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# PROGRAMS FOR CALCULATING A DYNAMIC MODE MAP ON THE EXAMPLE OF A SYSTEM WITH CHAOTIC MODES

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#### **ABSTRACT**

**Background**. Dynamic mode maps are a visualization tool used to analyze and classify the behavior of complex nonlinear dynamic systems as parameters change. They allow us to identify how the system's operating mode (steady state, periodicity, chaos, etc.) changes when one or more parameters are varied.

**Materials and Methods**. The paper proposes algorithms for constructing dynamic mode maps based on the convergence of periodicities and the minimum value function. The first is based on selecting the last element of the set and comparing this element in turn with all the previous ones. If the last element coincides with the previous one, then it is stated that the resulting set has a period of 1, which means that with these parameters, the system has a limit point. The second algorithm is based on creating arrays of standard deviations. Software has been developed for constructing dynamic mode maps using the convergence of periodicities and the minimum value function.

Results and Discussion. Based on the analysis of dynamic mode maps obtained by these methods under the condition of the existence of the Lifshitz invariant at n=3, it was established that the method of periodicity convergence more fully describes the existing dynamics of the incommensurate superstructure, which is experimentally traced in tetramethylammonium tetrachlorocuprate crystals. It is shown that the dynamic mode maps calculated by the method of periodicity convergence have a significant number of existing periodicities and most fully describe the dynamics of the incommensurate superstructure. It is established that the palette of existing periodicities is more represented under the condition when the increment of the phase function acts as the arguments of the recurrent relations. The dynamic mode map deserves special attention when the increment of both the amplitude and phase functions acts as the arguments of the recurrent relations.

**Conclusion.** It has been established that the considered algorithm for constructing dynamic regime maps is effective for analyzing the dynamics of an incommensurate superstructure, which is described by a system of differential equations, and the appearance of an incommensurate superstructure is due to the existence of the Lifshitz invariant.

**Keywords:** dynamical regime maps, incommensurate superstructure, incommensurate superstructure regimes, anisotropic interaction.

# **INTRODUCTION**

Dynamic mode maps, which are diagrams on a plane with two parameters on the coordinate axes, provide a fairly complete and visual representation of a dynamic system's behavior, showing the boundaries of areas of different dynamic modes. [1]. Constructed maps of dynamic modes are correlated with other ways of presenting this information, such



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Two-dimensional mappings, like one-dimensional mappings, are given by recurrence relations of the form:

$$\begin{aligned}
x_{n+1} &= f(x_n, y_n), \\
y_{n+1} &= g(x_n, y_n).
\end{aligned} \tag{1}$$

In two-dimensional mappings, it will be necessary to deal with points on the plane, that is, with several numbers that specify the coordinates of the points. Two-dimensional mappings come into consideration in various ways. Some of them are the result of generalization of one-dimensional mappings, others model some phenomenon characterized by discrete time. Two-dimensional mappings often arise as difference schemes during the numerical solution of systems of differential equations.

Let's construct dynamic mode maps for an incommensurate superstructure described by two second-order differential equations [3]:

$$R'' - R^3 + (1 - \varphi^2 + T\varphi')R - R^{n-1}K(\cos n\varphi + 1) = 0,$$
 (2)

$$\varphi'' + 2\frac{R'}{R}\left(\varphi' - \frac{T}{2}\right) + R^{n-2}K\sin n\varphi = 0,$$
(3)

where R,  $\varphi$  are dimensionless variables characterizing the amplitude and phase functions, T and K are dimensionless parameters, n is an integer characterizing the symmetry of the potential. In this system of differential equations, the appearance of an incommensurate superstructure is described by the Lifshitz invariant, T and K the parameters describe the long-range and anisotropic interaction, respectively. Anisotropic interaction in this system of differential equations is represented by the Dzyaloshynsky invariant [4].

The calculation of the spatial behavior of the amplitude and phase functions and the construction of dynamic mode maps is going to be performed in the Python software environment [5].

When constructing dynamic mode maps, a function describing the behavior of the disproportionation wave amplitude R or/and its change R' acted as the function  $f(x_n,y_n)$ . A function describing the behavior of the disproportionation wave phase  $\varphi$  or/and its change  $\varphi'$  acted as the function  $g(x_n,y_n)$ . The two-dimensional mapping constructed in this way depends on the values of parameters a=K and b=T. The choice of these parameters K and K' as K' and K' and K' is due to the dependence of the non-commensurate superstructure dynamics on the parameter: K' is the parameter that determines a long-range interaction magnitude; K' is the parameter that determines an anisotropic interaction magnitude.

In this study, we are going to consider dynamic mode maps for the incommensurate superstructure that occurs in crystals of the tetramethylammonium tetrachlorometallate(II) group ( $[N(CH_3)_4]_2MeCl_4$ , where Me = Zn; Cu; Co; Fe; Ni), and its appearance is due to the presence of the Lifshitz invariant. The spatial variation of the order parameter amplitude and phase in these crystals can be described by expressions (2), (3). Dynamic mode maps will start to be observed, provided that the amplitude and phase functions, as well as their changes (first integral of the motion) will act as recurrence relations, in order to follow the full picture of disproportionate superstructure dynamics.

# **MATERIALS AND METHODS**

#### Periodicity convergence method.

The following algorithm can be used to construct the dynamic mode maps.

