*METHODOLOGICAL NOTES*

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# Information capacity of condensed systems

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## Contents

**Abstract. The problem of copying a polyatomic system is analyzed from first principles quantum mechanically to show the number of minima of the adiabatic electron term to be the factor determining the storage capacity.**

## 1. Introduction

Informational aspects of physical processes are nowadays becoming a subject of basic research [1 – 4]. Many of these are based on ideal imaginary experiments with a single particle, which may be a particle of an ideal gas, a Brownian particle, etc. Naturally, condensed systems are equally interesting.

The practical side of this problem is associated with the urgent necessity to develop the scientific basis of nanotechnology [5, 6], which would specifically make it possible to obtain functional elements of microelectronics of nanometre scale. In principle, investigation of the informational aspect of the formation mechanism of nonequilibrium structures is a logically unavoidable stage in the further development of condensed matter physics.

The problem of copying acquires a special significance because of the necessity to prepare numerous identical nanostructures. Its essence consists in the development of processes capable of yielding systems that would be exact copies of the initial system [7]. The informational aspect of the copying problem is closely related to the task of determining the maximum large amount of information that could be recorded and preserved over a long time interval $t_{max}$ in a system containing $M$ atoms. One can easily become convinced that the copying is a specific case of information recording.

It may be argued *a priori* that if $M$ is finite the amount of recorded information $I$ is also finite. Furthermore, all other

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conditions being equal, the numerical value of $I$ increases linearly with respect to $M$. The amount of information increases in an analogous manner as the number of printed characters in the text grows [1]. Therefore, the value of $I$ is enclosed in the interval

$$0 \leqslant I \leqslant \frac{M\beta(t_{max}, \mathbf{n})}{\ln 2} ; \tag{1}$$

where $\beta(t_{max}, \mathbf{n})$ is the specific informational capacity; the components of the vector $\mathbf{n}$ are the relative concentrations of atoms of each species which form the system under consideration, $\sum_l n_l = 1$; the amount of information $I$ and $\beta(t_{max}, \mathbf{n})$ are expressed in bytes and nats, respectively [1]; the transition from one type of unit to another is done using the factor $\ln 2$.

The magnitude $I$ is taken to mean the amount of memorized information which is also called *macroinformation*. It is this term that is meant in information science, usually omitting the prefix 'macro'. An alternative is *microinformation*, which is the choice of one of the possible variants which is in principle not memorized by the system. Apparently, an ideal gas does not 'remember' the choice of one of the microstates because of the permanent chaotic motion of its constituent particles.

The numerical values of $I$ from interval (1) may be varied using definite technical means. In contrast, the upper limit of $M\beta(t_{max}, \mathbf{n})/\ln 2$ of this interval is independent of such means since the function $\beta(t_{max}, \mathbf{n})$ is determined by fundamental equations of quantum theory.

But by which equations and how? What is the precise upper limit

$$L^{(I)}(t_{max}) = \sup_{\mathbf{n}} \beta(t_{max}, \mathbf{n}) \tag{2}$$

of values of the function $\beta(t_{max}, \mathbf{n})$ for condensed systems of possible chemical compositions $\mathbf{n}$? By how much will the time $t_{max}$ of information preservation be reduced upon action of the external perturbation $\hat{W}$?

Hereafter, $\hat{W}$ is considered to mean the perturbation operator used in conventional quantum mechanics [8]. It can also be the 'measurement' operator in the generalized Schrödinger equation that considers the informational connection of the system with the outer world [1]. In the general

case, the $\widehat{W}$ operator is random [1], and this should be borne in mind when trying to answer the questions listed above.

The macroinformation $I$ (1) memorized by the system is a macroscopic concept. However, its maximum possible amount proportional to $\beta(t_{max}, \mathbf{n})$ is determined by microscopic parameters. This is not surprising because a sufficiently large number of microscopic states correspond to each macroscopic state. They form a quasiclosed ensemble which is given a mathematical definition in Section 5.

## 2. Exact copy

All elementary particles of the same kind (e.g., all electrons) are indiscernible in view of the principle of identity of microparticles [9]. The same may also be said about isotopes of the same kind. It is not problematic to make protium isotopes form hydrogen molecules which are exact copies of each other [1].

The situation is radically changed as the number $M$ of atoms forming the system increases. As a rule, it is impossible to get an exact copy of a macroscopic ($M \geqslant 10^4$ [10]) system using conventional physical and chemical methods. Glasses of the same chemical composition synthesized in absolutely identical conditions of heating and nonequilibrium cooling of the melt have virtually the same macroscopic properties but they are not exact copies of each other. The point is that it is rather difficult to repeat absolutely exactly the specific mutual disposition of structural fluctuations fixed upon glass transition.

