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Abstract

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PHYSICS

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THE PROBLEM OF JUSTIFYING STATISTICAL PHYSICS AND THE QUANTUM THEORY OF DECAY*

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1. In this work, by means of the quantum theory of decay ([1,2]), the problem of the justification of statistical physics is investigated ([3,5]) contains a detailed bibliography)—whether or not a description according to the axioms of statistical physics can be embedded in a dynamical theory (in particular, in quantum theory). Here we shall be mainly interested in whether the asymptotic (in time $t \to \infty$) predictions of statistical physics and of dynamical theory coincide.

2. As the profound analysis of the problem by N. S. Krylov ([3]) showed, an attempt at a complete justification of statistical physics in classical physics (mechanics) is logically contradictory. It is natural, therefore, to proceed from quantum theory as a dynamical theory, especially since, owing to the specifics of the limiting transition ($t \to \infty,\ \hbar \to 0$), the asymptotic predictions (as $t \to \infty$) of quantum and classical theory do not coincide.

3. In the fundamental works of L. Van Hove ([7]), under certain minimal assumptions concerning the operators of physical quantities (whose eigenfunctions determine the states of the physical system, numbered by the index k) and the vectors of initial states, there were obtained, in the limit $\lambda \to 0,\ t \to \infty,\ \lambda^2 t = \text{const}$, where λ is the interaction constant responsible for nonequilibrium, the governing equations

$$\frac{dP_k(t)}{dt} = \sum_m [P_m(t)W_{mk} - P_k(t)W_{km}], \tag{1}$$

where $P_k(t)$ are the probabilities of finding the system at time t in the k-th state, and $W_{km} = W_{mk}$ are the symmetric (as follows from the reversibility in time of the original Schrödinger equation) transition probabilities per unit time from state k to state m and conversely. Equation (1) is nothing other than the balance equation of a homogeneous Markov chain with symmetric nonzero transition probabilities, from which all the basic laws of statistical physics already follow automatically ([4,8]). Thus the problem is in fact reduced to an exact investigation of when equations of type (1) are obtained from quantum theory, especially since in ([7]) they were obtained with the aid of nonstationary perturbation theory together with the adiabatic hypothesis, the applicability of which in studying the nonstationary behavior of closed physical systems is open to objection. In ([7]), equations for $P_k(t)$ were also obtained without using perturbation theory, from which, in any case, it follows that $P_k(t)$, in contrast to (1), are, generally speaking, not connected with a Markov chain.

4. The irreversible behavior of closed conservative physical systems finds a consistent explanation within the framework of the quantum theory of decay ([1,2]).

A nonstationary (in particular, nonequilibrium) closed conservative physical system is specified** together with the operator of the total energy

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* A preliminary communication on this topic was reported at the Symposium on Limit Theorems (June 1963, Palanga) ([6]).

** We adhere to the meaning of the notation of works ([1,2]).

$\hat{H} = \text{const}(t)$ and the vector of the initial state $\Psi_0 = \Psi(x, t = 0)$, and its behavior is completely described by the vector $\Psi(x, t)$, which is the solution of the Cauchy problem for the Schrödinger equation. Let $\{\varphi_E(x), \varphi_k(x)\}$ be a complete orthonormal system of eigenfunctions of the operator $\hat{H}$ ($\varphi_E(x)$ of the continuous spectrum, $\varphi_k(x)$ of the discrete spectrum*). Then the probability $L(t)$ of finding the system at time t in the initial state is, on the basis of the Fock-Krylov theorem ([1]), $L(t) = |p(t)|^2$, where

$$p(t) = \sum_k c_k^* c_k e^{-\frac{i}{\hbar}E_k t} + \int_{E_{\min}}^{\infty} c^*(E)c(E)e^{-\frac{i}{\hbar}Et}\, dE, \tag{2}$$

where $c_{kc}k^*$ and $\omega(E) \equiv c^*(E)c(E)$ are the time-conserved (law of conservation of energy) weights of the discrete levels and the density of the energy distribution in the continuous spectrum

$$\Psi_0 = \sum_k c_k \varphi_k(x) + \int_{E_{\min}}^{\infty} c(E)\varphi_E(x)\, dE. \tag{3}$$