- **Step 1.** For some initial pair of values  $(x_0; y_0)$  and some pair of values (a, b) according  $d_i$  to formula (1), a set of iterative values  $(x_1; y_1), (x_2; y_2), \dots, (x_n; y_n)$ , is obtained.
- **Step 2.** A few q last points are selected. For example, 8 or 16. q is a number that represents the maximum period that can be determined by this algorithm. Selected points form a set  $(x_{n-q+1}; y_{n-q+2}), (x_{n-q+2}; y_{n-q+2}), \dots, (x_{n-1}; y_{n-1}), (x_n; y_n)$ .
- form a set  $(x_{n-q+1};y_{n-q+1}), (x_{n-q+2};y_{n-q+2}), \ldots, (x_{n-1};y_{n-1}), (x_n;y_n)$ . **Step 3.** Working with a set of points that have 2 coordinates is not very convenient in our case. To do this, you need to replace 2 coordinates with some single number. For example, replace with the square of the modulus of the vector corresponding to the given coordinate. That is, instead of the point  $(x_i;y_i)$ , the value  $d_i=x_i^2+y_i^2$  is used. As a result, the set  $d=(d_1,d_2,\ldots,d_q)$  is obtained. Further actions will require  $d_i$  displaying some specific  $(x_i;y_i)$  and not allow repeats. But this cannot be achieved if the points form a certain symmetrical figure, for example, a circle distances to the middle of the coordinates center of which will be the same. Therefore, it makes sense to introduce some asymmetry in the above operation. For example:  $d_i=(x_i+k_1)^2+(y_i+k_2)^2$ .
- **Step 4.** Work with a set d is the next. The last element of the set is highlighted and this element is compared one by one with all the previous ones. If the last q element matches q-1, then it is claimed that the obtained set d has a period of 1, which means that the system has a limit point with the parameters (a,b). If the match is on q-2, then it is believed that a cycle with a period of 2 is implemented in the system. And so on, until the period is not detected. That is, upon reaching a situation where none of the numbers in set d will match the last element. In this case, the presence of chaos is asserted. Although in reality it can turn out to be a period of higher order, or the system has not yet moved to stable behavior, and we ourselves have the right to choose what accuracy the behavior of the system is considered with. In a situation where the period was not detected, it is reasonable to record it as zero. The method of determining the period listed above can be called a *simple comparison* method or a *periodicity convergence* method.
- **Step 5.** Next, it is necessary to save the obtained result. Values are stored in 3 precreated arrays according to the following rule: in the first array the value of a, in the second the value of b, and finally, in the third the value of the received period. Of course, serial numbers of the data must match.
- **Step 6.** All the previous points are performed with other a and b values. It is necessary to walk through all possible combinations (a, b) from the interval with a certain step.
- **Step 7.** The last step is displaying the image. Points corresponding to different period values must be displayed using different colors. Validation loops or logical operations can be used for this.

#### Method of minimum value function

However, there is also a slightly different approach to determining the periods that appear in the image. This algorithm repeats the above one except **Step 4.** The fact is that in the new algorithm, a special function that analyzes the array according to its algorithm will be used to determine the periodicity in the array d. Let's call this function  $\textit{Min\_value}$  and see how it works.

- **Step 1.** The function  $Min_value$  accepts an array  $d = (d_1, d_2, ..., d_n)$ . The choice of number n is quite arbitrary, but for working with the function  $Min_value$ , it will be very beneficial to take n = 8, 16 or 32. Taking a greater number does not make sense.
- **Step 2.** Arrays of the following form are constructed from the array d:  $d_1=(d_1,d_1,\ldots,d_1),\ d_2=(d_1,d_2,d_1,d_2,\ldots,d_1,d_2),\ d_3=(d_1,d_2,d_3,\ldots),$  and so on, up to  $d_{n/2}=(d_1,d_2,\ldots,d_{n/2},d_1,d_2,\ldots,d_{n/2},\ldots)$ . That is, arrays consisting of the first

element d, the first two, the first three, and so on are formed. The length of all arrays is equal n.

**Step 3.** Next, an element-by-element difference between d and  $d_i$  is taken. For example, the difference between d and  $d_1$ :  $\Delta d_1 = d - d_1 = (d_1 - d_1, d_2 - d_1, \ldots, d_n - d_1)$ . After that, the standard deviation of the set  $\Delta d_1$  is taken and written as  $\lambda_1$  a number. And this is repeated with all  $\Delta d$ .

**Step 4.** An array is formed from the set  $\lambda_1, \lambda_2, \dots, \lambda_{n/2}$  and is presented as a result of a **Min\_value** function.

The function **Min\_value** outputs an array  $\lambda$ , and the closer  $\lambda_i$  is to zero, the more likely d has period i.

It is clear that the task is to select the smallest element from the set  $\lambda$ . However, it is more suitable to choose the first element i, which satisfies the condition  $\lambda_i < \varepsilon$ , where  $\varepsilon$  is a pre-set small value.

There are several remarks about the algorithms. The fact is that the systems used are non-linear, so sometimes values of points coordinates go beyond some reasonable limits, and the program writes the coordinates as (±inf, ±inf) or (NaN, NaN). However, it is better to exclude both cases from consideration and not to display them on the plane, because when comparing two inf values, the program will show that they are equal, and in our case, it is a period equal to one.

The second remark concerns accuracy. If a sufficient number of iterations is taken, there is no doubt that the system has arrived at its stable behavior mode, be it a periodic mode, a chaotic mode, or a stable point. In this case, it is not necessary to require the last element of the sequence to match with some previous elements exactly. It is enough that their difference is less than some given small  $\epsilon$  value. In this case, it is possible to avoid various difficulties with "long convergent" sequences, which often arise when the period is equal to one.

The construction of dynamic mode maps is a task in itself and requires a fairly large amount of machine time, so when building the program, displaying the image inside the cycle in the period calculation should be avoided. In addition, during the initial debugging of the program, a small step of changing parameter values should not be used - the execution time of the program strongly depends on this [2].

The process of developing software code for calculating the dynamic mode map using the minimum value function is presented in the **Appendix**.

# **RESULTS AND DISCUSSION**

# Dynamic mode maps of incommensurate superstructures described by the Lifshitz invariant and obtained using the function of minimum values

Let's consider the constructed dynamic mode maps for crystals of group  $A_2BX_4$  constructed according to the above methods.

