

3. Information and scientific laws

Consider how information is connected with scientific laws [7, 8]. Let us set up an experiment measuring two variables x and y . At that the quantity x changes in the range from 0 to a , and the quantity y in the range from 0 to b (Fig. 1). After a series of measurements we found that x and y were always inside the shaded area that characterizes some empirical law (dotted line) and the limits of errors $\beta_2 - \beta_1$. If $n_0 = ab$ is the full area of changes for x and y , n_1 is the square of shaded area, then the quantity of information is

$$I = k \ln \frac{n_0}{n_1}.$$

Here we suppose that all the parts of area are equi-probabilistic.

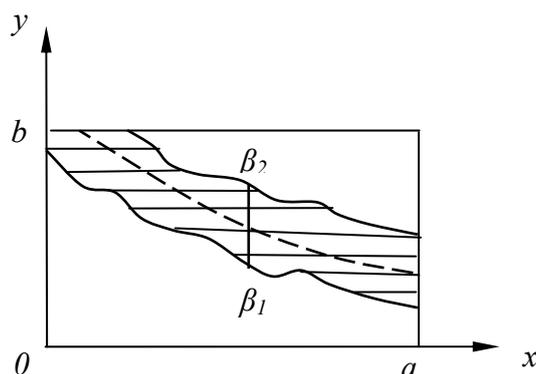


Fig. 1. Empirical law.

Therefore, to count information, we need to know:

- General field of observations,
- Field of random errors.

Consequently,

- Scientific law has always a limited sphere of application.
- Scientific law is correct within the boundaries of possible errors.

Leon Brillouin in his book “Scientific uncertainty and information” emphasized the following. “More than once philosophers paid attention to these two conditions. If the conditions are not concretized, the definition of scientific law has no sense. Many physicists think that one can do an experimental error to be arbitrarily small, and therefore it can be neglected in a theory. Physics is not mathematics. There are many sources of experimental errors for which one is unable to introduce corrections, e.g. Brown motion, principle of uncertainty, principle of isolation (it is impossible to shield from many unknown influences).”

In the general case, according to Brillouin, we can say the following. Let one carries out some experiment and obtains some quantity of information ΔI . According to Carnot’s principle (1824) this leads to the entropy increase $\Delta S \geq \Delta I$ in an experimental set. Let the experimental error approaches to zero. Then the quantity of information, and consequently entropy, tend to infinity. Inasmuch as the entropy characterizes lost energy, it means that in order to get zero error, we need to waist infinite amount of energy that is impossible.

An empirical law can be expressed with the help of figure, table or formula. Suppose we have several empirical laws α , β , and γ , each of them containing some quantity of information I_α , I_β , I_γ . If these laws were discovered independently, the total information equals to

$$I_\Sigma = I_\alpha + I_\beta + I_\gamma.$$

For example, for ideal gas the following laws are valid:

dered the phenomenon as “*insignificant discovery*”, but later it was called ‘*Fermi-Pasta-Ulam problem*’ and gave impetus to numerous studies of nonlinear vibrations done with the purpose to understand the phenomenon. Later it has been established that the phenomenon could be described with the help of solitons [20–22].

One of the authors of this paper was interested to find out that molecular dynamics can give to physics of strength; in particular what processes, being developed at the atomic level, lead to the time dependence of solids strength. For this purpose, tension of anharmonic chains of atoms was studied as well as behavior of chains under constant deformation [14, 19]. In the latter, the initial and boundary conditions were taken in the form

$$x_0 = 0, \quad x_n = na(1 + \varepsilon), \quad x_i(t=0) = ia(1 + \varepsilon), \quad \dot{x}_i(t=0) = A(\varepsilon) \sin \frac{\pi i}{n},$$

where ε is the given deformation of tension. The interaction of atoms was described with the help of Morse potential; in addition to the study of atomic trajectories, spectral density of vibrations was also investigated.

The spectral analysis of atomic vibrations in chains having different length, temperature, and tension revealed resettability of spectrum. The analysis of atomic trajectories, done in parallel, has discovered new quasi-particles. They were named dilatons; the name derives from the fact that the quasi-particles represented anomalously stretched atomic bonds [14, 19, and 23]. Their trajectories have also revealed resettability that correlated with the resettability of spectrum. To exclude the dilatons, Fermi-Pasta-Ulam calculations were repeated for nondeformed anharmonic chains with Morse potential in a significantly wider time interval. In the first cycle of resettability, the picture was the same as discovered by the pioneers, i.e. only some low modes were excited [20–22]. However, during the second cycle there appeared high modes which weakened the low modes, and the resettability has disappeared.

