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Computer modeling as a new method of research in natural science

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Presently, computer networks are actively used for scientific research. That has significantly increased the capabilities of the researcher who analyzes processes and performs modeling, has brought new research opportunities, and therefore led to qualitative changes in scientific research. Both the speed of research and analysis of its results have sharply increased and, as a result of numerous experiments, it became possible to find new, previously unknown solutions, discover new effects and phenomena. The results of the work conducted by the scientific group of the Department of Artificial Intelligence and Software of V.N. Karazin National University are presented in the article as the example of the new approach to scientific research. It shows that with the help of computer modeling, the physical phenomena previously unknown to researchers can be discovered.

Keywords: Numerical simulation, unstable convective medium, strategies with memory.

Комп'ютерне моделювання - новий метод досліджень у природничих науках

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На даний час комп'ютери, зв'язані мережею, почали активно використовуватись для наукових досліджень. Це суттєво збільшило можливості дослідника, який проводить аналіз процесів та виконує розрахунки. Таке збільшення кількості доступних операцій призвело до якісних змін у наукових дослідженнях: вчені отримали нові можливості для дослідження процесів та пристроїв. Різко збільшилась швидкість проведення досліджень та аналізу їх результатів. Збільшення на порядки темпів всіх дослідницьких процедур, починаючи від постановки проблеми та закінчуючи детальним аналізом отриманого рішення та внесенням змін до структури досліджуваних моделей призвели до того, що в результаті чисельних експериментів стало можливим знаходити нові, раніше невідомі рішення, відкривати нові ефекти та явища. Персональний комп'ютер дозволив на багато порядків посилити індивідуальні можливості людини. Це дало можливість обробляти величезну кількість інформації, забезпечивши доступ через мережу до великої кількості наукових та технічних даних, до різноманітних літературних джерел, а також дозволило досліднику швидко знаходити експертів в різних галузях, незалежно від відстані. З'явились нові методи та технології розрахунків, розширились можливості діагностики отриманих результатів, суттєво зросли темпи аналізу як аналітичних конструкцій так і числових рішень, значно поліпшився доступ до великого масиву наукових даних, різко пришвидшилось усвідомлення дослідниками результатів своїх експериментів. Все це свідчить про новий характер наукових досліджень. Так, з'явились такі дисципліни, як "комп'ютерна хімія", що змогла швидко створювати необхідні речовини із заданими властивостями, "комп'ютерна фізика", що дозволяє отримувати складні рішення, діагностувати їх, вносити зміни та вибирати параметри для моделей. Виникла нова реальність наукових досліджень - «людина-комп'ютер-мережа». В статті на прикладі результатів роботи наукової групи кафедри штучного інтелекту та програмного забезпечення Харківського Національного університету імені В.Н. Каразіна наведено результати нових підходів до наукових досліджень. Показано, як завдяки проведеному комп'ютерному моделюванню колективних процесів взаємодії заряджених частинок з полями та інших процесів було виявлено ряд фізичних явищ, що раніше не були відомі дослідникам.

Ключові слова: *комп'ютерне моделювання, нестійке конвективне середовище, стратегії з пам'яттю.*

Компьютерное моделирование - новый метод исследований в естественных науках

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В настоящее время компьютеры, связанные сетью, начали активно использоваться для научных исследований. Это существенно увеличило возможности исследователя, который проводит анализ процессов и выполняет моделирование и привело к качественным изменениям в научных исследованиях: ученые получили новые возможности для исследования процессов и устройств. Резко увеличилась как скорость проведения исследований, так и скорость анализа их результатов, что привело к тому, что в результате многочисленных экспериментов стало возможным находить новые, ранее неизвестные решения, открывать новые эффекты и явления. Персональный компьютер позволил на много порядков усилить индивидуальные возможности человека. Это дало возможность обрабатывать огромное количество информации, обеспечив доступ через сеть к большому количеству научных и технических данных, к различным литературным источникам, а также позволило исследователю быстро находить экспертов в различных областях. Все это свидетельствует о новом характере научных исследований. В результате упомянутых изменений появились такие дисциплины, как "компьютерная химия", которая смогла быстро создавать необходимые вещества с заданными свойствами, "компьютерная физика", которая позволяет получать сложные решения, диагностировать их, вносить изменения и выбирать параметры моделей. Возникла новая реальность научных исследований - «человек-компьютер-сеть». В статье на примере результатов работы научной группы кафедры искусственного интеллекта и программного обеспечения Харьковского Национального университета имени В.Н. Каразина приведены результаты новых подходов к научным исследованиям. Показано, как благодаря компьютерному моделированию были открыты физические явления, которые ранее не были известны исследователям.

Ключевые слова: компьютерное моделирование, неустойчивая конвективная среда, стратегии памятью.

