A CONTRIBUTION TO VON NEUMANN'S APPROACH TO THE QUANTAL ERGODIC THEOREM

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In the paper the Schrödinger equation is transformed into a system of differential equations similar to the Hamiltonian equations in classical mechanics. In this way it is possible to solve the ergodic problem in quantum mechanics analogically to Khinchin's method in classical mechanics. The physical observables are averaged on the phase surface G with the density of the probability which is the time invariant. It was shown that the sufficient condition for the justification of the ergodic theorem is that the dimension of the energy shell must be sufficiently large according to unity.

I. INTRODUCTION

The fundamental problem in statistical mechanics is to justify the use of the Gibbsian canonical ensembles. There are many ways of solving this problem. One of them starts under the assumption of the validity of the ergodic theorem. The ergodic theorem asserts that the time average of the physical observable characterizing one system is equal to the microcanonical average of the same observable. Thus it logically follows that the main problem of this method is to show under which assumptions the above mentioned theorem is valid.

J. von Neumann was the first to formulate the ergodic theorem in quantum statistical mechanics in paper [13] showing simultaneously under what conditions the theorem is valid. Paper [13] was followed by some other papers, especially [1—5]. The authors of the papers, after the critical evaluation of certain weak points of paper [13], partly simplified the method of the proof and partly showed that the ergodic theorem is valid under weaker conditions than those introduced by J. von Neumann. The criticism refers mainly to the method of averaging by means of which J. von Neumann determined an upper bound for the time mean of the expression

$$(\langle \hat{F} \rangle - \langle \hat{F} \rangle_M)^2,$$

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where $\langle \hat{F} \rangle$ is the quantum-mechanical expectation value of a macro-operator $\hat{F}$, $\langle \hat{F} \rangle_M$ is the microcanonical average of a macro-operator $\hat{F}$.

The authors come to the conclusion that the method of averaging over all possible macro-observers does not respect consistently the equation of motion and therefore is unable to give the microscopic criterion for distinguishing the ergodic systems from nonergodic ones.

We suppose that it will be useful to show the following fact: The use of J. von Neumann's method of averaging is limited only to trivial operators in the case when we accept this method exactly. That fact can be proved by the following consideration:

Proceeding according to Farquhar [3], let the isolated system be characterized by the Hamiltonian operator $\hat{H}$, whose orthonormal set of the eigenfunctions we denote by $\{\varphi_k\}$. Further let $\{\varphi_{nvl}\}$ be an orthonormal set of eigenfunctions of the macro-operators[1]; n indicates the energy shell, v indicates the phase cell and l indicates the functions within some phase cell. We shall assume the quantum state of the system to be in a certain energy shell, characterized by a wave function which we can write either in the form

$$\Psi(t) = \sum_k a_k \varphi_k \exp\left[-\frac{iE_k t}{\hbar}\right] \tag{1}$$

or in the form

$$\Psi(t) = \sum_{v=1}^{N} \sum_{l=1}^{s_v} b_{vl}(t) \Phi_{nvl}, \tag{2}$$

where

$$\sum_{v=1}^{N} s_v = S.$$

The sets of the functions $\{\varphi_k\}$ and $\{\Phi_{nvl}\}$ are connected by the following unitary transformations

$$\varphi_k = \sum_{v=1}^{N} \sum_{l=1}^{s_v} U_{k,vl}\, \Phi_{nvl} = \sum_{v=1}^{N} \sum_{l}^{s_v} \langle \Phi_{nvl} \mid \varphi_k \rangle\, \Phi_{nvl} \tag{3}$$

and

$$\Phi_{nvl} = \sum_{k=1}^{S} U^*_{k,nvl}\, \varphi_k = \sum_{k=1}^{S} \langle \varphi_k \mid \Phi_{nvl} \rangle\, \varphi_k,$$

where $U_{k,nvl}$ are the elements of an unitary matrix. From the relations (1), (2) and (3) we obtain

[1] The construction of the macro-operators is described in papers [8] and [12].

$$b_{nvl} = \sum_{k=1}^{S} a_k U_{k,nvl} \exp\left[-\frac{iE_k t}{\hbar}\right].$$