Indeed, as a result of each glass transition, which is a nonequilibrium transition from the liquid to the vitreous state, one of the structural modifications realized in the liquid is frozen (memorized by the system). Let it be the $i$-th modification (Fig. 1). Certainly, next time this will be another, e.g. the $k$-th, modification but again the only one.

Despite the identity of their macroscopic properties (internal energy, refractive index, density, etc.), these modifications are not exact copies of each other since, as seen from Fig. 1, it is impossible to make the coincident superimposition of the disordered $i$-th atomic network on the $k$-th one. If one bears in mind that a virtually infinite number of such modifications exist, then each time the process of glass transition will most probably result in structural modifications different from the preceding ones. Consequently, nonequilibrium cooling of the melt cannot yield even two macrosamples of glass which are exact copies of each other.

Thus, in order to perform copying it is not sufficient to have the required elements of the Mendeleev periodic table. This process also stands in need of the information which was memorized by the initial system and is indispensable for the purpose of copying. Such situations are considered in relation to so-called chemical-informational synthesis [11].

When solving the problem of copying, it is necessary in the first place to reproduce the required structure because the information about individual features of a polyatomic system is eventually stored in the mutual disposition of its atomic
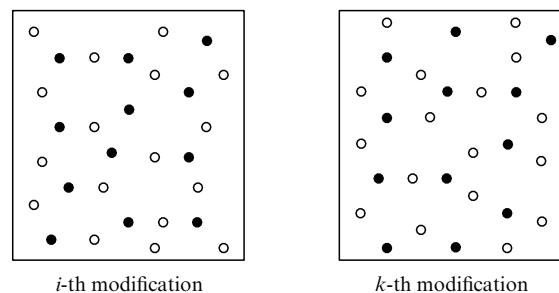
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[1] Evidently, exact copies are systems whose wave functions are identical. However, the identity of wave functions is a very rigorous requirement. Their collapse is induced even by a minor interaction [1]. For this reason, it is advisable to take exact copies to mean systems whose dynamics, including collapses, are described in the framework of the same quasiclosed ensemble. In this case, two hydrogen molecules will be regarded as exact copies even when, for example, their rotatory wave functions [8] are different.



**Figure 1.** Disordered atomic networks (structural modifications $i$ and $k$) which are not exact copies of each other. The sites of localization of atomic nuclei of different species are denoted by ○ and ●, respectively.

nuclei. In the framework of classical physics each structural modification (see Fig. 1) is set by the vector

$$\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_i, \dots, \mathbf{r}_M), \tag{3}$$

where $\mathbf{r}_i$ are the radius vectors of all atomic nuclei of the system. But the atomic nucleus is not a mathematical point whose position is unambiguously determined by the vector $\mathbf{r}_i$. The motion of microparticles is not characterized by the trajectory $\mathbf{r}_i(t)$ [8]. One can speak solely about the sites of their localization. In the case of condensed systems the size of the sites of atomic nucleus localization is much smaller than the interatomic distances and is a tenth-hundredth of an angstrom [12]. Therefore, one of the ways to make a brief [7] quantum-mechanical description of the structure R consists in setting the coordinates $\mathbf{r}_i$ (3) of the centers of these sites.

As a rule, numerous quantum states forming a quasiclosed ensemble correspond to each memorized macrostate (to each structural modification of $\mathbf{R}_k$; see Fig. 1). This raises the question about the number $G$ of different quasiclosed ensembles. It is useful to know $G$ not only in relation to the copying problem. It is the magnitude of $(\ln G)/\ln 2$ that determines the exact upper limit of possible values of the amount of information $I$ (1) since the recording of information consists in its essence in realization of the memorized choice of a single variant of the $G$ possible ones.

In order to find the numerical value of $G$, it is necessary to consider primarily the problem of distribution of quantum states over different quasiclosed ensembles. Some of these are formed by the microstates corresponding to one of the free energy minima. The latter holds only for stable and metastable systems [13]. In the overwhelming majority of cases we are dealing however the with nonequilibrium systems, the thermodynamic potentials of which are far from being extreme.

Thus structural modifications of the vitreous state (see Fig. 1) are not characterized by the Gibbs energy minimum. Each of them is described by its intrinsic quasiclosed ensemble. Their macroscopic properties are invariable because a quite definite structural modification corresponds to each ensemble. It is for this reason that glasses are kinetically frozen nonequilibrium systems, the properties of which virtually do not change over the long time interval $t_{max}$ (1). The same may also be said about the overwhelming majority of noncrystalline substances, many of which are already widely used for recording information [15].

Thus, the class of various quasiclosed ensembles (different macrostates memorized by the system with a fixed chemical

composition) is extraordinarily broad. Their number is substantially larger than the number of Gibbs energy minima.