Introduction

No only new, previously unknown effects and phenomena, but even drastically stronger manifestations of the previously known phenomena in certain conditions are recognized as new scientific achievements. There are a number of examples of the latter such as laser-induced phenomena which are tens of orders of magnitude faster and more intense than spontaneous ones; nuclear chain reactions, which are orders of magnitude more powerful than ordinary spontaneous radioactive decay, as well as, collective processes of particle-field interactions, which promise a revolution in power engineering and already making presence in high-current electronics.

The widespread use of computer networks for scientific research is one of such phenomena. Improved analysis and calculation capabilities, as well as an increase in the number of available operations have led to qualitative changes in scientific research. An unprecedented level of interaction with personal computers has opened completely new and unexpected opportunities for researching process.

The speed of human-computer interaction, diagnostic analysis and visualization have been dramatically increased. Nowadays it has become possible not only to illustrate, refine and revise the results obtained as a result of numerical experiments, but also to find new, previously unknown solutions, and to discover new effects and phenomena. That has been facilitated by greatly increased pace of research; from setting the problem to obtaining a solution, its immediate analysis, updating the structure of models and ascertaining their influence immediately (in real-time), etc.

A personal computer has strengthened a researcher’s individual capabilities by orders of magnitude. It has made it possible to process huge amounts of information, provide network access to a variety of literary sources, and connect a researcher with their associates, regardless of distance. It allows us to use new methods and technologies for calculations and expand our capabilities for diagnostics of the results obtained. The human awareness of the experimental results and analysis of models have increased dramatically.

The new approaches to the research have been appeared using the capabilities of personal computers and their network connection: “computer chemistry”, which is able to search for the substances with given properties quickly, “computer physics”, which allows obtaining complex solutions, diagnosing them, making changes and selecting the parameters of description models, as well as other new scientific directions.

Those changes in scientific research are illustrated below by using the results of the work conducted by the scientific group of the Department of Artificial Intelligence of V.N. Karazin Kharkiv National University. It shows that computer simulation has made it possible to discover a number of physical and other phenomena previously unknown to researchers.

Modeling the Ion heating phenomena with the development of modulation instability of an intensive Langmuir wave in plasma. Diagnostic possibilities.

The main problem in describing the processes of wave propagation in a plasma was the ambiguity of the nature of the absorption of RF energy by particles and the mechanism of their thermalization, that is, the formation of a normal energy distribution of particles, which only allows talking about their temperature. In [1], it is shown that the mechanism of formation of the normal energy distribution of particles is scattering by field inhomogeneities (the Fermi effect), which turned out to be more important than the mechanism of energy exchange between the field and particles traditionally explaining this phenomenon, known as Landau damping. The computerization made it possible to create a diagnostic stand demonstrating the process in real time (Fig. 1).

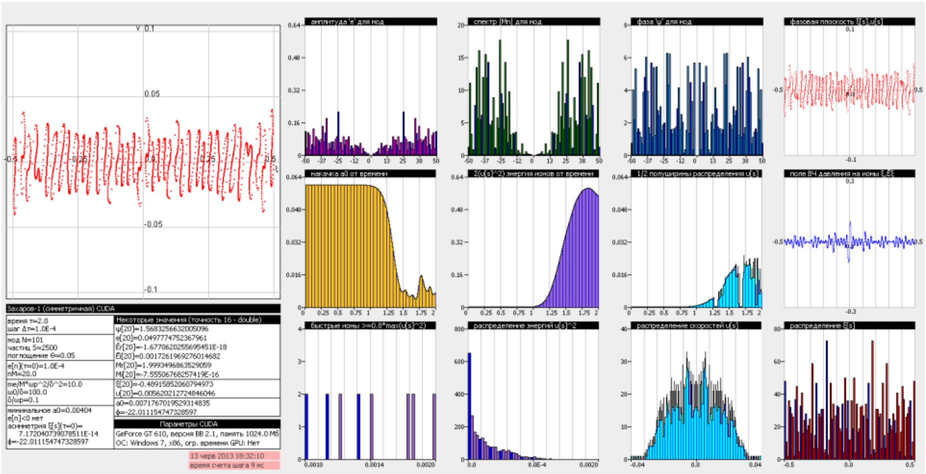


Fig. 1. Diagnostic stand for calculating systems of integro-differential equations on a computer (400 modes, 20,000 particles).