Crystals of  $A_2BX_4$  group, particularly tetramethylammonium tetrachlorometalates, are characterized by a complex sequence of phase transitions, including a transition to an incommensurate phase with nanoperiodicity (with a period ~ 100..160 nm). Such a wealth of commensurate (long-periodic) phases set and incommensurate phases sequence in these objects stimulated the study of dynamic mode maps of these systems.

These objects are characterized by different multiplications of elementary cell n. This parameter also characterizes the symmetry of the thermodynamic potential. That is, depending on the symmetry (multiplication of elementary cell n), one or another sequence of phase transitions will be observed in the crystal. The first representative of this family is the crystal of tetramethylammonium tetrachlorocuprate (TMATCC, chemical formula [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>CuCl<sub>4</sub>), which in the ferroelastic phase is characterized by elementary

multiplication equal to n=3. At the phase transition  $T_i=297 \mathrm{K}$  in a special point of Brillouin zone (m/n, where n=3, m=1) an incommensurate superstructure with a wave vector  $q=(1/3-\delta)/c$  appears. Changes of  $\delta$  value are insignificant ( $\delta\approx0.007..0.0075$ ). At the same time, the modulation wavelength near  $T_i$  is  $L_i\approx1617 \,\mathrm{Å}$ . With a decrease in temperature, down to the transition to a commensurate ferroelastic phase ( $T_c=291 \,\mathrm{K}$ ), the process is accompanied by an increase in anisotropic interaction, which is described by the Dzyaloshynskyi invariant and determined by the parameter K. The value of T parameter describes the long-range interaction process and may decrease as the temperature in the incommensurate phase decreases. Therefore, the T and K parameters describe the dynamics of the disproportionate superstructure.

Fig. 1 and Fig. 2 show dynamic mode maps for the following parameters of the system under study: T = c0 = 0.01..1.0, with a step of 0.01, c2 = 3, T = 200, K = c1 = 0.01..1.0, with a step of 0.01, provided n = 3

- d.append((data2[i-1]+k1)\*\*2+(data3[i-1]+k2)\*\*2) for Fig.1
- d.append((data0[i-1]+k1)\*\*2+(data1[i-1]+k1)\*\*2+(data2[i-1]+k1)\*\*2+(data3[i-1]+k2)\*\*2) for Fig.2

Visualizations made it possible to trace the dependence of existing periodicities on the system parameters values. If c0 = 0.01..1.0, with a step of 0.01, c2 = 3, T = 200, c1 = 0.01..1.0, with a step of 0.01, then the existence of a cascade of periodicities is

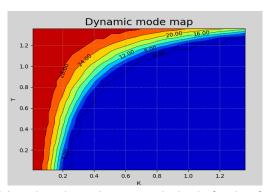


Fig. 1. The two-dimensional dynamic mode map is constructed using the function of minimum values for a system with the existence of a non-commensurate superstructure with n = 3, provided c0 = 0.01..1.4, with a step of 0.01, c2 = 3, c1 = 0.01..1.4, with a step of 0.01.

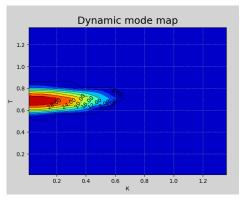


Fig. 2. The four-dimensional dynamic mode map is constructed using the function of minimum values for a system with the existence of a non-commensurate superstructure with n = 3, under the condition c0 = 0.01..1.4, with a step of 0.01, c2 = 3, c1 = 0.01..1.4, with a step of 0.01.

observed. This indicates the presence of stable and unstable system movement trajectories in different areas.

From conducted studies of the influence of system parameters c0, c1 on existing modes, it was established that c0 parameter determines the scale and number of existing periodicities, while c1 is their interval. This allows us to control the surface shape by specifying different combinations of parameters.

According to Fig.1, areas with different values, where red zones indicate high values, which may indicate the existence of periodicities with a longer period, and blue zones - with a smaller value, which indicates more stable areas. This distribution demonstrates the complexity of system dynamics and possible transitions between different behavior modes.

The resulting dynamic mode map of the system under research described by the system of differential equations (1.2, 1.3) does not correspond to the experimentally observed modes obtained in [7] provided n=3. Namely, the existence of two incommensurate structures and corresponding dependence of incommensurate superstructure modes on the amount of anisotropic interaction cannot be traced [8]. Therefore, let's consider the four-dimensional dynamic mode map, which is shown in Fig. 2. In Fig. 2, it is possible to observe a cluster of values in the upper part, closer to the central axis, which indicates an important role in appearance of periodicities in the magnitude of long-range interaction. Analysis of dynamic modes on such maps helps to understand where the system may be unstable and where it becomes stable, which is important for development of effective management and forecasting strategies.

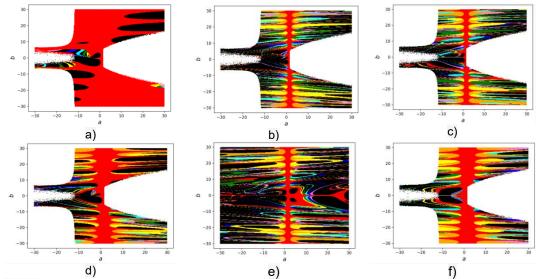
The resulting four-dimensional dynamic mode map also does not fully describe the behavior of Lyapunov coefficients for systems with n=3 [7,8]. Namely, if T=1, then this system is characterized by the existence of two chaotic regimes, which are spatially separated by the magnitude of anisotropic interaction. The dynamic mode map shown in Fig. 2 is characterized by the existence of the cascade of periodicities in the vicinity of T=0.7 and K=0.0.6. An absence of the chaotic regime proves that this method of constructing dynamic mode maps is not perfect. Therefore, let's consider the construction of dynamic mode maps obtained using periodicity convergence method.