The magnitude of $G$ cannot be evaluated without application of quantum-mechanical methods. The point is that the components $\mathbf{r}_i$ of the vector $\mathbf{R}$ (3) can vary continuously, i.e. there exists a continuum of various structures (different vectors $\mathbf{R}_k$), which cannot even be numbered with the help of the index $k$, if it has solely integer values. This hampers the determination of the number $G$ of different structural modifications. In a quantum-mechanical description [8] of a structure the superfluous detailing is useless altogether since according to quantum mechanics, a system is usually localized not at one point $\mathbf{R}_k$ but in a certain volume (cell $\Omega_k$). The set of all cells $\Omega_k$ is countable. It is this circumstance that allows one to speak about the number $G$ of different structural modifications of the condensed system with a fixed ($M = \text{const}$, $\mathbf{n} = \text{const}$) chemical composition.

All atomic configurations $\mathbf{R}_k$ (3) of an ideal monatomic gas are equiprobable. Condensed systems are characterized by the totally opposite situation. Therefore, it is not surprising that some of their structural modifications may be frozen (memorized) for a long time interval $t_{max}$ (1). Let us illustrate what has been said above in the framework of the adiabatic approximation.

## 3. Description in the framework of the adiabatic approximation

The adiabatic approximation [16] is based on the considerable differences in the masses of electrons and nuclei, which makes it possible to describe their motions separately well. Being light particles, the electrons 'succeed' in adapting themselves to the instantaneous configuration $\mathbf{R}$ (3) of the atomic nuclei, the latter in turn 'notice' only the averaged disposition of electrons.

In the zero approximation the atomic nuclei are regarded to be at rest [$\mathbf{R} = \text{const}$ (3)]. In this case, the wave function $\Phi_j(\mathbf{R}, \mathbf{X})$ of the $j$-th stationary quantum state of the electron subsystem satisfies the equation [17]

$$\widehat{H}\Phi_j(\mathbf{R}, \mathbf{X}) = U_M^{(j)}(\mathbf{R})\,\Phi_j(\mathbf{R}, \mathbf{X})\,; \qquad (4)$$

where $\widehat{H}$ is the Hamiltonian of electrons at fixed nuclei, which represents the sum of the total Coulomb energy of the interaction of atomic nuclei and electrons, the operator of the spin-orbital interaction of electrons and the operator of the kinetic energy of electrons; $\mathbf{X}$ is the sum of spatial and spin variables of all electrons of the system under consideration; $U_M^{(j)}(\mathbf{R})$ is the adiabatic electron term, which in the case of a polyatomic system ($M \gg 1$) usually has a great number of different physically non-equivalent minima $\mathbf{R}_k$ [7, 18]. The Hamiltonian $\widehat{H}$ does not contain any operator of the kinetic energy of atomic nuclei and, consequently, is the operator of the energy of the system under consideration for the fixed atomic configuration $\mathbf{R}$.

When the motion of atomic nuclei does not induce any transitions between different electronic states, the function $U_M^{(j)}(\mathbf{R})$ (4) may be interpreted as the potential energy of the nuclei corresponding to the $j$-th electronic state. In this case their motion takes place in the potential field of $U_M^{(j)}(\mathbf{R})$. Therefore, the nuclear wave function $\chi_j(\mathbf{R}, E)$ satisfies the Schrödinger equation [17]

$$\left(\widehat{T} + U_M^{(j)}(\mathbf{R})\right)\chi_j(\mathbf{R}, E) = E\chi_j(\mathbf{R}, E)\,, \qquad (5)$$

in which in contrast to (4), there is no variable $\mathbf{X}$ corresponding to the electron subsystem. Here, $\widehat{T}$ is the operator of the kinetic energy of atomic nuclei; $E$ is the energy of the stationary quantum state.

The chemical composition determines unequivocally the explicit form of equations (4) and (5). Their different solutions describe various modifications of a substance with a fixed composition. This can serve as the basis for classification of these solutions. Thus in the case of selenium some solutions may be attributed to the fluid state, others — to definite crystalline modifications, to amorphous modifications, to the vitreous state, to films, etc. However, it is most advisable to base the discussed classification of solutions of equations (4) and (5) on the structure $\mathbf{R}$ (3) because, as noted above, the information about individual peculiarities of a polyatomic system is eventually stored in the mutual disposition of its atomic nuclei. Any structural modification (e.g., the $k$-th modification, see Fig. 1), which is preserved at least over the time interval $t_{max}$ (1) is described by the wave functions $\Phi_j(\mathbf{R}, \mathbf{X})$ (4) and $\chi_j(\mathbf{R}, E)$ localized near the point $\mathbf{R}_k$. The diversity of the latter actually determines all the states belonging to the $k$-th quasi-ensemble.