The occurrence of waves with abnormally large amplitude (> 20 meters)

Arising as a result of nonlinear interference of strong sea waves (an average wave amplitude in unrest ocean is 4-6 m., a period is 10-12 sec, phase velocity is more than 20 m/sec, group velocity is half as much, and wave decay lengths are measured in thousands of kilometers) the perturbation of anomalous amplitude is a sequence (group) of usually 3 waves, one of which is the largest, the frequency of occurrence (ensemble statistics and time) of such wave group is one for 10-20 thousand waves. For such long waves (200-250 m), the maximum achievable amplitude before collapse is about 30 m. They are most likely to appear when the modulation instability is starts to develop (in the range of hundreds of kilometers from the boundary of the zone of wind excitation of waves, the development time of the instability is 10 reverse increments i.e., about 2.5-3 hours). It is shown in [2] that the perturbation of the ocean surface arising during the development of modulation instability is similar to the Peregrine breather/soliton. These killer waves can propagate for the hundreds of kilometers [3].

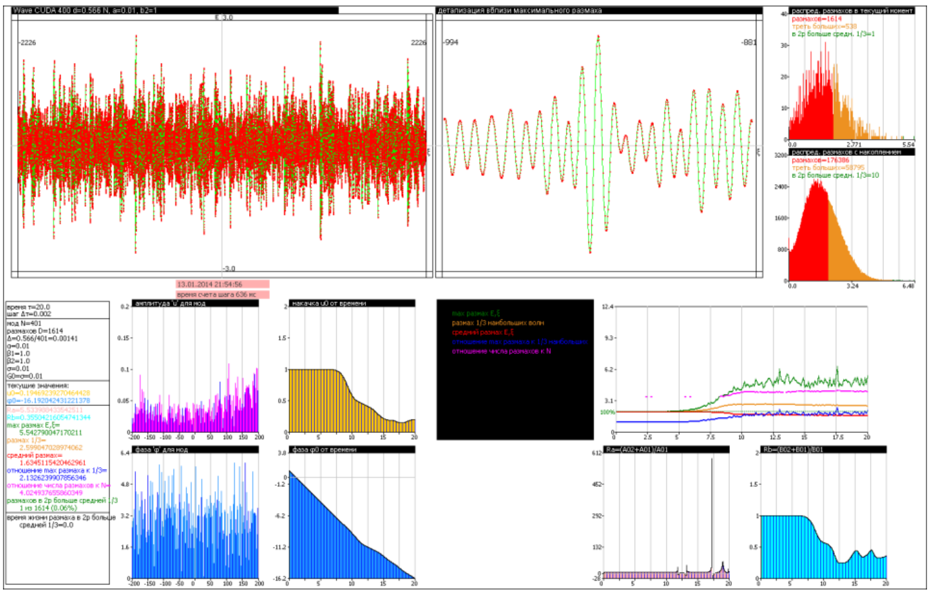


Fig. 2. A diagnostic stand for analyzing the behavior of individual wave packets and statistical processing of the results of modeling the behavior of waves of anomalous amplitude in the ocean.

Process of computer modeling has been carried out by using JCUDA technology which provides Java interoperability with CUDA (Fig. 2). The programs created by JCUDA provide the execution of program code written

in the "C" programming language with addition of the code specific to CUDA technology.

Phase transitions in unstable convective medium

The results of the study [4] on the models of convective instability near the boundary of thin layers of liquid and gas are presented. All spatial perturbations of the same spatial scale, but of different orientations, interact with each other. In the case of a more realistic model of convection described by the Proctor-Sivashinsky equation, it is possible to observe both the first-order phase transition and the second-order phase transition and detect the form of the state function, which is responsible for the topology of the resulting convective structures: metastable rolls and stable square cells (Fig. 3-4). The phase transition times are inversely proportional to the difference in the values of state function $I = \sum_{m=1}^{N} A_m^2$ for two consecutive states.

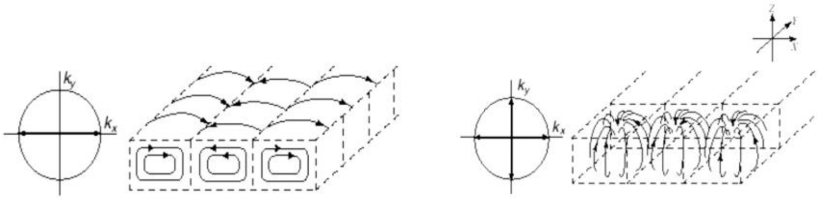
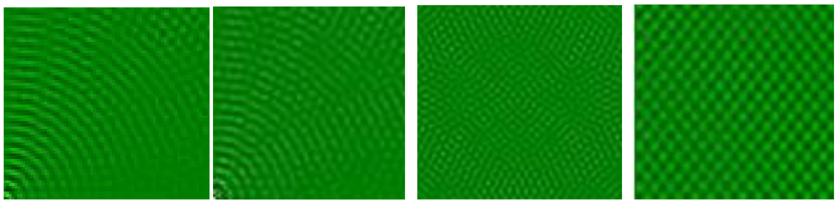