# Dynamic mode maps of non-commensurate superstructures described by the Lifshitz invariant obtained using the periodicity convergence method, provided n=3

Fig. 3 shows dynamic mode maps depending on values of parameters a = K and b = T with n = 3 obtained using the periodicity convergence method. Dynamic mode maps are given, where amplitude (R) and phase  $(\varphi)$  functions of the non-interchangeable superstructure, and their changes (R' and  $\varphi'$  respectively) are the arguments of recurrence relations. Thus, Fig. 3 shows dynamic mode maps under the condition of consideration as function arguments: R,  $\varphi$  (Fig.3a); R',  $\varphi'$  (Fig.3b); R,  $\varphi'$  (Fig.3c); R',  $\varphi$  (Fig.3d).

Analyzing the obtained dynamic mode maps, it should be noted that a palette of existing periodicities is more represented if the increment of phase function  $(\varphi')$  acts as the argument of the recurrence relations. The dynamic mode map deserves special attention when increase in both amplitude (R') and phase  $(\varphi')$  functions acts as arguments of recurrence relations (Fig. 3b). This is not surprising, because for this system the Lyapunov coefficients, characterized by the largest changes, are described by spatial changes in the amplitude (R') and phase  $(\varphi')$  of the order parameter [4]. The given dynamic mode map in Fig. 3, b,c,e is characterized by a richer palette of colors corresponding to different periodicities. This is especially evident when the phase and its change act as arguments of recurrence relations (Fig. 3, e).

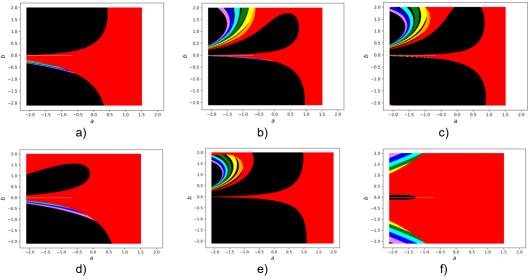
When constructing dynamic mode maps, we chose only the first eight possible periodicities (red - 1, orange - 2, yellow - 3, green - 4, cyan - 5, blue - 6, violet - 7, black - all others). The absence of any periodicities is marked in white. Periodicities with the



**Fig. 3.** Dynamic regime map along axes a and b. Here, a = K represents the value of the anisotropic interaction parameter described by the Dzyaloshinskii invariant, and b = T corresponds to the value of the long-range interaction parameter of the system, under the condition n = 3, with variations of the following pairs of variables: a) R,  $\varphi$ ; b) R',  $\varphi'$ ; c) R,  $\varphi'$ ; d) R',  $\varphi$ ; e)  $\varphi$ ,  $\varphi'$ ; f) R, R'.

smallest period (red - 1; orange - 2; yellow - 3; green - 4) are dominant on the dynamic mode maps.

Based on the dependence of the value of Lyapunov coefficients [4] on anisotropic interaction value (K), if n = 3, and K > 1.0, then a transition to a chaotic state is observed. Therefore, Fig. 4 shows dynamic mode maps when the parameters a = K and b = T are changed in the range from -2 to 2.



**Fig. 4.** Dynamic regime map along axes a and b. Here, a = K denotes the value of the anisotropic interaction parameter described by the Dzyaloshinskii invariant, and b = T represents the value of the long-range interaction parameter of the system, under the condition n = 3,  $\varepsilon = 0.1$ , and variations of the following pairs of variables: a) R,  $\varphi$ ; b) R',  $\varphi'$ ; c) R,  $\varphi'$ ; d) R',  $\varphi$ ; e)  $\varphi$ ,  $\varphi'$ ; f) R, R'.

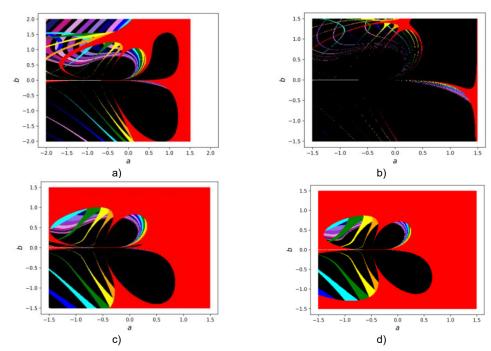
The dynamic mode maps shown in Fig. 4 are similar to those shown in Fig. 3. For these dynamic mode maps, the same regularity is observed. Namely, dynamic mode maps are characterized by a greater number of periodicities, provided that the phase increase value ( $\varphi'$ ) acts as the argument of recurrence relations. When the amplitude value or its increase value acts as an argument of recurrence relations, then the dynamic mode maps show a sharp transition to a state characterized by an increase in the amplitude function value and its change (K > 1.5). It is known [8] that such an increase in the amplitude of spontaneous deformation in TMATCC crystals is associated with a transition to a commensurate ferroelastic phase. At the same time, spatial incommensurate modulation disappears. It should also be noted that the incommensurate phase in the TMATCC crystals is one, but its structure is different ( $I_1$  and  $I_2$ ) in different areas of the phase diagram.

Since on dynamic mode maps black color corresponds to periodicities with a period greater than N=8, then periodicities with periods greater than this value (N>8) may exist in this spatial area. Therefore, this area can be considered as an area of possible coexistence of incommensurate phases with different structures. Exiting the black area and transitioning to the red area indicates the transition to the first periodicity. It can be assumed that this transition is associated with a change in the superstructure mode from sinusoidal to soliton. But, as is known, the soliton mode is characterized by wave harmonics of incommensurate modulation caused by the anharmonicity of oscillations of structural units, as well as the existence of anisotropic interaction. That is, the spectrum of existing oscillations is richer than in the sinusoidal mode. Therefore, the reason for such an obtained result (Fig. 4.) may be in the choice of  $\varepsilon$  value. The value of the  $\varepsilon$  variable indicates the permissible difference between  $d_1$  values and consecutive values  $d_2...d_8$ . When calculating the mapping, only the last 8 values of d are determined, which depend on x, y coordinates:

$$d_i = (x_i + m_1) + (y_i + m_2),$$

where  $m_1$  and  $m_2$  are constants necessary to introduce some asymmetry.