Usually one or a series of potential $\mathbf{R}_k$ minima correspond to the points $U_M^{(j)}(\mathbf{R})$, near which the motion of one or other structural modification takes place. In order to estimate the number of such points (the number $G$ of different quasiclosed ensembles), it is, as a rule, sufficient to consider only the minima of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ corresponding to the ground ($j = 0$) state of the electron subsystem [2].

The point is that the lifetimes $\tau_e$ of most excited states of the electron subsystem are relatively short ($\tau_e \ll t_{max}$). Therefore, these states alone cannot form a quasiclosed ensemble, in the framework of which the $k$-th structural modification can be described over a long time interval $t_{max}$ (see Fig. 1). Its preservation is favored by the potential barriers surrounding the minimum $\mathbf{R}_k$ of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ (Fig. 2). If they are sufficiently high, then even the low-energy quasi-steady [8] states localized in the potential well $\mathbf{R}_k$ under consideration have larger [compared to $t_{max}$ (1)] lifetimes $\tau_l$ which satisfy the inequalities

$$\tau_r \ll t_{max} \ll \tau_l\,. \qquad (6)$$

where $\tau_r$ is the relaxation time of the phonon subsystem, which is usually appreciably shorter than the time $t_{max}$ required for the preservation of information.

Consequently, quasiclosed ensembles may be formed by the stationary and quasi-steady [8] states with large lifetimes $\tau_l$ (6). Usually these are low-energy states, which describe vibrational motion of atomic nuclei near one of the minima of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ (see Fig. 2). Transitions

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[2] Each minimum of the function $U_M^{(0)}(\mathbf{R})$ sets one of the equilibrium configurations $\mathbf{R}_k$. Crystals correspond to the deepest minima (potential wells). Most minima correspond to different noncrystalline structures. Transition from one potential well to another ($\mathbf{R}_i \to \mathbf{R}_k$) means in the general case the rearrangement of all of the $M$ atomic nuclei of the system since the components of the vector $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_M)$ are radius vectors $\mathbf{r}_j$ of these nuclei (3). Each point in Fig. 2 sets the internal energy $E$ of the system and the coordinates of all its nuclei. In the framework of classical physics the translocation of this point can characterize various processes occurring in the system. The adiabatic electron term $U_M^{(0)}(\mathbf{R})$ does not depend either on temperature or on the thermal prehistory, etc. According to (4), it is unequivocally determined only by the chemical composition. Various scenarios of the system behavior consist in the sequence of passage over potential wells [the minima of the function $U_M^{(0)}(\mathbf{R})$].
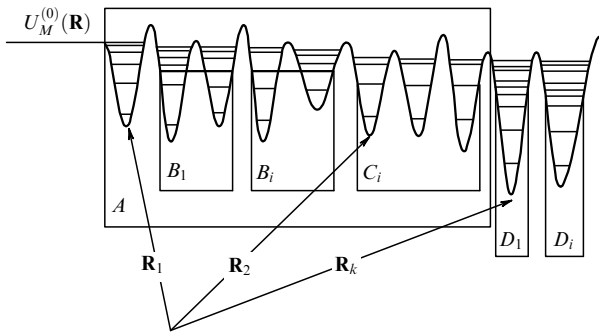
**Figure 2.** Adiabatic electron term $U_M^{(0)}(\mathbf{R})$. The rectangles $A$, $B_i$, $C_i$ and $D_i$ indicate the potential wells corresponding to the $\mathbf{R}_k$ structures (quasiclosed ensembles) of liquid, glass, amorphous substance and crystal. The segments of horizontal straight lines set the values of energies of quantum states. This figure is rather conditional because for polyatomic systems ($M \gg 1$) the function $U_M^{(0)}(\mathbf{R})$ is set, in conformity with (3), in the multidimensional space.

between these states are not accompanied by any substantial changes in the $\mathbf{R}_k$ structure. The $k$-th structural modification is preserved when only such transitions take place (see Fig. 1).

The same may also be said about the macroinformation $I$ (1) which is the choice of a quasiclosed ensemble memorized by the system. This information is preserved as long as all changes occurring spontaneously or owing to the action of the external perturbation $\widehat{W}$ are described in the framework of the same quasiclosed ensemble. This means that with the probability $P(t)$ close to unity

$$P(t) > 1 - \varepsilon \quad \text{at} \quad 0 \leqslant t \leqslant t_{\max} \quad \text{and} \quad 0 < \varepsilon \ll 1, \qquad (7)$$

the system 'stays' in this quasiclosed ensemble during the long time interval $t_{\max}$ and, consequently, the transition from the ensemble under consideration to other ensembles may be disregarded. Relations (7) are in full agreement with the definition of a quasiclosed ensemble given below.