Fig. 3. Convective structures: rolls and square cells



a b c d

Fig. 4. The appearance of fragments of the spatial structure of the temperature field distribution on the surface of layer: a) after the structural phase transition of the first kind with the formation of convective rolls, b) with the transverse modulation of the rolls, c) during the formation of domains – a metastable spatial structure, after the destruction of the roll system, d) with the formation of a stable convective structure – square convective cells

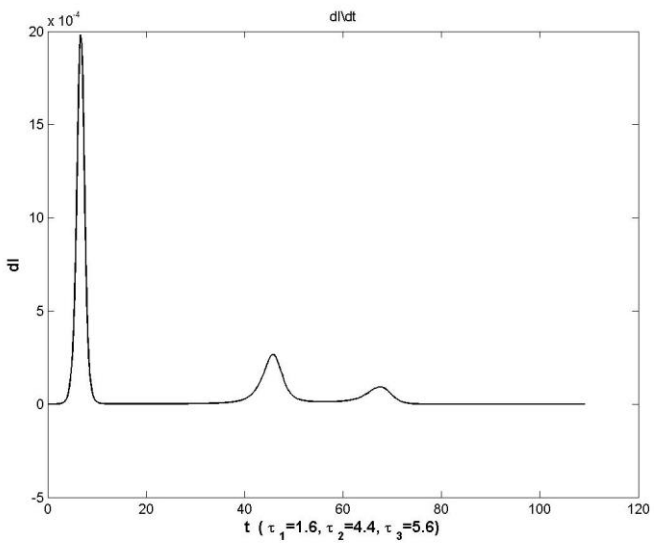


Fig. 5. The behavior of a state function derivative as a function of time. The characteristic times of transient processes $\tau_1 = 1.6$ are the time of occurrence of the "amorphous" state, $\tau_2 = 4.4$ the time of formation of pronounced shaft-like structures $\tau_3 \approx 5.6$, and the time of forming a system of cells for one of the implementations of the process of establishing convective motion.

From the graph (Fig. 5) it is possible to verify that the relative times of formation of states I (spatial structures) are

$$\tau_3 / \tau_2 \approx \Delta I_2 / \Delta I_3$$

inversely proportional to the difference between the values of the state function. A similar description of phase transitions which does not use phenomenological approaches and various speculative considerations, allows for a closer look at the nature of transients [5].

The physical nature of the second order phase transition.

The onset of longitudinal modulation of convective rolls leads to the occurrence of convective motion in a plane parallel to the direction of the rolls, which adds to the strong convection across the rolls. A decrease in the spatial period of the roll modulation leads to an increase in convection as a whole and its equalization in two perpendicular planes, an increase in the temperature on the upper surface of the layer and, accordingly, increase in the energy value, and therefore in the state function value, which indicates a change in the structure and a second-order phase transition.

If we assume that domains with a dominant structure arise and propagate in the convective zone, then we will have to admit that the correlation rate of spatial perturbations in this case is extremely high. This paradox is explained by the fact that the process of a second-order phase transition is described, at least here, by the equations, whose solutions form the set of eigenfunctions with different wave vectors:

$$\Phi = \varepsilon \sum_j A_j \exp(i\vec{k}_j \vec{r}) \cdot$$

The process of phase transformations does not cover individual local regions, but the entire convection zone, where the conditions for the phase transition are satisfied. In this case the formation of local domains with a homogeneous spatial structure in different places of the convective layer is the result of the interference of these eigenfunctions.

Discovery of new phenomena: dynamo effects in hydrodynamic

As a result of the secondary modulation instability of the structure in Fig.4(d), large-scale structures consisting of convective vortices and poloidal vortices [6] are formed (Fig. 6-7) (similar vortices are considered in [7]). The latter which are the effect of a regular hydrodynamic dynamo, predicted by S.S. Moiseev are of the greatest interest.

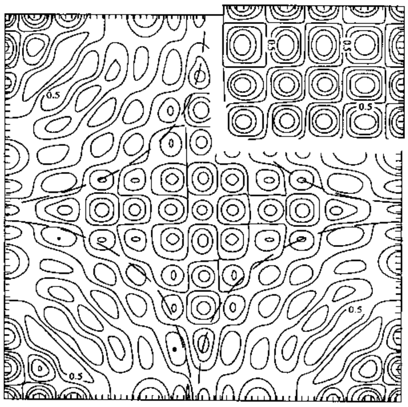


Fig. 6. *It is a regular defect in the convective structure. In the upper corner is a fragment of the primary unperturbed structure. The dashed lines show the characteristic lines of the current of large-scale vortices.*