The appearance of high modes is connected with calculation errors that occur by the following reasons [14, 24]. They are: a) change of differential equations by difference ones (truncation error); b) iteration method of calculation (iteration error); c) discontinuity or sharp change of a derivative (discontinuity error); d) finite length of computer registers (round off error). The errors are inevitable; they lead to motion instability and, as a consequence, to irreversibility. The measure of motion stability is Krylov-Kolmogorov entropy or K -entropy [9]. It is defined by the formula

$$K(t) = \frac{1}{t} \ln \frac{D(t)}{D(0)},$$

where t is a time,

$$D(t) = \sqrt{[\mathbf{x}_1(t) - \mathbf{x}_2(t)]^2}$$

is the distance in a phase space between points of two trajectories 1 and 2, and $D(0)$ is the distance at the initial moment. If the motion is stable, $K(t)$ is approximates to zero with time t . It is well to bear in mind the formula to be of theoretical interest because it leaves out account discrete nature of a computer.

The practical way of estimating the motion stability is to check keeping a phase trajectory up. It is as follows [14, 25]. For simplicity, consider one-dimensional case. On integrating the equations of motion at the same initial and boundary conditions but with different time steps Δt_1 and Δt_2 , e.g. $\Delta t_2 = \Delta t_1 / 2$, we will have different noises. Let us calculate the values

$$\frac{x(t, \Delta t_1) - x(t, \Delta t_2)}{x(t, \Delta t_1)} = \frac{\Delta x(t)}{x(t)}, \quad \frac{v(t, \Delta t_1) - v(t, \Delta t_2)}{v(t, \Delta t_1)} = \frac{\Delta v(t)}{v(t)}.$$

Here $\mathbf{x}(t)$, $\mathbf{v}(t)$ is the coordinate and velocity of some atom. The norm of deflection vector

$$\delta u(t) = \sqrt{\left(\frac{\Delta x(t)}{x(t)}\right)^2 + \left(\frac{\Delta v(t)}{v(t)}\right)^2}$$

gives the deflection error of phase trajectory

$$D(t) = \sqrt{[x_1(t) - x_2(t)]^2},$$

i.e. characterizes the accuracy of computational algorithm or, in other words, its calculating entropy.

As in the case of spectral analysis, we have carefully considered methodical questions. The reason is that in the majority of work on molecular dynamics of conservative systems the law of conservation of energy is usually taken as the criterion of calculation accuracy. However the conservation of energy does not mean that the phase trajectories conserve too.

Let us return to Fermi-Pasta-Ulam problem. The problem has again attracted attention to the question how a system of particles comes to equilibrium. In this connection there appeared a lot of new terms and hypotheses. This makes difficulties when reading scientific literature, so briefly review these notions [5, 10, and 19]. The transition of a system in the state of thermal equilibrium is called *thermalization* [from gr. *θερμη* – heat + *λειτουργία* – release, decomposition]. At this, dynamic characteristics of the system are changing with time in a *random way*, and the system acquires *statistical properties*. The word *statist* originates from Greek word *στατος* that signifies standing; supernumeraries in a theatre are usually standing so that the word *statistics* has the meaning of a mass phenomenon. As a result, deterministic mechanics behaves as though it were *statistical* and obeying to random laws. In this connection a transition from determinism to randomness is also spoken of as a transition to *stochasticity* [from gr. *στοχος* – guess, supposition]. Besides, under the influence of Ludwig Boltzmann and Josiah Willard Gibbs, one uses terms *ergodicity* [from gr. *εργον* – work + *οδος* – way, road] and *mixing*.

According to Boltzmann, a system is ergodic if, during transition to an equilibrium state, the phase trajectories begin to cover uniformly all accessible energy surface. Ergodicity in physics is connected with ergodicity hypothesis that consists in the following assumption: time average of a physical value is equal to its statistical average. The hypothesis is the substantiation of statistical physics. In mathematics, one says about ergodic theory. Here classical dynamic systems are considered, the motion of which is described with differential equations, but these systems have strong statistical properties resembling the properties of a random process. In this case, one says that the classical dynamic system is isomorphous to probabilistic one.

