solvable ideals, then it is called **semisimple**. Obviously that every simple algebra is semisimple. One can prove that every non1-dimensional Lie algebra is simple.

Theorem (Levi Maltsev) Each Lie algebra can be decomposed into a semidirect sum of a radical and a semisimple algebra, the latter is defined ambiguously

$$L = R \bigoplus^{s} N$$

Theorem (decomposition of a semisimple algebra) Each semisimple Lie algebra decomposes into a direct sum of its simple ideals

A

Invariant solutions

Lets consider the system $\mathrm{E}\colon \mathrm{F}^{\sigma}(\mathrm{x},\mathrm{u},\mathrm{u1},\mathrm{u2},\dots,\mathrm{uk}) = 0 \quad \sigma = 1..\mathrm{s}$

which admits a group of transformations $G_r = \{T_a\}$

Its corresponding Lie algebra is generated by the operators

$$L_r = \left\{X_\mu = \xi_\mu^i(x,u)\partial_{x^i} + \eta_\mu^j(x,u)\partial_{u^j}\right\}$$

A certain solution of this equation is invariant with respect to a certain subgroup, if the corresponding manifold is invariant with respect to this subgroup. In order for such a solution to exist without peculiarities, it is enough to fulfill the following conditions

$$o.p.\left\|\frac{\partial I^s}{\partial u^j}\right\| = m$$

$$r(\xi,\eta) = r(\xi)$$

where $r(\xi) = o.p.M(\xi)$, $r(\xi,\eta) = o.p.M(\xi,\eta)$ and

$$M(\xi) = \begin{matrix} \xi_1^1(x,u) & \dots & \xi_1^n(x,u) \\ \dots & \dots & \dots \\ \xi_r^1(x,u) & \dots & \xi_r^n(x,u) \end{matrix} \qquad M(\xi,\eta) = \begin{matrix} \xi_1^1(x,u) & \dots & \xi_1^n(x,u)\eta_1^1(x,u) & \dots & \dots & \eta_1^m(x,u) \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \xi_r^1(x,u) & \dots & \xi_r^n(x,u)\eta_r^1(x,u) & \dots & \dots & \eta_r^m(x,u) \end{matrix}$$

Invariant solutions

Theorem 4. Let the system of differential equations E admits a group K, while the conditions written on the previous slide are fulfilled. Then there is a factor system E/K, which depends only on invariants $I^m, m = 1..t$, functions expressed through these invariants and their derivatives. Hence, the representation of an invariant manifold has the form

$$I^\alpha(x,u) = U^\alpha\left(v^1(x), \dots, v^{n-r}(x)\right) \quad \alpha = 1..m$$

$$I = \{I^1(x,u), \dots, I^m(x,u), \lambda^1 = I^{m+1}(x), \dots, \qquad \lambda^{n-r} = I^t(x)\}$$

Then we can obtain the factor system E/M by substituting the resulting invariant representation into the initial system E.

Since an invariant equation can only be expressed in terms of invariants and functions of them, there will be fewer independent variables, and thus the equation will be simplified

For example, when n-r=1, we get a factor system in the form of a system of ordinary differential equations, and in the case of n-r=0, a system of algebraic equations.

Invariant solutions (an example)

Lets consider, for example, KdV equation. $u_t + uu_x + u_{xxx} = 0$

It can be shown that it admits a 4-dimensional Lie algebra

$$X_1 = \partial_t \quad X_2 = \partial_x \quad X_3 = t\partial_x + \partial_u \quad X_4 = 3t\partial_t + x\partial_x - 2u\partial_u$$

Lets find the factor equation for the subalgebra generated by elements X_1 ,X_3

The corresponding invariant variables will have the form

$$I = \left\{x - \frac{bt^2}{2}, u - bt\right\} = \{\lambda, u(\lambda)\}$$

After the appropriate replacement of variables in the E system and further simplifications, we obtain the factor of the E/M system

$$u''' + uu' + \beta = 0 \qquad \Rightarrow u'' + \frac{U^2}{2} + \beta\lambda + C_1 = 0$$