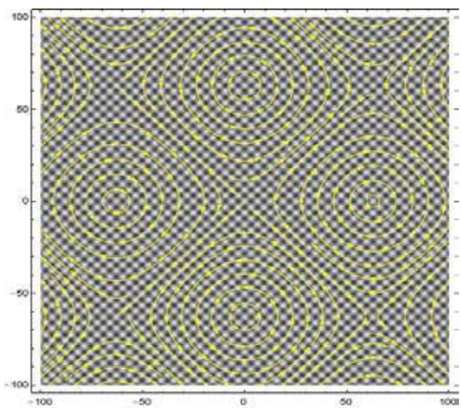


Fig. 7*. In the background of a field of modulated convective cells, is the appearance of large poloidal vortices.*

The detection of the effect of self-profiling of the electron bunch.

The effect of self-profiling (grouping) of a short (less than the wavelength of the wakefield) electron bunch moving in the plasma, which leads to an anomalous value of the field of its wake radiation is considered [8].

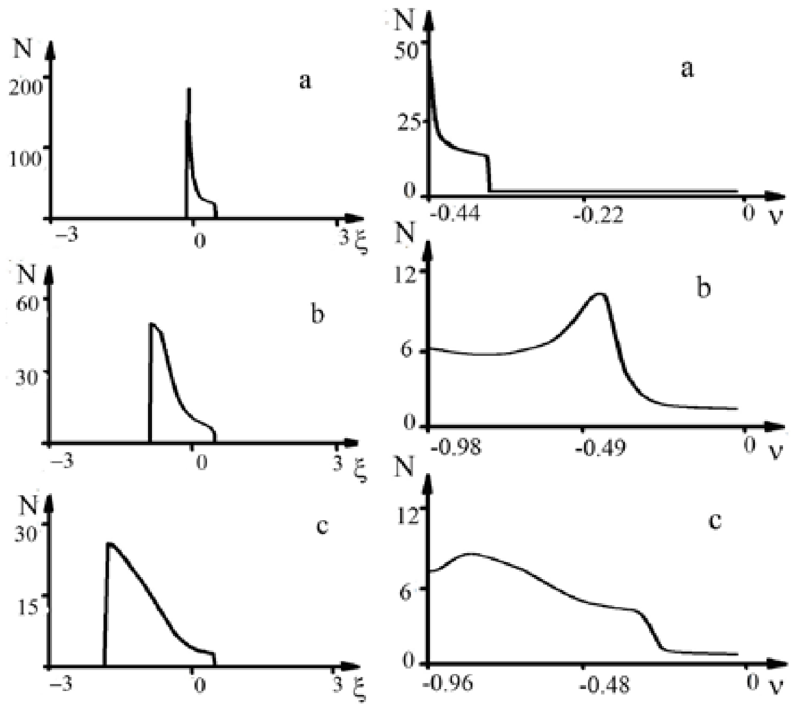


Fig. 8. Change in the distribution of particles in space ξ (left), and in velocities ν (right) at different times

It is shown that the field amplitude in the extended region behind the bunch is the same for the case of the short bunch, and for the case when all particles of the bunch are gathered at one point. Previously, such profiling of density and speed has been done artificially, which is extremely difficult, and requires complex equipment and noticeable efforts. Computer modeling allows us to see the possibility of such self-profiling without any additional devices. This is extremely important for creating an effective acceleration regime in the wakefields of such a bunch.

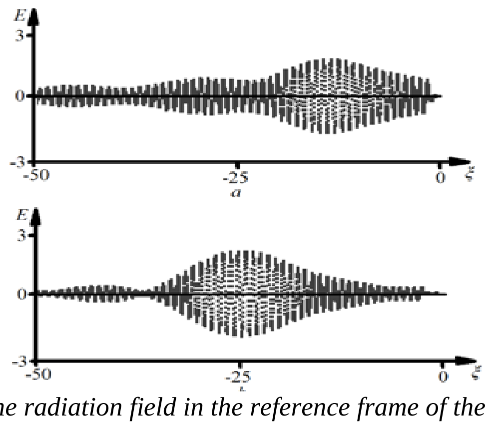


Fig. 9. View of the radiation field in the reference frame of the beam as a whole at different points in time (beam boundary at zero)

Detection of a new induced radiation threshold (due to the competition between spontaneous and induced processes).

Detecting the behavior changes $\ln\{dN_1 / N_1 dT\}$ (N_1 is the number of quanta) by numerical methods has made it possible to clarify the conditions for the appearance of induced radiation of a two-level system [9]. The threshold of occurrence is determined by the condition $N_0 = (n_1 + n_2)/(n_2 - n_1)^2 = 1$, where n_1 and n_2 are the number of states at the lower and upper energy levels, respectively.