The same ensemble of quantum states may be quasiclosed relative to a single quite definite operator $\widehat{W}$ or a group of operators and, generally speaking, not be quasiclosed relative to other operators. The latter include the recording operator $\widehat{W}^{(m_k)}$ which brings about the transition to the preset $k$-th quasiclosed ensemble. Therefore, the ensembles under consideration are usually 'closed' only during the storage and reading of information. It is this circumstance that determines the choice of the term *quasiclosed*.

Measurement is performed in the course of information reading. It is known [1] that any measurement is an irreversible process fixing one of the possible states. The measurement process proper, which in principle permits an extremely small energy exchange between the system and the measuring instrument, exerts nonetheless a substantial effect on the dynamics of the quantum system. The initial state of the system "is broken, i.e. it is transformed into something that cannot be regarded as a pure state or into another pure state which differs explicitly from the initial one" [1, p. 472]. To preserve the information recorded previously, it is necessary that during the reading this 'something' does not go beyond the frames of the initial quasiclosed ensemble. This condition is met in many cases.

Indeed, let us assume that the nuclear wave function $\chi_0(\mathbf{R}, E_1)$ describes the low-energy vibrational motion of

atomic nuclei in the potential well $\mathbf{R}_k$ (see Fig. 2). Reading (measurement) is done by the collapse $\chi_0(\mathbf{R}, E_1) \rightarrow \chi_0(\mathbf{R}, E_2)$. If the energy variation ($|E_1 - E_2|$) is much smaller than the magnitudes of most potential barriers separating the $\mathbf{R}_k$ minimum from other minima of the potential $U_M^{(0)}(\mathbf{R})$, there is overwhelming probability of localization of the wave $\chi_0(\mathbf{R}, E_2)$ of the final state in the initial potential well $\mathbf{R}_k$. This can be easily seen since in this case, when applying the theory of perturbations [8, 9], it is sufficient to take into consideration only the matrix elements $\langle \chi_0(\mathbf{R}, E_1) | \widehat{W}^{(r)} | \chi_0(\mathbf{R}, E_s) \rangle$ of the reading operator [3] $\widehat{W}^{(r)}$ for the wave functions $\chi_0(\mathbf{R}, E_s)$ localized in the same potential well [4] $\mathbf{R}_k$.

Thus, in order to preserve a polyatomic system, an exact copy and also the recorded information, it is sufficient that all changes occurring in the system do not extend outside the limits of one and the same quasiclosed ensemble. It is this ensemble that characterizes the properties of the system displayed during informational interaction. In fact, the behavior of a quantum system can be interpreted in classical terms with an accuracy up to its belonging to a definite quasiclosed ensemble. It is for this reason that $I$ (1) is regarded as macroinformation.

The amount of information $I^{(s)}$ indicating that the state of the system belongs to a given quasiclosed ensemble is equal to

$$I^{(s)} = \frac{\ln G}{\ln 2} ; \qquad (8)$$

where $G$ is the number of quasiclosed ensembles. Naturally, the magnitude of $G(t_{\max}, \varepsilon, \widehat{W}, \mathbf{n}, M)$ is a function of many arguments. Its explicit form is unknown and this impedes the direct application of equation (8) for calculating the numerical value of $I^{(s)}$.

The magnitude of $G(t_{\max}, \varepsilon, \widehat{W}, \mathbf{n}, M)$ can be estimated proceeding from the number $J(\mathbf{n}, M)$ of different minima of the potential $U_M^{(0)}(\mathbf{R})$. This approach allows a relatively simple derivation of numerical estimates as the function $J(\mathbf{n}, M)$ depends on only two arguments and, in addition, its determination is actually based on equation (4) when $j = 0$. This unambiguous mathematical definition is useful not only for the problem of information copying and recording but also for considering a wide range of other issues [7].

## 4. Estimation of the number of different quasiclosed ensembles

For the number $J(\mathbf{n}, M)$ of different physically non-equivalent local minima of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$, which corresponds to the ground electronic state of the electroneutral system consisting of $M$ atoms, the following asymptotic formula [7] is valid as $M \rightarrow \infty$

$$\frac{1}{M} \ln J(\mathbf{n}, M) \sim \alpha_{\mathbf{n}} ; \qquad (9)$$

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[3] Strictly speaking, the reduction (collapse) is not described by the Schrödinger equation [4]. Nonetheless, approaches are known which allow a highly accurate interpretation of the measurement in terms of quantum-mechanical interaction of the system with an instrument (environment) [19]. This makes it possible to introduce the operator of interaction of the two subsystems $\widehat{W}^{(r)}$ and then to use the Schrödinger equation.