According to Gibbs, transition to an equilibrium state is equivalent to integration of several identical systems, initially isolated, into one. At that, the equations of motion produce in the phase space a flow of initial states which mixing leads to uniform distribution of final states on the energy surface. At first, mixing was illustrated with the example given by Gibbs – dilution of ink with water. Now one uses more strong drinks and mixing is illustrated as preparation of cocktail from gin and vermouth.

8. Temperature and variance

Earlier [1] we have considered the evolution of such notions as heat and temperature, but the definition was given only for the temperature of ideal gas. Here, a temperature is a value that is proportional to the variance of distribution function for velocities of ideal gas molecules. In the recent paper [26], the authors criticized the definition given in the Physical Encyclopedic Dictionary: “In equilibrium state temperature is proportional to average kinetic energy of particles of a body”. The authors [26] point out that “this statement is valid for gases, but is rejected vigorously for solids”. Having considered carefully thermal equilibrium in solids, the

authors came to conclusion; “inasmuch as the attempts to come to the simple notion ‘temperature’ on the basis of quantum dynamics in solids have not been successful, we suggest as a temperature of solid to consider a temperature of a gas that is in equilibrium with the solid”. With the criticism of the definition given in the Dictionary, it is hard not to be agree, however what is suggested in fact is the way of measuring but not definition of the notion.

State our point of view. At the beginning of the XX century, solid state physics is characterized by two major achievements: the theory of X-ray scattering and the theory of vibrations of crystal lattice [27]. The latter theory proceeds from the assumption that thermal vibrations of solids represent superposition of elastic vibrations similar to sound waves. In order to describe the decrease of scattering intensity with increasing temperature, one was compelled to combine both theories. As a result, it has been possible to describe the decrease with the help of factor $\exp(-2W)$ depending on a temperature. The factor was developed by Debye and Waller and is referred to by their names [27–29]. The value of W is defined with the formula

$$W = \frac{3}{2} \frac{(h/2\pi)^2 K^2 T^2}{m k \theta^3} \int_0^{\theta/T} \left\{ \frac{1}{\exp x - 1} + \frac{1}{2} \right\} x dx.$$

Here h is Planck constant, K^2 is the vector of reciprocal lattice squared, m is the mass of atom, k is the Boltzmann constant, and θ is the Debye temperature. Recall that Debye temperature is the temperature above which all the normal vibrations are excited and below which some modes begin to freeze out. For us it is important that the value W in the state of thermal equilibrium is proportional to the mean square amplitude of atomic vibrations $\langle u^2 \rangle$ at temperature T [29]

$$2W = \frac{1}{3} K^2 \langle u^2 \rangle.$$

From these formulae it follows that above Debye temperature

$$\langle u^2 \rangle \cong \frac{9(h/2\pi)^2 T}{m k \theta^2}.$$

The mean square displacement of an atom from the equilibrium position – this is just the variance. Consequently, at high temperatures, as in the case of ideal gas, the temperature is proportional to the variance of distribution function; but these distribution functions are different. For ideal gases, it is the distribution function for velocities of ideal gas molecules; for solids it is the distribution function for atomic displacements from the equilibrium position. Below Debye temperature, the temperature is connected with variance by more complex dependence that is given by Debye–Waller factor.

The mean square displacement of atom from the equilibrium position associated with zero vibrations does not depend on a temperature and has the form [30]

$$\langle u_0^2 \rangle \cong \frac{(h/2\pi)^2}{m k \theta}.$$

Here the variance is connected not with a temperature (since there is no temperature) but with the variance of the wave function of oscillator. The wave function has the form of Gaussian distribution

$$A \exp(-\alpha^2 u^2 / 2);$$

its variance is equal to α^{-2} . The square of wave function gives the probability to find the oscillator at the distance u from a center of equilibrium.

In radiation solid state physics, the main subject of investigation are real crystals that contain a lot of various defects created by irradiation [31–34]. The structure of damage zones and behavior of radiation defects are strongly influenced by a temperature; therefore serious ef-

forts were made to develop a corresponding theory. The frontal attack had no success; theoretical results were not in agreement with experiment. The viable alternative consists in the following [14, 35, and 36]. From the two last formulae it follows:

- a) Amplitude of vibration increases with increasing temperature,
- b) Amplitude of vibration increases with decreasing mass of an atom.