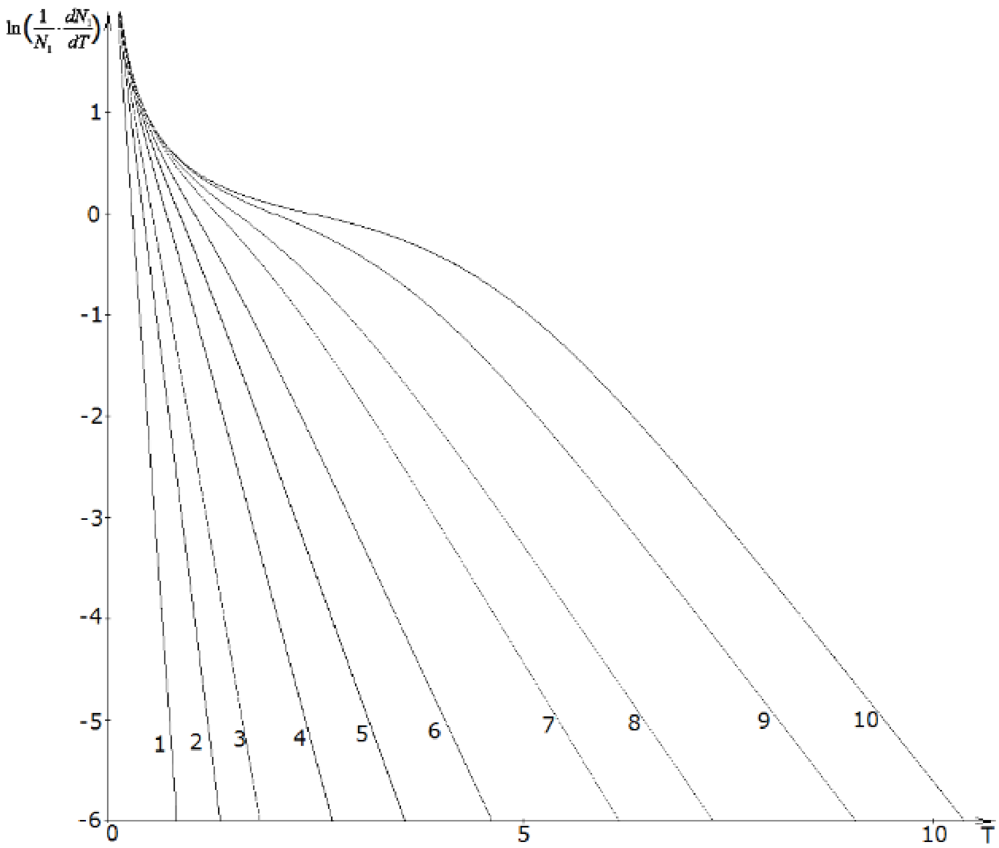


Fig. 10. A change in the nature of the process demonstrates a curve in the graph of the value $\ln\{dN_1 / N_1 dT\}$ *depending on the ratio of the number of states of a two-level system to the square of the population inversion.* *$N_0=(n_1-n_2)/(n_2-n_1)$: 1) $N_0=30$; 2) $N_0=10$; 3) $N_0=5$; 4) $N_0=2$; 5) $N_0=1$; 6) $N_0=0.5$; 7) $N_0=0.2$; 8) $N_0=0.1$; 9) $N_0=0.03$; 10) $N_0=0.01$.*

Periodic changes in the luminosity of quantum sources

In the equilibrium state, heated gas radiation sources are located near the threshold of the induced radiation $n_2 \geq n_1$. In this case the induced radiation can be comparable to spontaneous radiation, but only if there is a source of population inversion, which can be convection from denser heated layers $-v \cdot \partial\mu / \partial x \approx v \cdot \mu / l$ (here, v, l is the average velocity and the characteristic height of the convective layer). The conditions of this generation regime are discussed in [10,11]. A one-parameter system of equations that describes the generation of only induced radiation of a quantum source is reduced to two equations

$$\frac{\partial M}{\partial \tau} = K \cdot M - 2M \cdot N$$

$$\frac{\partial N}{\partial \tau} = M \cdot N - 2N ,$$

where $N = (N_c / \mu_0)(\frac{4\pi\omega\mu_0 \, | d_{ab} |^2}{\gamma_{12}\delta_D \hbar^2})$, $M = (\mu / \mu_0)(\frac{4\pi\omega\mu_0 \, | d_{ab} |^2}{\delta_D \gamma_{12} \hbar^2})$, $\tau = \delta_D t$, $K = (v / \delta_D l)$, where N_c and μ are the density of quanta of induced radiation and the population inversion per unit volume. The population inversion scale $\mu_0^2 \sim (n_1 + n_2)$ is chosen so that $n_2 \geq n_1$, δ_D is the effective decrement of the source, γ_{12} is the line width, d_{ab} is the dipole moment of the active particle. The solution of the system of equations is presented in Fig.11. The phase plane (N, M) is shown in Fig. 12. The bold line on the graph represents a periodic change in the number of quanta, $N_{\max} = 20.188$, $N_{\min} = 4$, $N_{\max} - N_{\min} = 16.188$. It is seen that the constant component of the induced radiation is not zero.