Since the natural requirement of irreversibility is $L(t) \to 0$ as $t \to \infty$, it follows from (3) that for this it is necessary ([1]) that the operator $\hat{H}$ have a continuous spectrum** (and, consequently, that $\omega(E)$ be integrable) and that the initial state have no contribution from the possible discrete spectrum ($c_k = 0$). If, however, $c_k \neq 0$, then we immediately arrive at the Poincaré recurrence theorem. Thus, for a decaying (irreversibly) nonequilibrium physical system,

$$p(t) = \int_0^\infty \omega(E) e^{-\frac{i}{\hbar}Et}\, dE; \qquad \int_0^\infty \omega(E)\, dE = 1, \tag{4}$$

where we have explicitly taken into account the spectrality principle fundamental to our investigation—the existence of a lowest energy state $E_{\min} = 0$. On the basis of the spectrality principle it follows ([2]) that $p(t)$ is the boundary value of a function analytic in the complex half-plane t, which leads to essential restrictions on the possible behavior of $p(t)$. In particular, using dispersion relations, one can solve the inverse problem ([2]): knowing the physically measurable $L(t) = |p(t)|^2$, determine $\omega(E)$. It follows from this that a nonstationary physical system, generally speaking, remembers the initial state. Still more important restrictions follow from the criterion of physical realizability ([2])

$$\int_{-\infty}^\infty \frac{|\log|p(t)||}{1+t^2}\, dt < \infty, \tag{5}$$

namely: a) decay—a transition to an equilibrium state in a finite time T—is impossible, $p(t) \neq 0,\ t \geq T < \infty$; b) "breathing" decay is impossible, i.e., it is inadmissible for $p(t)$ to vanish only on finite intervals $t \in (t_1, t_2)$; c) finally, contrary to the conclusions usually adopted, an exponential law of decay is asymptotically impossible; more precisely, an exponential law of transition to an equilibrium state cannot be valid for all $t \in [0, \infty)$. In particular, if the density of the energy distribution is a dispersion one $\omega(E) = C[(E - E_0)^2 + \Gamma^2]^{-1}$, then, as shown in ([2]), in addition to the principal exponential term

$$\exp\left[-\frac{i}{\hbar}E_0 t - \frac{\Gamma}{\hbar}|t|\right]$$

(where $\hbar/2\Gamma \equiv \tau$ naturally has the meaning of the relaxation time), in $p(t)$ there is also a term that does not vanish even for

* To avoid complicating the notation, we do not write other quantum numbers for $\varphi_E(x)$; where necessary, summation or integration over them is assumed.

** In the present work we do not dwell on the interesting problem of how to obtain such properties of the operator H for model problems and, in particular, by means of the limiting transition $N \to \infty,\ V \to \infty,\ N/V = \text{const}$.

for what t^* an additional term, decreasing only as a polynomial with negative powers and, consequently, determining the true asymptotics of $p(t)$ as $t \to \infty$. The exact determination of the time interval where the exponential term is dominant depends on the detailed behavior of $\omega(E)$, i.e., on the detailed specification of the initial state. In particular, for dispersive $\omega(E)$ these are those t for which

$$\frac{\Gamma t}{\hbar} e^{-\Gamma t/\hbar} \gg \frac{\Gamma^2}{E_0^2 + \Gamma^2}. \tag{6}$$

Thus, the development of a nonequilibrium system in time is determined, if the relaxation time is not very small $(\Gamma^2/(E_0^2 + \Gamma^2) < e^{-1})$, by two terms: one, dominant over a finite time interval and weakly dependent on the initial state, which determines the memory of the initial state. From the nonexponential character of the decay law there also follows the fundamental conclusion that the very concept of a transition probability per unit time that is independent of time —the homogeneity of decay in time, which arises naturally within nonstationary perturbation theory (see the derivation of (1) in (7))—is a highly approximate concept.

5. Let us make the quantum theory of decay more concrete for our problems. Let A be the operator of a physical quantity whose measurements single out the corresponding statistical ensemble,** and let $\xi_k(x)$ be eigenfunctions***

$$A\xi_k(x) = a_k \xi_k(x). \tag{7}$$

The natural condition for A to belong to the system described by the operator H and by the vector of the initial state Ψ_0 consists in requiring that

$$A = B + G; \qquad [B, H] = 0; \qquad [G, H] \neq 0. \tag{8}$$

Consider the mean value of the operator A at the time t, $\bar{A}(t) = (\Psi(t), A\Psi(t))$. On the basis of the irreversibility condition ($c_k \equiv 0$), it is not difficult to obtain

$$\bar{A}(t) = \int_0^\infty \int_0^\infty e^{-\frac{i}{\hbar}Et + \frac{i}{\hbar}E't} c^*(E) c(E') (\varphi_E, A\varphi_{E'})\, dE\, dE', \tag{9}$$