[4] Since the wave functions localized in different potential wells virtually do not overlap, all other matrix elements may be neglected.

where $\alpha_{\mathbf{n}}$ is the positive parameter dependent solely on the chemical composition $\mathbf{n}$ (1). It follows from (9) that

$$J(\mathbf{n}, M) = \exp\left(\alpha_{\mathbf{n}}M + o(M)\right), \qquad (10)$$

the function $o(M)$ satisfying the condition $\lim_{M \to \infty} o(M)/M = 0$. In other words, the number $J(\mathbf{n}, M)$ of different physically nonequivalent minima of the $U_M^{(0)}(\mathbf{R})$ potential exhibits a rapid exponential growth with the increasing number $M$ of atoms forming the system with a fixed ($\mathbf{n} = \text{const}$) chemical composition.

This fact is not surprising because the magnitude $J(\mathbf{n}, M)$ (10) takes into account all potentially possible structural modifications $\mathbf{R}_k$ (3) of a polyatomic system. These are structures of liquid, glass, perfect crystal, crystals with different concentrations of particular defects, polycrystals, amorphous substances, amorphous and vitreous films, glass-ceramics and many others, including the structures of microheterogeneous materials storing the recorded information. The diversity of minima of the function $U_M^{(0)}(\mathbf{R})$ makes it possible to explain the possibility to vary properties of a material of the same chemical composition through preparation of its various modifications described by different quasiclosed ensembles. Thus glass fits not one but many physically nonequivalent quasiclosed ensembles $B_1, B_2, \ldots, B_i, \ldots$ (see Fig. 2). Therefore, the properties of glasses vary depending on the cooling rate of the glass-forming melt [7].

In practice, technical limitations allow, as a rule, the use of only some quasiclosed ensembles. For this reason, the amount of recorded information $I$ (1) is usually smaller than the maximum possible $I^{(s)}$ value (8):

$$I \leqslant \frac{\ln G(t_{\max}, \varepsilon, \widehat{W}, \mathbf{n}, M)}{\ln 2}. \qquad (11)$$

The right side of inequality (11) is simple to estimate, if one takes into account only the quasiclosed ensembles which fit the ground state of the electron subsystem. Indeed, when there are $G^{(0)}$ of them the following relations are satisfied:

$$\ln G^{(0)}(t_{\max}, \varepsilon, \widehat{W}, \mathbf{n}, M) \leqslant \ln J(\mathbf{n}, M)$$
$$= \left(\alpha_{\mathbf{n}}M + o(M)\right) \leqslant \left(BM + o(M)\right), \qquad (12)$$

where constant $B$ is determined by the identity

$$B \equiv \sup_{\mathbf{n}} \alpha_{\mathbf{n}}. \qquad (13)$$

Let us demonstrate the validity of transformations (12). At low temperatures the motion of atomic nuclei takes place in the proximity of one or a series of minima (potential wells) of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ (see Fig. 2). If all low-energy states $\Phi_0(\mathbf{R}, \mathbf{X})\chi_0(\mathbf{R}, E_s)$ localized in each potential well are stationary or quasi-steady and have long lifetimes $\tau_l$ satisfying inequality (6), then such states seem to form one of the quasiclosed ensembles. In this case, their number is equal to the number $J(\mathbf{n}, M)$ (10) of potential wells. In all other cases when a part of the quasiclosed ensembles describe the motion of atomic nuclei near a series of potential $U_M^{(0)}(\mathbf{R})$ minima, the strict inequality $G^{(0)} < J(\mathbf{n}, M)$ is satisfied. We have thereby demonstrated the validity of the inequality $G^{(0)} \leqslant J(\mathbf{n}, M)$ which in combination with (10) and (13) directly yields relations

(12) which allow the estimation of $G^{(0)}$ from above, if one proceeds from the numerical values of $\alpha_{\mathbf{n}}$ or $B$.

It would not be particularly difficult to find the exact value of constant $B$ (13) if the solutions of equation (4) at $j = 0$ were known for the systems of various chemical compositions. Since this is not the case, one has to use model approaches [7]. In their frameworks it is possible to calculate numerical values of the parameter $\alpha_{\mathbf{n}}$ (9), (13) for specific systems. The results of such computations [7, 18] support the following estimate:

$$B \approx 3. \qquad (14)$$

The constant $B$ is also useful for the estimation of the upper limit of the specific information capacity $\beta(t_{\max}, \mathbf{n})$ (1), (2):

$$0 \leqslant \beta(t_{\max}, \mathbf{n}) \leqslant \sup_{\tau_r \ll t_{\max}} L^{(I)}(t_{\max}) \equiv B^{(I)} \approx B. \qquad (15)$$

Indeed, in contrast to $B$ (13), the calculation of $B^{(I)}$ (15) requires consideration not only of the minima of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ corresponding to the ground state of the electron subsystem but also, generally speaking, of the minima of all other potentials $U_M^{(j)}(\mathbf{R})$ (4). However, as noted above, the lifetimes $\tau_e$ of most excited states of the electron subsystem are relatively short ($\tau_e \ll t_{\max}$). States of this kind are unsuitable for information storage. The potentials corresponding to them may be neglected. Then the estimate (15) is derived directly from (10) – (13).