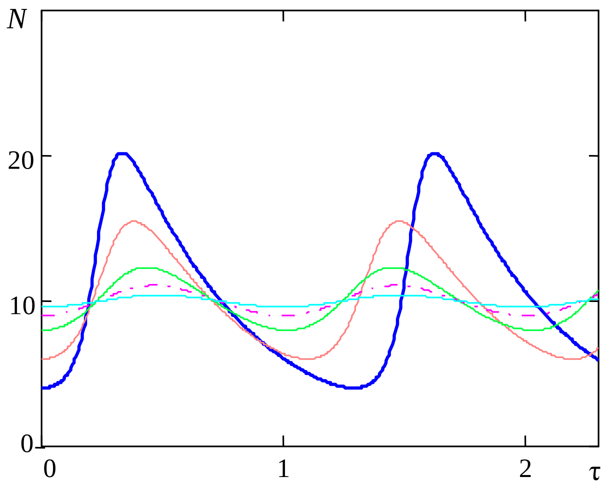


Fig. 11 Behavior of the field intensity N (ordinate axis) with time (abscissa axis).

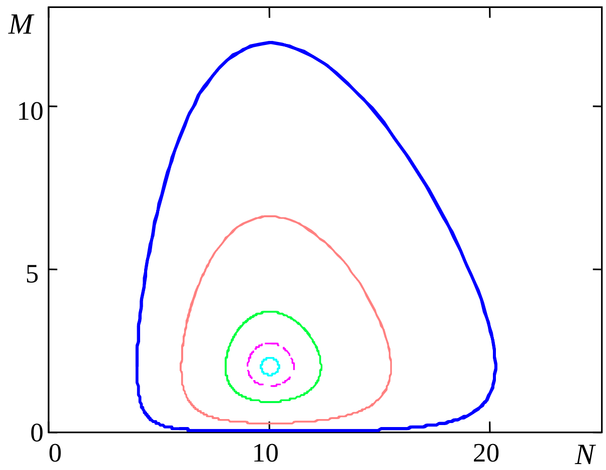


Fig. 12. Phase plane.

The model presented above can be used to describe changes in the luminosity of Cepheid stars. If we assume that the spontaneous emission of the cantilever source and the rest of the heated source is equal to $\mathrm{Nb} = 8.748$, multiplying by $84,507 \cdot L_{\odot}$, where $L_{\odot}$ is the luminosity of the Sun, we get the Delta Cephei, the star which is 272 parsec from us and has a maximum luminosity of 2000 $L_{\odot}$ and using the relations $M = m - 5\lg(d/d_0)$, $m = M + 5\lg(d/d_0)$, $d_0 = 10$, $m_1 - m_2 = -2{,}5\lg(L_1/L_2)$, to change the stellar values, we obtain the following graph (see Fig.13), which coincides with the observational data presented in the literature.

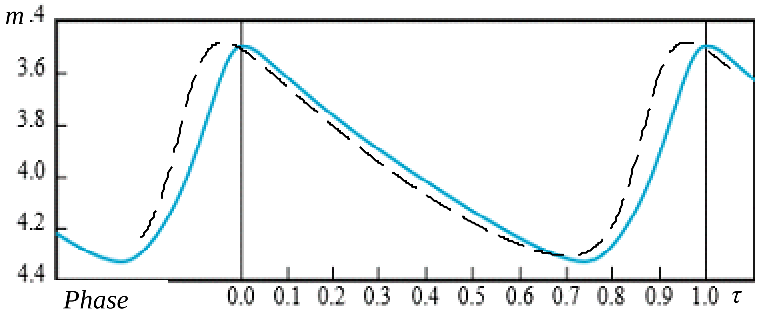


Fig.13. The change in the stellar magnitude of the star of the Delta Cephei with time. (solid curve received in the 1930s by N.F. Florey using a visual photometer) and the solution of equations of system in the same variables (dashed line) [11]