This is an ordinary differentiation, which can be solved to obtain solutions in the form of elliptic functions. In this way, taking into account the action of the group, we obtained a whole class of solutions invariant with respect to the algebra stretched over the subalgebra

Invariant solutions (an example)

The resulting factor system may turn out to be contradictive, then the invariant solution for this subalgebra will not exist. Consider as an example the equation $tu_t + xu_x = 1$

This equation admits a uniform expansion of the variables t and x with an operator

$$X = t\partial_t + x\partial_x \qquad \Rightarrow I = \left(\frac{x}{t}, u\right)$$

Substituting $u = U\left(\lambda = \frac{x}{t}\right)$ into the original equation leads to a contradictive factor equation

E/H: 0=1

Thus, this equation does not have a solution that is invariant under uniform tensions of t and x.

Properties of the factor system E/H

Let the initial system E admits a Lie algebra G. Let's take a subgroup H from it. We take a subgroup H from it and construct a factor system. It is interesting to know what part of the elements from the initial group will be allowed by the factor system.

Theorem (**<u>symmetry of E/H</u>**) factor system allows transformations generated by the normalizer Nor $_L$ H. Although the factor system may allow other transformations not contained in the normalizer

Theorem: if subgroups H,H' are conjugate i.e. $H = THT^{-1}$ than for arbitrary H--invariant solution , the solution F' =TF is also an invariant H' --solution

Thus, conjugate subgroups generate conjugate invariant solutions.

Application of the Ovsyannikov-Lie method to solving the GLD equation for a multiferroic film

In the simplest case, when the components of the polarization vector are $p_1=p_2$ then we obtain a simplification of the original system to one differentiation:

$$\frac{\partial^2 u}{\partial t^2} + a\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} - u + (1+b)u^3 = 0$$

where a,b=const. In the case of $a\neq 0$, $b\neq -1$, we will have a trivial two-dimensional algebra which corresponds to the ansatz of running wave $u = \varphi(x-ct)$. The corresponding invariant solution:

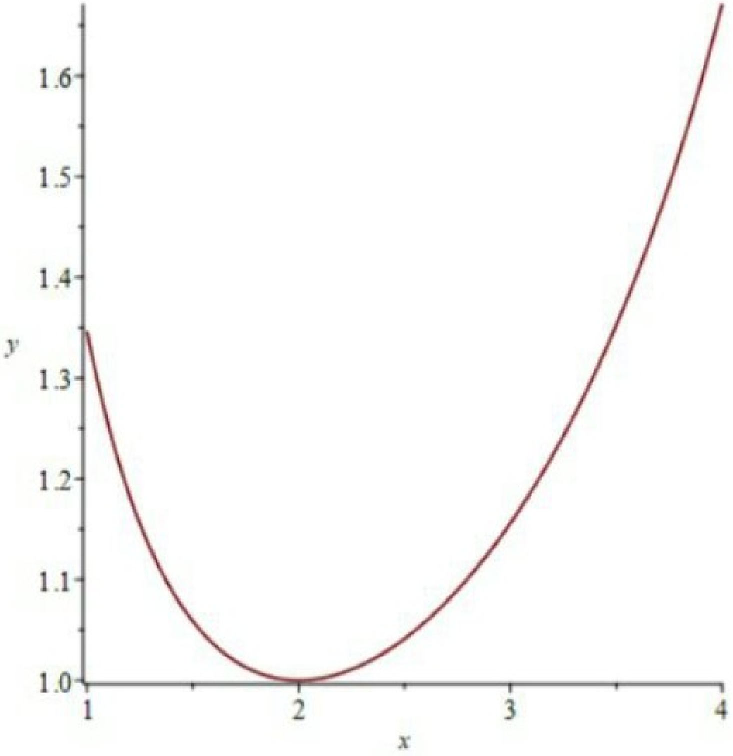
$$x(t) = \left(C + C^{-\frac{3}{4}}\right) BtF\left(\frac{1}{2}, \frac{3}{4}, \frac{3}{2}, \frac{2t^2}{c}\right)\left(C - 2t^2\right)^{-\frac{1}{4}}$$

$$y(t) = \varphi'(t) = \varphi(\varphi t + B),$$

where $x(t)\equiv u(x,t)$, $y(t)\equiv u'(x,t)$, B i C – constants which are determined from the initial conditions.