Until now no strict definition of the notion 'quasiclosed ensemble' has been given. It was believed that each structural modification (see Fig. 1) of the system with a fixed chemical composition has an intrinsic set of microscopic states, which form one of the quasiclosed ensembles. This is an illustrative, though somewhat simplified interpretation. It is possible to carry out a more strict consideration based on the definition of a quasiclosed ensemble outside the framework of the adiabatic approximation. This approach requires consideration of many important nuances which were not discussed here. For this reason, it appears advisable to give a definition of a quasiclosed ensemble.

## 5. Definition of a quasiclosed ensemble

Any state of a system is described by the corresponding statistical operator (density matrix [8]) $\hat{\rho}(t)$ in the Hilbert space $\mathbb{I}$. A *quasiclosed ensemble* is perceived as a non-empty set of system states meeting the two following conditions.

1. It is possible to establish a one-to-one correspondence between the elements of this set and various statistical operators $\hat{\rho}^{(\mathbb{N})}$ for a certain subspace $\mathbb{N}$ of the Hilbert space $\mathbb{I}$. Each state of the quasiclosed ensemble is set by a single operator $\hat{\rho}^{(\mathbb{N})}$ and, conversely, each operator $\hat{\rho}^{(\mathbb{N})}$ of the subspace $\mathbb{N}$ sets a single state from this ensemble.

2. Any state of $\hat{\rho}(t)$ of the system, which belongs initially ($t = 0$) to the quasiclosed ensemble [$\hat{\rho}(0) = \hat{\rho}^{(\mathbb{N})}$], is described in the $\varepsilon$-approximation in the subspace $\mathbb{N}$ even in the presence of the external perturbation $\widehat{W}$. This means that the inequalities $0 \leqslant t \leqslant t_{\max}$ are satisfied

$$\left| \text{Sp}\left(\hat{\rho}(t)\hat{f}_l\right) - \text{Sp}_{(\mathbb{N})}\left(\hat{\rho}(t)\hat{f}_l\right) \right| < C_l \varepsilon, \quad l = 1, 2, \ldots \qquad (16)$$

where $\hat{f}_l$ are the operators of physical quantities; $\text{Sp}_{(\mathbb{N})}\left(\hat{\rho}(t)\hat{f}_l\right)$ is the sum of the diagonal matrix elements of the operator $\hat{\rho}(t)\hat{f}_l$ in an arbitrary orthonormal basis of the subspace $\mathbb{N}$;

$\mathrm{Sp}\left(\hat{\rho}(t)\hat{f}_l\right)$ is an analogous sum for the Hilbert space $\mathbb{F}$; $C_l$ are constants. In addition, it is assumed that at $t > t_{\max}$ at least one of the inequalities (16) is not respected.

It is known that these definitions are not proven. Let us give a number of arguments in favor of the quasiclosed ensemble definition formulated above. The advisability of setting a given ensemble in the corresponding subspace $\mathbb{N}$ of the Hilbert space $\mathbb{F}$ follows from the superposition principle [8]. In full agreement with this principle, all the solutions of the Schrödinger equation form a linear manifold with time [8]. If we are interested in only some of these solutions, then again bearing in mind the superimposition principle, it is convenient that these represent a closed linear manifold. The latter is called a subspace [20].

The satisfaction of inequalities (16) means that in order to calculate (with the arbitrarily small error $C_l\,\varepsilon$) the mean values

$$\bar{f}_l(t) = \mathrm{Sp}\left(\hat{\rho}(t)\hat{f}_l\right), \quad l = 1, 2, \ldots, \tag{17}$$

of physical quantities $\hat{f}_l$ that are of interest to us, it is sufficient to know the corresponding matrix elements only for the subspace $\mathbb{N}$. This is not surprising because the probability $P(t)$ of the system staying in any state of the quasiclosed ensemble is close to unity, or more precisely

$$P(t) > 1 - \varepsilon \quad \text{at} \quad 0 \leqslant t \leqslant t_{\max}\,. \tag{18}$$

Inequality (18) follows directly from relations (16) and (17), if we assume in the latter that $\hat{f}_1 = C_1 = 1$ and take also into account that $P(t) = \mathrm{Sp}_{(\mathbb{N})}\left(\hat{\rho}(t)\right)$. Relations (18) virtually coincide with inequalities (7), which were used for substantiating the advisability of introducing the concept of a 'quasiclosed ensemble'.