If the difference  $|d_1 - d_2| < \varepsilon$ , then we consider that the cycle is equal to one iteration and the corresponding dot is colored in the first color (red). If the cycle is equal to two iterations, then the color of the dot is orange, etc. For the cycle equal to 7, the dot color is purple. If the cycle is greater than 7, then we consider that the transition between iterations is chaotic, and such a point is colored black. If d goes to infinity, the calculation of the iteration cycle is interrupted, and the dot color is considered white. That is, the  $\varepsilon$  variable essentially determines the existence of periodicities with the value  $\varepsilon$ . So, returning to the appearance of periodicity, which is determined by the red color when K > 1 (Fig. 4, b,c,e), according to the authors, it can be associated with the non-optimized value of the  $\varepsilon$  variable. For this purpose, a study of the effect of  $\varepsilon$  value on the dynamic mode maps character was carried out. Since the studied system, which determines the appearance and dynamics of the incommensurate superstructure, is described by a system of second-order differential equations, let's consider a four-dimensional mapping. The amplitude function (R), its spatial variation (R'), the phase function  $(\varphi)$ , and its spatial variation  $(\varphi')$  are the arguments of the recurrence relations. Fig. 5 shows four-dimensional dynamic mode maps for different  $\varepsilon$ values, provided that only the last 14 values of d are determined (that is, an increase in the number of possible periodicities from 8 to 16). Based on the analysis of obtained dynamic mode maps (Fig. 5), it follows that at  $\varepsilon = 0.01$ , under the condition that (T) parameter describing the long-range interaction is equal to a = T = 1, the consistency between the behavior of Lyapunov parameters is observed under the condition of changing the anisotropic interaction b = K. Namely, the existence of two "black" areas describing the presence of two incommensurate phases, and disappearance of the incommensurate phase at K = 1.5. At other values of  $\varepsilon$  ( $\varepsilon = 1$  Fig. 5d;  $\varepsilon = 0.1$  Fig. 5a;  $\varepsilon = 0.001$  Fig. 5c),

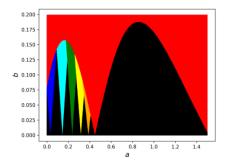


**Fig. 5.** Four-dimensional dynamic regime maps along axes a and b. Here, a = K represents the value of the anisotropic interaction parameter described by the Dzyaloshinskii invariant, and b = T denotes the value of the long-range interaction parameter of the system, under the condition n = 3, with varying values of  $\varepsilon$ :

a)  $\varepsilon = 0.1$ ; b)  $\varepsilon = 0.01$ ; c)  $\varepsilon = 0.001$ ; d)  $\varepsilon = 1.0$ .

dynamic mode maps are characterized by the existence of narrowed spatial areas that describe chaotic states, that is, existing incommensurate phases, and by expanding the spatial areas of periodicities with lower periods. Since the existing periodicities can be associated with localizations of the wave incommensurability vector on commensurate high-order values, then the presence of narrow intervals of their existence (periodicities) on the dynamic mode maps is in favor of the variable  $\varepsilon = 0.01$ .

Fig. 6 shows a map of the existence of possible periodicities from the anisotropic interaction value a = K, under the condition of the maximum long-range interaction value T = 1. According to Fig. 6, an increase in the  $\varepsilon$  variable leads to a decrease in the intervals of existence of periodicities. It should also be noted that two intervals (by K) of the existence of chaotic states (incommensurate phases), which are characterized by different periodicity



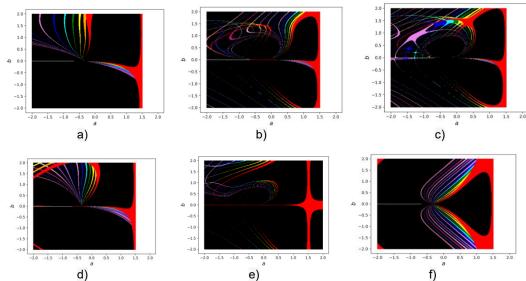
**Fig. 6.** Two-dimensional map of the existence of possible periodicities. Where a = K is the anisotropic interaction parameter value, which is described by the Dzyaloshynsky invariant,  $b = \varepsilon$ , provided that n = 3 and the maximum value of the long-range interaction T = 1.

dynamics, are observed. The first interval (K = 0..0.4) is characterized by the existence of periodicities both with N < 14 and with N > 14, and the other interval (K = 0.4..1.5) is characterized by periodicities with N > 14.

Proceeding from such dynamics of the existing periodicities from the anisotropic interaction parameter, it can be assumed that there is one incommensurate phase in this crystal, and at K=0.4 there is only a change of incommensurate superstructure mode from sinusoidal to soliton. Based on Fourier studies of spectra of amplitude and phase functions of the incommensurate superstructure [7], the soliton mode is described by the existence of several periodicities. Dependence of harmonics of a wave vector (q) of incommensurate modulation on the amount of anisotropic interaction (parameter K), described by the Dzyaloshynskyi invariant, indicates complex transformations that occur during transition from sinusoidal mode to soliton mode at K=0.4. At the same time, both the disappearance of existing periodicities and the appearance of new ones were traced.