The probability of the state of the system being in the v-phase cell is then given by the relation

$$u_v = \sum_{l=1}^{s_v} |b(t)|^2 = \sum_k \sum_{k'} a_k^* a_{k'} \exp\left[-\frac{i(E_{k'} - E_k)t}{\hbar}\right] \sum_{l=1}^{s_v} U_{k,nvl}^* U_{k',nvl}.$$

The quantum mechanical expectation value of the macro-operator $\hat{F}$ is given by the relation

$$\langle \hat{F} \rangle = \langle \Psi | \hat{F} | \Psi \rangle = \sum_{v=1}^{N} F_v u_v.$$

The ergodic theorem formulated by J. von Neumann asserts that

$$\langle \hat{F} \rangle_T \stackrel{!}{=} \langle \hat{F} \rangle_M \tag{4}$$

is valid, where

$$\langle \hat{F} \rangle_T = \lim_{T \to \infty} \frac{1}{T} \int_0^T \sum_{v=1}^{N} F_v u_v \, dt$$

and

$$\langle \hat{F} \rangle_M = \sum_{v=1}^{N} F_v \frac{s_v}{S}$$

for all macro-operators. Since the relation (4) is to be valid for an arbitrary macro-operator, it is enough to prove that

$$\langle u_v \rangle_T = \langle u_v \rangle_M$$

is valid. It is possible to show [3] that

$$\langle u_v \rangle_T = \sum_{k=1}^{S} a_k^2 \sum_{l=1}^{s_v} |U_{k,vl}|^2 + \sum_k \sum_{k'} a_k^* a_{k'} \sum_{l=1}^{s_v} U_{k,vl}^* U_{k',vl}$$

is valid. It is evident that the second term is not zero only in the case of energy degeneracies.

The construction of the macro-operators from the micro-operators is not an unambigous operation and therefore J. von Neumann assumed that with the given accuracy of the experimental set-up, it is possible to divide

the energy shell in many ways into phase cells so that their number will be the same. Each such subdivision is connected with some macro-observer. J. von Neumann removes this ambiguity so that the quantity $\langle u_v \rangle_T$ averages over the unitary continuous group[2]. If we denote this averaging process by the symbol $\langle \ \rangle_0$, then for the validity of the ergodic theorem it is necessary to show that

$$\langle \langle \hat{F} \rangle_T \rangle_0 = \sum_{v=1}^{N} \langle F_v \langle u_v \rangle_T \rangle_0 \stackrel{!}{=} \langle \hat{F} \rangle_M \tag{5}$$

is valid. In J. von Neumann 's method instead of the relation (5) the relation

$$\langle \langle F \rangle_T \rangle_0 = \sum_{v=1}^{N} F_v \langle \langle u_v \rangle_T \rangle_0 = \langle \hat{F} \rangle_M \tag{6}$$

is proved.

If we realize that each basis $\{\Phi_{nvl}\}$ is connected with the standard basis $\{\varphi_k\}$ by the unitary matrix, it is evident that the basis $\{\Phi_{nvl}\}$ arises by spinning from the basis $\{\varphi_k\}$. With the application of all elements of the unitary group in the standard basis any phase cell fills up the whole energy shell. If thus during the averaging process we assume the eigenvalue of the operator $\hat{F}$ to be a constant, the relation (6) is correct only in the case if an operator $\hat{F}$, reduced to an energy shell is a trivial operator, that means a unique operator multiplied by the arbitrary constant.

One can remove this lack in the following manner: We choose the definite basis as a fixed one and the inaccuracies of the definition of the macro-operators are described by a definite distribution of the initial states of the system. P. Bocchieri and A. Loinger proceeded similary in papers [1—2]. The above authors assumed all initial states of the macroscopic system to be a priori equally probably distributed over the whole energy shell. The aim of this paper is the same. The method of solving the ergodic theorem described in this paper brings however some improvement which can be summarized in the following points:

1. It justifies statistical mechanics, both classical and quantum mechanics from a common point of view

2. The measure of averaging in the phase surface is choosen as the time invariant and in this sense it respects the equation of motion.

3. A sufficient condidion for the validity of the ergodic theorem in quantum mechanics is weaker than those introduced in the preceding papers.