In the case a=0, we have an algebra $\langle \partial_t, \partial_x, x\partial_t + t\partial_x \rangle$ which corresponds to the ansatz $\varphi = u\left(x^2 - t^2\right)$

Plot of the numerical solution of the reduced equation:



For the stationary case, the original system of equations can be written in the form:

$$-p+\frac{1+\mu}{4}p^3+\frac{3-\mu}{8}p\,a^2-\frac{\partial^2 p}{\partial x^2}=0,$$

$$-a+\frac{1+\mu}{4}a^3+\frac{3-\mu}{8}a\,p^2-\frac{\partial^2 a}{\partial x^2}=0.$$

here $p=p_1+p_2$, $a=p_1-p_2$.

here $p=p_1+p_2$, $a=p_1-p_2$.

For the case $p_1=p_2$, the system is reduced to one equation:

$$-p+\frac{1+\mu}{4}p^3-\frac{\partial^2 p}{\partial x^2}=0$$

Its solution

$$p(x)=\frac{1}{2}\sqrt{\frac{2m}{1+m}}\,sn\left(\frac{x+X_{\omega 1}}{\sqrt{1+m}},m\right)$$

where parametrs $X_{\omega 1}$ and m are defined from boundary conditions

For the general case when $p_1 \neq p_2$, we get the solution:

$$p_1(x) = \frac{1}{2}\left[\sqrt{\frac{2m}{1+m}}\, sn\left(\frac{x+X_{\omega 1}}{\sqrt{1+m}}, m\right) + \sqrt{\frac{2n}{1+n}}\, sn\left(\frac{x+X_{\omega 2}}{\sqrt{1+n}}, n\right)\right]$$

$$p_2(x) = \frac{1}{2}\left[\sqrt{\frac{2m}{1+m}}\, sn\left(\frac{x+X_{\omega 1}}{\sqrt{1+m}}, m\right) - \sqrt{\frac{2n}{1+n}}\, sn\left(\frac{x+X_{\omega 2}}{\sqrt{1+n}}, n\right)\right]$$