To find out processes that occur at K=0.4, let's consider two-dimensional dynamic mode maps provided that  $\varepsilon=0.01$  (Fig. 7). According to Fig. 7, the transition from one chaotic state to another state passes through a cascade of periodicities. These periodicities determine the peculiarity of the first disproportionate area behavior (a chaotic state in the vicinity K=0..0.5).

It is known that as a result of the appearance of the incommensurate superstructure wave oscillations harmonic, it passes from the sinusoidal mode to the soliton mode. If it is assumed that in the sinusoidal mode, harmonics of the incommensurate superstructure, which causes its transition to the soliton mode, arise, then the range of sinusoidal mode and the mode transitional to the soliton mode should be characterized by the existence of periodicities, and in the ideal case, the soliton mode should have at least as many periodicities. The observed "black" area with increasing K value (K = 0.5..1.5), in the absence of any periodicities with N < 14, is possibly related to the formation of a chaotic superstructure. This is particularly indicated by the dependence of Lyapunov coefficients [3] on the K parameter. The appearance of the incommensurate superstructure chaotic



**Fig. 7.** Dynamic regime map along the axes a and b. Here, a = K represents the value of the anisotropic interaction parameter described by the Dzyaloshinskii invariant, and b = T denotes the value of the long-range interaction parameter of the system, under the conditions n = 3,  $\varepsilon = 0.01$ , and variations in the following pairs of variables: a) R,  $\varphi$ ; b) R',  $\varphi'$ ; c) R,  $\varphi'$ ; d) R',  $\varphi$ ; e)  $\varphi$ ,  $\varphi'$ ; f) R, R'.

state on these dependencies begins to manifest itself at  $K \ge 1.0$ . Taking into account the dynamic mode maps in Fig. 7, the transition to a chaotic state is caused by a change in the phase function of the incommensurate superstructure. The amplitude function is responsible for the presence of periodicities in the first chaotic phase.

#### CONCLUSION

Therefore, the considered algorithm for constructing dynamic mode maps is effective for analyzing the incommensurate superstructure dynamics, which is described by a system of differential equations, and the appearance of an incommensurate superstructure is due to Lifshitz invariant. The software for constructing dynamic mode maps using the periodicity convergence method and the function of minimum values was developed. Based on the analysis of dynamic mode maps obtained by these methods under the condition of Lifshitz invariant existence at n=3, it was established that the periodicity convergence method more fully describes the existing incommensurate superstructure dynamics, which is experimentally observed in TMATCC crystals. It was shown that the dynamic mode maps calculated by the periodicity convergence method have a significant number of existing periodicities and most fully describe the dynamics of the incommensurate superstructure. It was confirmed that the incommensurate phase in the TMATCC crystals is single, but its structure is different ( $I_1$  and  $I_2$ ) in various phase diagram areas.

## **COMPLIANCE WITH ETHICAL STANDARDS**

The authors declare that they have no competing interests.

#### **AUTHOR CONTRIBUTIONS**

Conceptualization, [S.S.]; formal analysis, [S.S., I.Ka., Y.S.,].; investigation, [I.Ku.]; resources, [I.Ku.]; writing – original draft preparation, [S.S., I.Ka., I.Ku.]; writing – review and editing, [I.Ka, I.Ku, Y.S.].

All authors have read and agreed to the published version of the manuscript.

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## **APPENDIX**

# Development of a program for calculating the dynamic mode map using the minimum values function.

This source code is intended for modeling dynamic systems and studying the dependence of the order parameter amplitude and phase on the system parameters. It uses numerical methods to solve systems of differential equations and visualize the results. The main parameters analyzed include long-range interaction (parameter  $c_0$ ) and anisotropic interaction (parameter  $c_0$ ). Influence of these parameters is studied through an integration of the system of equations with time. [6]

# 1. Import libraries:

Libraries provide functionality for calculating differential equations, data visualization, and numerical calculations.

```
from jitcdde import y, t
from symengine import sin, cos
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import numpy as np
from scipy.integrate import ode
from scipy.integrate import odeint
import array as arr
```

# 1. Definition of initial parameters:

- $c_0 = 1.0 long$ -range interaction
- c<sub>1</sub> = 0.1 anisotropic interaction
- c<sub>2</sub> = 3 symmetry of thermodynamic potential
- T = 1000, dt = 0.1 Initial values for system parameters.

```
y0 = [0.3, 0.0, 0.0, 0.0]
```

## 2. Definition of differential function:

```
def f(t, y):
   y0, y1, y2, y3 = y
   return [y1, y0**3 - (1 + c0 * y3 - y3**2) * y0 + c1 * (y0**(c2 - 1)) * (1 +
   np.cos(c2 * y2)), y3, -(y1 / y0) * (2 * y3 - c0) - c1 * (y0**(c2 - 2)) *
   np.sin(c2 * y2)]
```

This function defines a system of differential equations which describe the dynamics of the system under study (given by expressions (1.2) and (1.3)). Nonlinear terms, long-range interaction  $c_0$  and anisotropic interaction  $c_1$  are taken into account here.

# 3. Initialization of arrays for saving data:

Arrays are used to store data at various stages of calculations.

```
cz=arr.array('d',[])
y=arr.array('d',[])
```

```
t=arr.array('d',[])
d=arr.array('d',[])
aT=arr.array('d',[])
bK=arr.array('d',[])
H=arr.array('d',[])
```

# 4. Numerical integration of differential equations:

```
params = np.arange(0.01, 1.41, 0.01)
for c0 in np.arange(0.01, 1.01, 0.01):
for c1 in params:
r = ode(f).set_integrator("vode", method="adams", order=10, rtol=0, atol=1e-
8, with_jacobian=False)
y0 = [0.3, 0.0, 0.0, 0.0]
r.set initial value(y0, 0)
T = 200
dt = 0.1
t = []
y = []
while r.successful() and r.t <= T:
r.integrate(r.t + dt)
y.append(r.y)
t.append(r.t)
t = np.array(t)
y = np.array(y)
```

Numerical integration of differential equations is performed using the Adams method.