[2] The definition of the integral over this domain of the parameters defining the elements of the continuous group is described in papers [6—7].

II. „CLASSICAL" FORM OF QUANTUM MECHANICS

For further aims it will be advantageous to transform Schrödinger's equation into the system of Hamiltonian equations [5]. We consider again an isolated system characterized by the Hamiltonian operator $\hat{H}$ and the wave function $\Psi(t)$, which describes the quantum state existing in some energy shell. Further let $\{\Phi_k\}$ be an orthonormal set of the eigenfunctions of the makro-operators belonging to a definite energy shell. The wave function can be written in the form

$$\Psi(t) = \sum_{k=1}^{S} c_k(t)\, \Phi_k.$$

When the function $\Psi(t)$ is substituted into the Schrödinger equation and an operation is performed, we obtain

$$i\hbar \frac{dc_m(t)}{dt} = \sum_{k=1}^{S} c_k(t)\, H_{mk}, \tag{7}$$

where $H_{mk} = \langle \Phi_m | \hat{H} | \Phi_k \rangle$. For every m we introduce real variables by the following transformation

$$q_m = \frac{1}{\sqrt{2}} [c_m^*(t) + c_m(t)] \tag{8}$$

$$p_m = \frac{i}{\sqrt{2}} [c_m^*(t) - c_m(t)]. \tag{9}$$

If we calculate $c_m(t)$ from the system of equations (8—9) and substitute it into the equation (7), then after zeroing the real and imaginary part we obtain, for an arbitrary m, the following system of equations

$$\frac{dq_m}{dt} = \frac{\partial H}{\partial p_m}$$

$$\frac{dp_m}{dt} = \frac{\partial H}{\partial q_m} \qquad m = 1, 2, \ldots, S,$$

where the function

$$H(p_k, q_k) = \frac{1}{\hbar} \langle \Psi | \hat{H} | \Psi \rangle = \frac{1}{2} \sum_k \sum_j \frac{H_{kj}}{\hbar} \{(p_k p_j + q_k q_j) + i(q_k q_j - q_j p_k)\} \tag{10}$$

is called formally „the Hamiltonian function".

Analogically, according to relation (10), we can express also the quantum-mechanical expectation value of an arbitrary Hermitian operator $\hat{F}$. Its form, expressed by the quantities $\{p_k, q_k\}$, is

$$F(p_k, q_k) = \langle \Psi | \hat{F} | \Psi \rangle = \tfrac{1}{2} \sum_k \sum_j F_{kj} \{(p_k p_j + q_k q_j) + i(q_k p_j - q_j p_k)\}. \tag{11}$$

In the case when the operator $\hat{F}$ is a macro-operator, relation (11) has the simple form

$$F(p_k, q_k) = \tfrac{1}{2} \sum_k F_k (p_k^2 + q_k^2). \tag{12}$$

From the condition that the norm of the wave functions is unique we obtain

$$\langle \Psi \mid \Psi \rangle = \tfrac{1}{2} \sum_{k=1}^{S} (p_k^2 + q_k^2) = G(p_k, q_k) = 1. \tag{13}$$

The formal agreement with the mathematical form of the entry of the quantum-mechanical equation with the equations of motion of classical mechanics enables us to solve the ergodic theorem in quantum mechanics analogically as in classical mechanics. The set of variables $\{p_k, q_k\}$ which defines the function $\Psi(t)$ in the representation $\{\Phi_k\}$ will be called „dynamical variables" and we choose them as coordinates of the $2S$-dimensional Euclidean space, which we call the phase space. The time course of the quantum states will be illustrated in the phase space by a trajectory. All possible trajectories are found on the surface G, of which the analytical form is given by relation (13). If we observe the relations (10—11), we see that the Hamiltonian function and the quantum-mechanical expectation value of the operator $\hat{F}$ have a relatively simple mathematical form — a bilinear function — contrary to classical mechanics, where especially the potential energy and analogically the physical quantity $F(p_k, q_k)$ can depend on dynamical variables in a complicated way.