Therefore, one and the same effect can be obtained if to increase the temperature at constant mass or at zero temperature to decrease the mass of atom. Consequently we can estimate the influence of temperature substituting a habitual mass for effective one that depends on temperature

$$m(T) = m \frac{\theta}{\theta T}.$$

This simple formula has an even greater impact on radiation solid state physics than one is inclined to think. With its help, temperature was incorporated into equations of mechanics. This allowed calculating the temperature dependence of such values that are crucial for radiation solid state physics; among them are transient energy, i.e. the kinetic energy of a fast particle above which a crystalline target behaves as an amorphous material; effective diameter of collisions, dimensions and form of subcascades, free path of crowdion etc. Apparently, unusual effectiveness of the formula and the expressions obtained on its base lies in the fact that it connects a measure of chaos (temperature) with a measure of inertia (mass).

9. Self-organization of chaos

A drawback of any statistical theory resides in the fact that it gives only general or averaged description, not providing all the necessary information on the behavior of many-body systems. A distinguishing characteristic of such systems is presence of fluctuations [10]. A fluctuation [from lat. *fluctuatio* – oscillation] is a random deviation of a physical value from its mean value. In statistical physics, the fluctuations are supposed to be connected with uncontrolled motion that is named chaotic or thermal [9]. Only Maxwell demon and molecular dynamics know everything about the motion of all particles. With the help of these tools it is possible “to gain a more penetrating insight into heat nature and even to develop some concepts”.

The main assumption of kinetic concept of strength is as follows: fracture is a successive break of interatomic bonds with thermal fluctuations, the process being referred to all solids irrespective of the nature of interatomic forces and peculiarity of material structure [37]. But what is meant by the thermal fluctuation that is able to break an interatomic bond? No response. Only molecular dynamics gave the possibility to gain a more penetrating insight into physical nature of rupture fluctuations [14, 19, and 38]. It turned out that the rupture fluctuation is not merely a thermal fluctuation, but has a very complex structure. It is a phenomenon in which there appear not only fluctuations of kinetic energy but also fluctuations of potential energy. But the most surprising was the fact that during interatomic bond rupture there formed a region of correlated motion. In this region, two groups of atoms surrounding the bond ruptured were moving in an antiphase and played the role of tension grips.

Consider the correlated motion in detail [14, 19, and 39]. To characterize this phenomenon quantitatively, the linear momentum P , averaged through the period of atomic vibrations τ_0 , was calculated

$$\langle P(x, t) \rangle_t = \frac{1}{\tau_0} \int_0^{\tau_0} P(x, t) dt.$$

Here x is the coordinate, t is the time. The linear momentum consists of two constituents

$$P(x, t) = P_0(x, t) + p(x, t).$$

The first constituent corresponds to smooth running and describes a trend; whereas the second one represents fluctuations with the frequency of the order of atomic vibration frequency around the trend. The average value of $p(x, t)$ in the time τ_0 is close to zero; so the function $P_0(x, t)$ changes very little in this time. For this reason, we can take as the order parameter η the dimensionless quantity

$$\eta(x, t) = P_0(x, t) / \frac{1}{L} \int_0^L P(x, t) dx \dots$$

Here L is the length of the region where the correlated motion takes place.

The distribution function for the order parameter that depends on coordinates has the form [40]

$$f(\eta(x)) = N \exp\left(-\frac{F}{kT}\right),$$

where F is Ginzburg–Landau functional which is equal to

$$F = \int \left\{ \frac{\alpha}{2} \eta^2(x) + \frac{\beta}{4} \eta^4(x) + \frac{\gamma}{2} \left[\frac{d\eta(x)}{dx} \right]^2 \right\} dx.$$

Here the coefficient α depends on the temperature T as $\alpha = \alpha_0(T - T_c)$ and changes the sign at some threshold value of parameter T_c , the positive coefficients α_0 , β do not depend on a temperature, and γ is the diffusion coefficient of the order parameter. From the relaxation equation

$$\dot{\eta}(x, t) = -\frac{\delta F}{\delta \eta(x)}$$

we obtain the time –dependent Ginzburg–Landau equation

$$\frac{\partial \eta}{\partial t} = -\alpha \eta - \beta \eta^3 + \gamma \frac{\partial^2 \eta}{\partial x^2}.$$