## 5. Analysis of results:

After integration, the data is analyzed to determine the frequency and amplitude characteristics. The change of phase and amplitude of the order parameter is calculated for each combination of parameters.

```
n=len(t)
y.shape=n,4
data1 = y[ :,1]
data0 = y[ :,0]
data3 = y[ :,3]
data2 = y[ :,2]
nn=len(data0)
x=data0
xx=data1
y=data2
yy=data3
d=[]
```

## 6. Calculation of standard deviation:

```
def Min_value (d):
    n = 32
    g = np.zeros((n, n))
    for i in range(1, int(n / 2)):
    p = d[1:i]
    for k in range(1, int(np.fix(n / i) + 1)):
    try:
    if (i + k * i) <= n:
    g[(k-1)*i+1:k*i, i] = d[k*i+1:i+k*i] = p
    else:
    g[(k-1)*i+1:(k-1)*i+n-k*i, i] = d[k*i+1:n] - p[1:n-k*i]
    except ValueError:
    continue</pre>
```

```
return round(np.std(g), 7)
```

**Min\_value** function calculates the standard deviation for the data used to analyze the stability of the dynamic system.

# 7. Data processing:

```
aT=np.array(aT)
bK=np.array(bK)
H=np.array(H)
eps=0.01
p3=[]
LL=sorted(set(H))
for i in range(len(LL)):
 for j in range(len(H)):
 if H[j]==LL[i]:
 if i<=16:
 H[j]=16-i
 if i>16:
 H[j]=0
p=np.arange(0.01,1.41,0.01)
q=np.arange(0.01,1.01,0.01)
l=len(p)
j=len(q)
x=aT
y=bK
print("j size", j)
print("l size", l)
H.shape=j,1
```

This code snippet converts **aT**, **bK** and **H** arrays to **numpy.array** type for further processing. The **eps** value is set to 0.01. The empty list **p3** is initialized. Then unique values from the **H** array are sorted and result is stored in the **LL** variable. For each value in **LL**, a double iteration on all elements of the **H** array is performed, comparing them with the current value from **LL**. If the values match, they are modified: for the first 16 values of index **i**, the value of **H** is reduced by **16 - i**, for other values, **H** is set to 0.

Arrays of **p** and **q** parameters are created, where **p** contains values from 0.01 to 1.41 with a step of 0.01, and **q** contains values from 0.01 to 1.01 with a step of 0.01. Lengths of these arrays are determined and stored in variables **i** and **j**. Variables **x** and **y** are assigned the values of the arrays **aT** and **bK** respectively. Sizes of **j** and **i** arrays are displayed on the screen for verification. Finally, the **H** array changes its shape according to **j** and **i** values, which is necessary for the correct data displaying in the form of 2D or 3D graphs.

# 8. Visualization of results:

```
fig = plt.figure()
ax = Axes3D(fig)
u = np.array(q)
Y, X = np.meshgrid(p, q)
z0 = H
contour = plt.contour(X, Y, z0)
plt.clabel(contour, colors = 'k', fmt = '%2.1f', fontsize=20)
c = ('#ff0000', '#ffff00', '#0000FF', '0.6', 'c', 'm')
contour_filled = plt.contourf(X, Y, z0, colors=c)
plt.colorbar(contour_filled)
plt.title('Dynamic mode map')
plt.xlabel(u'K')
plt.ylabel(u'T')
plt.savefig('R`,f`_32,eps=0.001,n=4_A.png', dpi=300)
plt.show()
```

Visualization of the results includes construction of contour diagrams and 3D graphs showing the dependence of dynamic modes on K (anisotropic interaction) and T (long-range interaction) parameters. This makes it possible to evaluate the influence of the parameters on system behavior and to determine areas of stability and instability.

In this code, parameters have the following values and interpretations:

- **T = 1000**: Total integration time a time limit up to which the numerical integration of differential equations is performed.
- **dt = 0.1**: Time step for the numerical integration an interval between points where values of the system variables are calculated.
- n = 32: Number of first selected periodicities.

# 1.2. Construction of dynamic mode maps using periodicity convergence method.

Let's look at the code that describes the method of conducting experiments to study the dependence of order parameter phase and amplitude on parameters of long-range interaction (c0) and anisotropic interaction (c1).

# 1. Import libraries:

The libraries provide functionality for working with differential equations, data visualization, and numerical calculations.

```
from jitcdde import y, t
from symengine import sin, cos
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
import numpy as np
from scipy.integrate import ode
from scipy.integrate import odeint
import array as arr
```

# 2. Definition of initial parameters:

- c0 = 1.0 long-range interaction
- c1 = 0.1 anisotropic interaction
- c2 = 3 variable parameter
- T = 1000, dt = 0.1

Initial values for system parameters.

```
y0 = [0.3, 0.0, 0.0, 0.0]
```

## 3. Definition of differential function:

```
def f(t, y):
   y0, y1, y2, y3 = y
   return [y1, y0**3 - (1 + c0 * y3 - y3**2) * y0 + c1 * (y0**(c2 - 1)) * (1 +
   np.cos(c2 * y2)), y3, -(y1 / y0) * (2 * y3 - c0) - c1 * (y0**(c2 - 2)) *
   np.sin(c2 * y2)]
```

The function defines a system of differential equations that describe the system dynamics taking into account nonlinear terms, long-range interaction (c0) and anisotropic interaction (c1).

# 4. Initialization of arrays to save data:

```
from scipy.integrate import ode
data=0.3
y=arr.array('d',[])
x=arr.array('d',[])
amplid=arr.array('d',[])
```

```
omega=arr.array('d',[])
chastota=arr.array('d',[])
chast1=arr.array('d',[])
d=arr.array('d',[])
crok=0.01
e=0.01
px=arr.array('d',[])
py=arr.array('d',[])
```

Arrays are used to store data at various stages of calculations.