III. JUSTIFICATION OF THE ERGODIC THEOREM

In classical mechanics the ergodic theorem asserts that if an isolated system, characterized by the Hamiltonian function $H(p_k, q_k)$, is ergodic, then

$$\overline{F(p_k, q_k)} = \frac{\int_{\Sigma_E} F(p_k, q_k)\, d\mu}{\int_{\Sigma_E} d\mu} \tag{14}$$

where $F(p_k, q_k)$ is a physical quantity characterizing the system in the dynamic state defined by the set of variables $\{p_k, q_k\}$,

$$\overline{F(p_k, q_k)} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{F}(p_k, q_k)\, \mathrm{d}t, \tag{15}$$

Σ_E is a surface in the phase space analytically expressed by the Hamiltonian function, the value of which is E, $\mathrm{d}\mu$ is the time invariant measure in the surface Σ_E and its expression is

$$\mathrm{d}\mu = \frac{\mathrm{d}\Sigma}{\sqrt{\sum_k \left[\left(\frac{\partial H}{\partial p_k}\right)^2 + \left(\frac{\partial H}{\partial q_k}\right)^2\right]}}, \tag{16}$$

where $\mathrm{d}\Sigma$ is the area of the elementary surface on the surface Σ_E.

In the quantum mechanical case the possible dynamic state are found in the phase space on the surface G. Analogically to relation (14), if the quantum system is ergodic,

$$\overline{F(p_k, q_k)} \overset{!}{=} \frac{\int_G F(p_k, q_k)\, \mathrm{d}\mu}{\int_G \mathrm{d}\mu} \tag{17}$$

should be valid.

We know from classical statistical mechanics that it is a necessary and sufficient condition for the validity of relation (17) that the surface G be metrically indecomposable. In our case it can be easily shown from the form of the Hamiltonian function that there are many analytical integrals of motion and therefore the surface G is metrically decomposable. To be exact relation (17) for this reason is not valid. Under certain condition we can prove however that relation (17) is valid with a sufficient approximation. For the proof of this assertion it is sufficient to realize that the quantum-mechanical expectation value of the operator in the representation $\{\Phi_k\}$ is the additive function. A. J. Khinchin in paper [6] showed that for additive functions the relative measure of the points on the surface Σ_E is $O(N^{-1/4})$ for which

$$\frac{|\overline{F} - \langle F\rangle_0}{\langle F\rangle_0} > KN^{-1/4} \tag{18}$$

is valid, where $\overline{F}$ is defined by the relation (15), $\langle F\rangle_0$ is defined by relation (17).

For $N \to \infty$ we can replace with a sufficient approximation the time average value with the phase average on the surface Σ_E. In our case $F(p_k, q_k)$ as well as the surface G have a simple analytical form and we can therefore calculate an estimate analogous to relation (18) more precisely.

According to relation (16) the measure $\mathrm{d}\mu$ has the form

$$\mathrm{d}\mu = \frac{\mathrm{d}\Sigma}{\sqrt{\sum_k \left[\left(\frac{\partial G}{\partial p_k}\right)^2 + \left(\frac{\partial G}{\partial q_k}\right)^2\right]}} = \frac{\mathrm{d}\Sigma}{\sqrt{2}} \tag{19}$$

and, as mentioned above, it is invariant along the trajectories. After substituting relations (12) and (19) into relation (14), we can write with regard to the spherical symmetry of the surface G on which we are averaging

$$\langle p_k p_i + q_k q_j\rangle_0 = \begin{cases} \frac{2}{S} & k = j \\ 0 & k \neq j \end{cases}$$

and

$$\ll \hat{F} \gg_0 = \frac{\sum_k F_k}{S}.$$

For the estimate of the measure of approximation of the interchange of the time average with the phase average, it is necessary to calculate the relative quadratic fluctuation. The relative quadratic fluctuation is defined by the relation

$$\delta_F = \frac{\sqrt{\langle(\langle \hat{F}\rangle - \ll \hat{F} \gg_0)^2\rangle_0}}{\ll \hat{F} \gg_0} = \frac{\sqrt{\langle\langle \hat{F}\rangle^2\rangle_0 - (\ll \hat{F} \gg_0)^2}}{\ll \hat{F} \gg_0}. \tag{20}$$