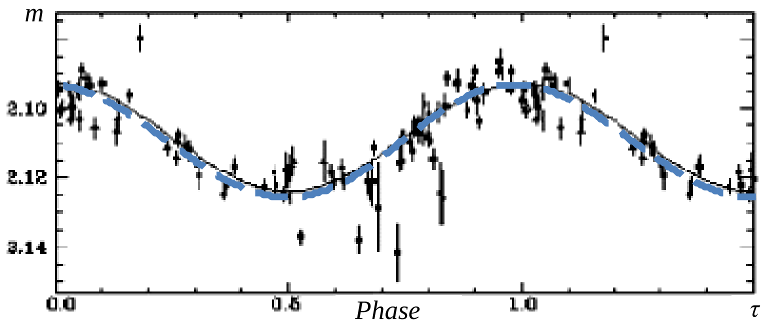


Fig. 14. The change in the magnitude of the North Star with time (solid curve) and the solution of the equations (dashed line) [11]

The attenuation of a wave packet in waveguides filled with an active medium, and plasma

When considering the processes of wave attenuation in a waveguide (resonator) filled with an active medium and in plasma with a finite electron temperature, the reason for the transition of the nature of the change in the field amplitude from oscillatory to monotonic with increasing line width of the wave packet is discussed [12].

The nature of the oscillations in a waveguide (resonator) filled with an active medium is associated with the interference of oscillations of the population inversion in local regions. Inversion changes occur with the Rabi frequency, which depends on the electric field of a standing wave formed as a result of reflections from the ends of the waveguide. In case of strong fields or with a significant population inversion, the line width can be neglected. In this case the field energy density is quite high $|E(t)|^2/4\pi >> \gamma_{12}^2\hbar^2/|d_{ab}|^2$ (a similar relation can be given for population inversion $\mu >> \gamma_{12}^2 \cdot \hbar/(\omega|d_{ab}|^2)$. At low levels of electric field intensity or a small population inversion, the inverse inequalities are satisfied and the line width should be taken into account, which leads to suppression of the interference of individual local inversion regions along the waveguide. The nature of the change in the field amplitude becomes monotonic.

In a similar way, the width of the spectrum of the wave packet affects the character of the Landau damping [6] on plasma electrons. In this case, the role of population inversion is played by the quantity $\mu = n_2 - n_1 = f(v_0 + \hbar k/m) - f(v_0) = (\hbar k/m)\cdot\partial f(v)/\partial v|_{v=v_0}$, where $f(v)$ is the velocity distribution function of the electrons, n_2, n_1 are the numbers of electrons whose velocity is less than and greater than the phase velocity of the wave.

The role of the Rabi frequency here is played by the oscillation frequency of the trapped particles in the potential well of the field $\Omega_{tr} = \sqrt{ekE/m_e}$ (here e, m_e is the charge and mass of the electron, a k is the wave number of oscillations, and $v_{ph} = \omega/k$ is the phase velocity of the wave).

In the case of a small spectral width of the packet $\Delta k \cdot v_{ph} \approx \Delta\omega << \Omega_{tr}$, the process of wave attenuation acquires a characteristic oscillatory form associated with the exchange of energy between the wave and plasma electrons captured by its field. In the case of the reverse inequality, the monotonic character of the field attenuation is observed with the formation of a characteristic "plateau" in the vicinity of the phase velocity of the wave on the electron velocity distribution function corresponding to the state with zero population inversion, which is presented in this case as $\mu = (\hbar k/m)\cdot\partial f(v)/\partial v|_{v=v_0} = 0$.

The superradiance of a bunch of rotating electrons

Equations describing the excitation of a TE wave by a beam of electrons rotating in an external magnetic field in a waveguide in two regimes have been considered. In the first regime the interaction of the oscillators − rotating electrons in the magnetic field − is neglected. It is assumed that the beam electrons interact only with the waveguide modes. In the second case, in the superradiance regime, the beam electrons interact with each other due to their spontaneous radiation. The basic features of the description of the gyrotron gain regime are discussed in the article [13].

The world of strategies with memory [14]

Understanding the nature of the emergence of cooperative behavior in different systems has been of interest to researchers. As part of a generalized "prisoners' dilemma", it is considered that the evolution of a population with a full set of behavioral strategies is limited only by the depth of memory. Each subsequent generation of the population successively loses the most disadvantageous strategies of behavior of the previous generation. It is shown that an increase in population memory is evolutionarily beneficial. The winners of evolutionary selection invariably refer to agents with maximum memory. The concept of strategy complexity is introduced. It is shown that strategies that win in natural selection have maximum or near maximum complexity. Despite the fact that according to the payout matrix the individual gain obtained from refusing to cooperate, exceeds the gain obtained from the cooperation at a separate stage of evolution, the winning strategies always belonged to the so-called respectable strategies that are clearly prone to cooperation. The changes in the average memory and complexity of a population with a fixed depth of strategy memory are insignificant during evolution. Aggression in the process of evolution decreases and tends to a minimum value.

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