# 5. Numerical integration of differential equations:

```
def Dynamic(c0, c1, e):
d = []
r = ode(f).set_integrator("vode", method="adams", order=10, rtol=0, atol=1e-
8, with jacobian=False)
y0 = [0.3, 0.0, 0.0, 0.0]
r.set_initial_value(y0, 10)
T = 100
dt = 0.1
t = []
y = []
while r.successful() and r.t <= T:
r.integrate(r.t + dt)
y.append(r.y)
t.append(r.t)
t = np.array(t)
y = np.array(y)
data0 = y[:, 0]
data1 = y[:, 1]
data2 = y[:, 2]
data3 = y[:, 3]
nn = len(data0)
x = data0
xx = data1
y = data2
yy = data3
for i in range(len(data0)):
d.append((x[i]+1)**2 + (xx[i]+1)**2 + (y[i]+1)**2 + (yy[i]+1)**2)
c = 'black
try:
if abs(d[14] - d[13]) < e: c = 'red'
elif abs(d[14] - d[12]) < e: c = 'orange'
elif abs(d[14] - d[11]) < e: c = 'yellow'
elif abs(d[14] - d[10]) < e: c = 'green'
elif abs(d[14] - d[9]) < e: c = 'cyan'
elif abs(d[14] - d[8]) < e: c = 'blue'
elif abs(d[14] - d[7]) < e: c = 'violet'
elif abs(d[14] - d[6]) < e: c = '#000080'
elif abs(d[14] - d[5]) < e: c = '#9370DB'
elif abs(d[14] - d[4]) < e: c = '#9932CC'
elif abs(d[14] - d[3]) < e: c = '#DDA0DD'
elif abs(d[14] - d[2]) < e: c = '#C71585'
elif abs(d[14] - d[1]) < e: c = '#191970'
elif abs(d[14] - d[0]) < e: c = '#DB7093'
except IndexError:
pass
```

#### return c

Numerical integration of differential equations is performed by the Adams method, using parameters c0 and c1. The Dynamic(c0, c1, e) function analyzes the system behavior and determines colors for visualization based on the calculated data.

# 6. Visualization of results:

```
for e in np.arange(0.0, 1.0, 0.01):
  for c1 in np.arange(-1.0, 1.5, 0.01):
    c = Dynamic(c0, c1, e)
    px.append(e)
    py.append(c1)
    pc.append(c)
plt.scatter(py, px, marker=',', s=0.2, color=pc)
plt.xlabel('$a$', fontsize=14)
plt.ylabel('$b$', fontsize=14)
plt.show()
```

Visualization of the results includes the construction of graphs showing the dependence of order parameter amplitude and phase on the magnitude of long-range interaction (c0) and anisotropic interaction (c1). Color coding is used to display different modes of dynamic behavior of the system.

# Parameters and their interpretations

- **T = 1000**: Total integration time a time limit up to which the numerical integration of differential equations is performed.
- **dt = 0.1**: Time step for the numerical integration an interval between the points where values of the system variables are calculated.

This code allows the analysis of dynamic systems, taking into account long-range and anisotropic interactions. Using numerical integration and visualization, it is possible to construct dynamic mode maps and investigate the influence of parameters on system behavior.

# ПРОГРАМИ РОЗРАХУНКУ КАРТИ ДИНАМІЧНИХ РЕЖИМІВ НА ПРИКЛАДІ СИСТЕМИ, ЩО ВОЛОДІЄ ХАОТИЧНИМИ РЕЖИМАМИ

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Вступ. Карти динамічних режимів — це інструмент візуалізації, який використовується для аналізу та класифікації поведінки складних нелінійних динамічних систем при зміні параметрів. Вони дозволяють нам визначити, як змінюється режим роботи системи (стаціонарний стан, періодичність, хаос тощо) при зміні одного або кількох параметрів.

**Матеріали та методи.** У статті запропоновано алгоритми побудови карт динамічних режимів на основі збіжності періодичностей та функції мінімального значення. Перший базується на виборі останнього елемента множини та порівнянні цього елемента по черзі з усіма попередніми. Якщо останній елемент збігається з попереднім, то стверджується, що результуюча множина має період 1, що означає, що

з цими параметрами система має граничну точку. Другий алгоритм базується на створенні масивів стандартних відхилень. Розроблено програмне забезпечення для побудови карт динамічних режимів з використанням збіжності періодичностей та функції мінімального значення.

**Результати.** На основі аналізу динамічних карт мод, отриманих цими методами за умови існування інваріанта Ліфшиця при n=3, було встановлено, що метод збіжності періодичності повніше описує існуючу динаміку неспівмірної надструктури, яка експериментально простежується в кристалах тетрахлоркупрату тетраметиламонію. Показано, що динамічні карти мод, розраховані методом збіжності періодичності, мають значну кількість існуючих періодичностей та найповніше описують динаміку неспівмірної надструктури. Встановлено, що палітра існуючих періодичностей більш представлена за умови, коли приріст фазової функції виступає аргументами рекурентних співвідношень. На особливу увагу заслуговує карта динамічних мод, коли приріст як амплітудної, так і фазової функцій виступає аргументами рекурентних співвідношень.

**Висновки.** Встановлено, що розглянутий алгоритм побудови карт динамічного режиму є ефективним для аналізу динаміки неспівмірної надструктури, яка описується системою диференціальних рівнянь, а поява неспівмірної надструктури зумовлена існуванням інваріанта Ліфшиця.

**Ключові слова**: карти динамічних режимів, неспівмірна надструктура, режими неспівмірних надструктур, анізотропна взаємодія