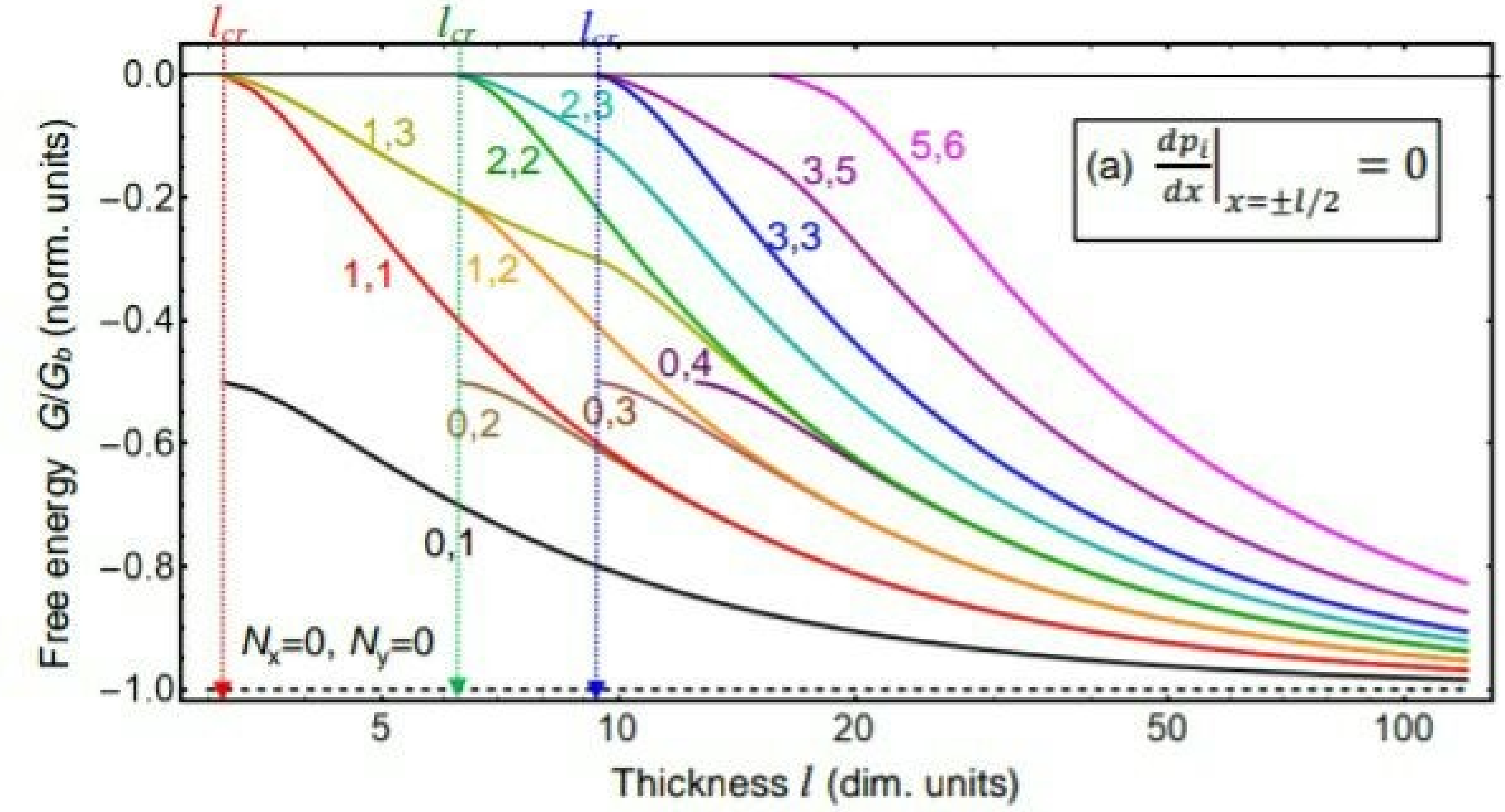
In turn, the free energy density in the GLD model is described by the expression:

$$G = \int_{-l/2}^{l/2} g_V(x)dx + \frac{p_1^2(-l/2)}{\lambda_1} + \frac{p_2^2(-l/2)}{\lambda_2} + \frac{p_1^2(l/2)}{\lambda_1} + \frac{p_2^2(l/2)}{\lambda_2},$$

$$g_V = -\frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{4}(p_1^4 + p_2^4) + \frac{\mu}{2}p_1^2 p_2^2 + \frac{1}{2}\left[\left(\frac{dp_1}{dx}\right)^2 + \left(\frac{dp_2}{dx}\right)^2\right]$$

where l is the film thickness, μ is the anisotropic factor, λ is the extrapolation length.

Analysis of the dependence of the free energy of a multiferroic film on its thickness [Morozovska, A. N., Eliseev, E. A., Fomichov, Y. M., & Kalinin, S. V. (2020). Mesoscopic structure of mixed type domain walls in multiaxial ferroelectrics. Phys. Rev. Materials, 4(11).]



Conclusions

1. Particular solutions of the Landau–Ginzburg–Devonshire system of dynamic equations for a free film of a multiferroic were found using the group-theoretic Ovsyannikov-Lie method.

2. Using the solutions, the dependence of the free energy of the film on its thickness and boundary conditions was analyzed. It was found that the resulting stable polydomain states have negative energy which monotonically decreases with increasing film thickness.

3. Finding general analytic solutions of the system of differential equations with *cubic nonlinearity* requires further research: to investigate the algebraic invariant solutions of this system and, possibly, to apply the method of non-classical symmetries.

Thanks for your attention !