## 6. Conclusion

Of course, the investigation of the informational aspect of the behavior of condensed systems is still in its infancy. The development of the macroscopic theory of information copying and recording is restricted by many factors. These are primarily a number of unsolved problems in natural sciences. Let us list some of them. Until now "the problem of the relationship between the quantum and classical descriptions of physical processes" remains open to debate [19, p. 1018]. There is no consensus regarding fundamental concepts, such as the wave function, reduction (collapse), etc. [21]. Finally, the subject of discussions continues to be "the question about irreversibility at the boundary between classical and quantum systems, in particular when measuring quantum systems" [2, p. 973]. The latter circumstance is of prime importance for dissipative and temporally irreversible processes, such as information recording and reading.

If the above-listed problems remain unsolved, it would hardly be possible to answer exhaustively all of the questions formulated in this work. It centered attention on the estimation of the number of different quasiclosed ensembles [various structural modifications (see Fig. 1) preserved over the long time interval $t_{\max}$ (1)]. As long as their dynamics, including collapses, is described by different quasiclosed ensembles, these modifications do not pass one into another even under the action of the unfavorable external perturbation $\hat{W}$. Therefore, there is the potential to use them for the recording and storage of information.

Indeed, there are no basic restrictions as to the practical realization of any state described by fundamental equations

of quantum mechanics [5]. The same may be argued in respect of various structural modifications (see Fig. 1) of the system with a fixed chemical composition [6]. They can be distinguished using a macroscopic instrument [7]. Naturally, in the course of information measuring (reading) the initial state of the system is obligatorily changed, whereas the structural modification (a quasiclosed ensemble) remains, generally speaking, invariable. The latter circumstance is important for the preservation of the information recorded earlier during its reading because it represents the choice of one of the possible quasi-ensembles memorized by the system.

The development of a microscopic theory of information copying and recording stands in need of various model systems. To this end, an ideal glass may prove to be useful [7]. It has already been used as a model in the analysis of peculiarities of the operation of neuronal networks [23] and in the description of cosmic objects known as black holes [24].

Naturally, an ideal glass is not yet used in theoretical studies as widely as the concept of an ideal gas. The main reason consists in that the development of theory of disordered systems, to which glasses are referred, is still far from completion [14]. Further progress in this field appears to be impossible without radically new approaches, in particular without using the methods of information theory [1–4, 25].

Indeed, the glass transition involves the internal measurement (self-measurement) and realization of one structural modification memorized by the system (see Fig. 1) of the $G$ possible modifications. As noted above, it is this that is meant when the macroinformation $I$ is discussed (1). It is essential that the memorized choice cannot be realized using an ideal gas or liquid because of their lability. Furthermore, a glass transition is a nonequilibrium process, while information "plays an important role in physical nonequilibrium processes" [1, p. 451].

It appears that the ideology of the vitreous state will henceforward serve as the base for constructing various models for the investigation of the informational aspect of the behavior of polyatomic systems. Liquid is "a stochastised system with zero information and maximum entropy, i.e. the system of the $C$ type" [1, p. 474]. Glass is precisely its antipode. Each glass macrosample memorizes the information indispensable for copying, it whereas the entropy of glass is substantially smaller than that of liquid [26, 27]. Liquids are not used for recording information. On the contrary, glasses, incidentally like many other disordered systems, are well-suited for this purpose [15].

The microscopic mechanism of information copying and recording is determined by elementary processes occurring in small-size fragments. These may be elementary structural transformations, elementary chemical transformations, etc. In their description, it is necessary to take into consideration primarily the potential barriers surrounding each minimum

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[5] Quantum mechanics [8] admits even the possibility of realization of a coherent superposition of any two states. Naturally, this is also valid for any two structural modifications (Fig. 1). However, due to the ever-occurring weak interaction with the environment their superimposition is rapidly transformed into one of the stable structural modifications. States of this kind are called *incoherent* [19].

[6] In its practical aspect, the task of obtaining a preset structural modification is considered in the framework of so-called chemical-information synthesis [11].

[7] This is also evidenced by the impressive progress, e.g., in the development of diffraction methods for studying disordered structures, made over the last 70 years [22].

of the adiabatic electron term $U_M^{(0)}(\mathbf{R})$ (see Fig. 2), or more precisely, the coefficients of passage through these barriers [28].

Most elementary processes occur in the nanometre-range fragments containing tens to hundreds of atoms [29]. Therefore, these processes are in particular responsible for the formation of condensed media-based nanostructures, the diversity of which virtually determines the level of specific information capacity $\beta(t_{max}, \mathbf{n})$ (1), (15).

The task of the targeted synthesis of individual nanostructures [1] dictates the need for developing the microscopic theory of information copying and recording. The solution of this particular problem is impossible without such a fundamental characteristic of any material object as information, without which it is in turn impossible to get an exact copy. In this field, studies of an applied character are moving ahead of basic research and stimulating its progress. We witnessed something similar in the middle of this century when information theory was taking shape [30].

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