Molecular dynamics dropped a hint that the solution of this equation should be searched in the form of the running wave

$$\eta(x, t) = \eta(x - Vt).$$

In this case the equation takes the form

$$\gamma \eta'' + V \eta' - \alpha \eta - \beta \eta^3 = 0,$$

where the prime means the differentiation with respect to x . The authors [39] have found the divergent solution of this nonlinear equation in the form of the rupture wave

$$\eta = \eta_0 \operatorname{cth}\left(\frac{x - Vt}{\Delta} \pm 1\right),$$

where η_0 is the amplitude and Δ is the correlation length. The solution was named the soliton of order parameter (Fig. 3).

The example shows that a soliton-like structure can be formed spontaneously in the chaos of thermal motion.

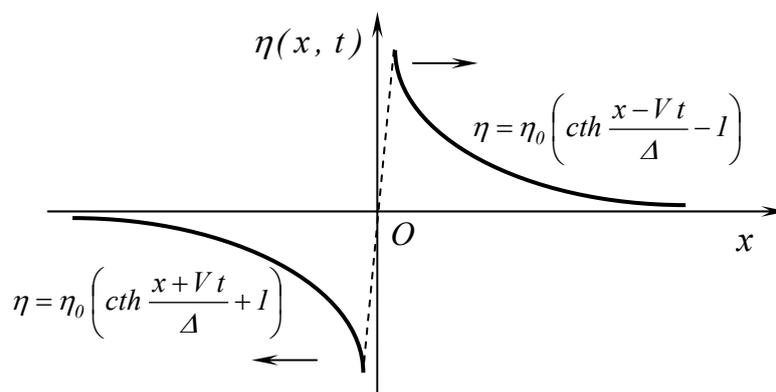


Fig. 3. Solitons of order parameter. Both waves appear simultaneously; two groups of atoms are moving in an antiphase and play the role of tensile grips that stretch an interatomic bond up to rupture.

10. Conclusions

In the previous lecture [1] we have considered how such notions as heat, temperature, and entropy originated beginning with the appearance of heat science and ending with the XIX century when the subject of investigation was at first vapor and then ideal and real gases. In this paper we have considered the evolution of those notions in the XX century when the subject of investigation in physics was mainly solids. Gases and solids are two limiting aggregate state of substance surrounding us. Along with them there are liquids and polymers. Polymers are the substances which molecules consist of a large number of repeating groups (monomers). If the number of atoms in a molecule exceeds 1000, the molecule is named a macromolecule (Hermann Staudinger, 1922). It is thought that the subsequent increasing of monomers does not change properties of a macromolecule significantly. Polymers have the properties that make them similar both to liquids and to solids; therefore they are marked out as a special class – soft condensed matter.

In parallel with physics, informatics was developing practically independently. It made significant contribution to better understanding of the notions, especially of entropy. At the second half of the XX century the informational approach began to penetrate into physics. That was induced by the fact that computers came into wide use in physical investigations. As a result, the new style of investigation was born: numerical experiment and subsequent analysis of results obtained. This style becomes more and more important in a scientific discovery. Ideally, the approach should be finished with a new theory.

The computational experiments done at the second half of the XX century, at first few in numbers, have shown that chaos, even in solids, had a structure. The computer simulations of polymers and biopolymers have revealed that this soft condensed matter was favorably disposed towards self-organization [41–43]. In this connection the new problems raise: what are the mechanisms of self-organization; how, with all this going on, behave themselves temperature and entropy; do they conserve their initial sense or change it. These questions are beyond the scope of this lecture.

Making the summary we can say the following. The evolution of notions is proceeding from particular to general. At the second half of the XX century, the most general definition of heat, temperature, and entropy in physics could be sound thus: *heat is a quantity of chaos, temperature is a variance of chaos, and entropy is a density of chaos*. These conclusions follow from the traditional study of different models of condensed matter. However, the main issue how chaos and heat are connected with the types of motion in a system of particle remains, as in Boltzmann's times, at the level of hypotheses.

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