First we calculate the quantity $\langle \hat{F}\rangle^2$. According to relation (11) we can write

$$\langle \hat{F}\rangle^2 = \tfrac{1}{4} \sum_k \sum_j (p_k^2 + q_k^2)(p_j^2 + q_j^2) F_k F_j. \tag{21}$$

Averaging over the surface G we obtain

$$\langle\langle F\rangle^2\rangle_0 = \tfrac{1}{4} \sum_k \sum_j \langle (p_k^2 + q_k^2)(p_j^2 + q_j^2)\rangle_0 F_k F_j. \tag{22}$$

From the spherical symmetry of the surface G it follows

$$a = \langle (p_k^2 + q_k^2)^2\rangle_0$$

$$b = \langle (p_k^2 + q_k^2)(p_j^2 + q_j^2)\rangle_0$$

$$a + (S-1)\, b = 2\langle (p_k^2 + q_k^2)\rangle_0 = \frac{4}{S} \tag{23}$$

is valid for all k and j. According to appendix 3 in the monograph [3] we can write

$$a = 4\,\frac{S}{S(S+1)}. \tag{24}$$

After substituting relations (24) into relation (23) we obtain

$$b = 4\,\frac{1}{S(S+1)}. \tag{25}$$

After substituting relations (24—25) into relation (22) we obtain

$$\langle\langle\hat{F}\rangle^2\rangle_0 = \frac{1}{S(S+1)}\sum_k F_k^2 + \frac{1}{S(S+1)}\left(\sum_k F_k\right)^2.$$

Finally, if we substitute relation (21) into relation (20), we obtain

$$\delta_F = \frac{\sqrt{\dfrac{1}{S(S+1)}\sum_k F_k^2 + \dfrac{1}{S(S+1)}\left(\sum_k F_k\right)^2 - \dfrac{1}{S^2}\left(\sum_k F_k\right)^2}}{\dfrac{\sum_k F_k}{S}} <$$

$$< \frac{1}{\sqrt{S+1}}\,\frac{\sqrt{\dfrac{\mathrm{Sp}\hat{F}^2}{S}}}{\dfrac{\mathrm{Sp}\hat{F}}{S}}. \tag{26}$$

The expression $\sqrt{\dfrac{\mathrm{Sp}\hat{F}^2}{S}}\Big/\dfrac{\mathrm{Sp}\hat{F}}{S} < \dfrac{F_{\max}}{F_{\min}}$, where $F_{\max}$ and $F_{\min}$ are the maximum and minimum values of the operator $\hat{F}$ in some energy shell. If we realize that $S = \exp 10^{20}$ [8], it follows from relation (26) that $\langle\hat{F}\rangle$ is nearly constant on the surface G without the set of the points of the measure zero. Therefore we can expect that $\overline{\langle\hat{F}\rangle}$ will differ from $\langle\langle\hat{F}\rangle\rangle_0$ only on the set of points of the surface G of an extremely small measure, which can be proved in the following way:

Let us calculate the expression

$$\frac{\sqrt{\langle(\overline{\langle\hat{F}\rangle} - \langle\langle\hat{F}\rangle\rangle_0)^2\rangle_0}}{\langle\langle\hat{F}\rangle\rangle_0}.$$

If we use Schwarz's inequality, we can write

$$(\overline{\langle\hat{F}\rangle} - \langle\langle\hat{F}\rangle\rangle_0)^2 \leqslant \overline{(\langle\hat{F}\rangle - \langle\langle\hat{F}\rangle\rangle_0)^2}.$$

The operations of the time averaging and averaging on the surface G are commutative operations as it was shown by P. Bocchieri and A. Loinger [2]. Using this fact we can write

$$\langle(\overline{\langle\hat{F}\rangle} - \langle\langle\hat{F}\rangle\rangle_0)^2\rangle_0 \leqslant \langle\overline{(\langle\hat{F}\rangle - \langle\langle\hat{F}\rangle\rangle_0)^2}\rangle_0 = \tag{27}$$

$$= \langle\overline{(\langle\hat{F}\rangle - \langle\langle\hat{F}\rangle\rangle_0)^2}\rangle_0 = \langle(\langle\hat{F}\rangle - \langle\langle\hat{F}\rangle\rangle_0)^2\rangle_0.$$