However, by virtue of the adopted restriction on the operator A (8):

$$(\varphi_E, A\varphi_{E'}) = b(E')\delta(E - E') + g(E, E'), \tag{10}$$

where $g(E, E')$ is absolutely integrable in its variables. Passing to the limit, we obtain

$$\lim_{t\to\infty} \bar{A}(t) = \bar{A}(\infty) = \int_0^\infty b(E) c^*(E) c(E)\, dE. \tag{11}$$

Thus, condition (8), to which we have subjected the operator A, is necessary for the existence of a limiting mean value of the operator A as $t \to \infty$ (in the equilibrium state), which ensures irreversibility in the behavior of the statistical ensemble singled out by measurements of A.

It is easy to see that

$$\bar{A}(t) = A_{\text{av}}(t) = \sum_k a_k |P_k(t)|^2, \tag{12}$$

where $|P_k(t)|^2$ are the probabilities of finding the system at time t in states in which the value of the physical quantity is equal to a_k:

$$P_k(t) = (\Psi(t), \xi_k) = \int_0^\infty e^{-\frac{i}{\hbar}Et} \alpha_k(E) c^*(E)\, dE, \qquad \xi_k(x) = \int_0^\infty \alpha_k(E) \varphi_E(x)\, dE. \tag{13}$$

* The presence of an additional term, not equal to zero for any t, is valid for arbitrary $\omega(E)$.

** The case in which the states are specified by a density matrix is considered analogously.

*** For simplicity, in ξ_k we do not write out the other quantum numbers; where necessary, summation or integration over them is assumed to have been performed.

It can be shown that, by virtue of condition (8),

$$a_k^*(E) a_k(E') = \beta(E') \delta(E - E') + \gamma(E, E'), \tag{14}$$

where $\beta(E)$, $\gamma(E, E')$ are absolutely integrable functions.

As follows from (13), $P_k(t)$ contains a term that is the boundary value of a function analytic in the complex half-plane t, and for its investigation the methods and results given in Sec. 4 are fully applicable. Let us list the main results that follow from this analysis: a) $P_k(t)$ cannot be associated with a Markov chain, since a nonequilibrium system explicitly remembers the "past" and, in general, the details of the initial state; b) only in a finite interval of time t can the behavior of $P_k(t)$ be close (they cannot coincide exactly for any t) to that predicted by statistical physics.

6. As follows from (10), (11), (12), the ergodic hypothesis within the framework of quantum theory is, strictly speaking, false, for the mean value of the operator A in the equilibrium (limiting as $t \to \infty$) state explicitly depends on the initial state. The degree of dependence on the details of the initial state depends, of course, on the behavior of $\omega(E)$ and $b(E)$.

From (11) it follows, however, that the ergodic theorem is approximately valid for not very nonequilibrium systems ($\hbar/2\Gamma = \tau \gg 1;\ E_0 \gg 0$), when, computing the integral in (11) by residues, one may neglect the presence of the lower limit $E_{\min}$, replacing it by $-\infty$. It is interesting to note that even in this particular case the mean value $\bar{A}(\infty)$ in the equilibrium state is determined by the value $b(E_0 - i\Gamma)$, i.e., not only the mean energy of the nonequilibrium system is essential (as follows from the Gibbs distribution), but also the relaxation time.

7. Thus, from dynamical theory, more precisely from quantum theory, the predictions of statistical physics do not, strictly speaking, follow, especially asymptotically as $t \to \infty$, and a dynamical system, while irreversibly tending toward the equilibrium state, does not "forget" the initial state; consequently, the ergodic hypothesis is, strictly speaking, false. However, in a finite interval of time the predictions of statistical physics and of dynamical theory can be sufficiently close (they cannot coincide exactly in any interval of time); moreover, as follows from (6), (11), this finite interval of time for commonly encountered nonequilibrium systems ($\hbar/2\Gamma = \tau \gg \hbar/E_0$) is large, practically "infinite."
8. As was already indicated above, the asymptotic predictions (as $t \to \infty$) of quantum and classical theories, owing to the specific character of the double limiting transition, do not coincide. Therefore the proof of the ergodic theorem for some model classical systems [9] in no way contradicts the falsity, proved above, of the ergodic hypothesis within the framework of quantum theory.

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Note: Figure translations are in progress. See original paper for figures.