Using relations (26—27), we obtain the required estimate

$$\frac{\sqrt{\langle(\overline{\langle\hat{F}\rangle} - \langle\langle\hat{F}\rangle\rangle_0)^2\rangle_0}}{\langle\langle\hat{F}\rangle\rangle_0} < \frac{1}{\sqrt{S}}K.$$

Relation (26) is valid not only for macro-operators but also for micro-operators used in concrete applications. This can be proved by the following consideration: The quantum-mechanical expectation value of the micro-operator $\hat{F}$ in the quantum state described by the wave function $\Psi(t)$ can be briefly written as $\mathrm{Sp}(\hat{P}_{\psi(t)}\hat{F})$, where $\hat{P}_{\psi(t)} = |\Psi\rangle\langle\Psi|$. If we use relations (14) and (16), the operation of averaging on the surface G will have a simple form

$$\langle\langle\hat{F}\rangle\rangle_0 = \int_G \mathrm{Sp}(\hat{P}_{\psi(t)}\hat{F})\,\frac{\mathrm{d}\Sigma}{\Sigma} = \mathrm{Sp}\int_G \hat{P}_{\psi(t)}\hat{F}\,\frac{\mathrm{d}\Sigma}{\Sigma} = \mathrm{Sp}\hat{W}_1\hat{F},$$

where

$$\hat{W}_1 = \int_G \hat{P}_{\psi(t)}\,\frac{\mathrm{d}\Sigma}{\Sigma}.$$

Analogically we can write also

$$\langle\hat{F}\rangle^2 = \langle\Psi|\hat{F}|\Psi\rangle\langle\Psi|\hat{F}|\Psi\rangle = \mathrm{Sp}(\hat{P}_\psi\hat{F}\hat{P}_\psi\hat{F})$$

and

$$\langle\langle F\rangle^2\rangle_0 = \int_G \mathrm{Sp}(\hat{P}_\psi\hat{F}\hat{P}_\psi\hat{F})\,\frac{\mathrm{d}\Sigma}{\Sigma} = \mathrm{Sp}\int_G \hat{P}_\psi\hat{F}\hat{P}_\psi\hat{F}\,\frac{\mathrm{d}\Sigma}{\Sigma} = \mathrm{Sp}\hat{W}_2\hat{F},$$

where

$$\hat{W}_2 = \int \hat{P}_\psi\hat{F}\hat{P}_\psi\,\frac{\mathrm{d}\Sigma}{\Sigma}.$$

We know from quantum mechanics that the addition of operatos is an invariant operation and Sp is invariant with regard to a unitary transformation of the orthonormal set. We choose such a transformation in which the bilinear

function expressed by relation (11) passes into the quadratic form ($\hat{F}$ is the Hermitian operator) and in this way we transform this case into the case of a macro-operator.

IV. CONCLUSION

J. von Neumann in paper [13] postulates three sufficient conditions for the validity of the ergodic theorem. These conditions are: the inequality $s_v \gg N$ for all v, a non-degeneracy of energy eigenvalues and non-zero differences between the energy eigenvalues. P. Bocchieri and A. Loinger [2] as well as J. E. Farquhar and P. T. Landsberg [4] postulate for the validity of the ergodic theorem the inequality $s_v \gg 1$ for all v. Relation (26) does not give any condition for the dimension of the phase cells but it requires the inequality $S \gg 1$ as a sufficient condition. It is evident that the last condition is weaker than those which are introduced in previous papers.

It is necessary to realize the fact that when evaluating these results, we are replacing one hypothesis by another. We suppose that it would be superfluous to describe in detail to what extent the obtained results justify the ergodic problem since, as it was shown, the solution of the ergodic theorem in quantum mechanics is analogous to a similar problem in classical mechanics and the discussion about the obtained results can be found complete in papers (6—7). It is worthwhile to mention that the obtained results enable us to state that the quantum-mechanical expectation values of the Hermitian operators are in a considerable majority of set of points of the surface G „almost constant" and equal to the microcanonical average. To justify the ergodic problem we must accept the hypothesis that on the surface G there do not exist trajectories which would to a considerable extent stay on the set of those points on which the quantum-mechanical expectation values considerably differ from the microcanonical average.

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