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Statistical Operator of von Neumann in the Wave Operator Formalism and Reduction of States in Subspaces when the Total System obeys the Schrödinger Equation

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加藤さんと量子力学

話は４０年前にさかのぼる．加藤さんが東京大学の大学院（旧制）におられた頃，私は東京文理科大学にのこり朝永先生の下で理論物理の勉強をはじめていた．学年次からは私の方が１年上に当たるが，その当時，東京都内各大学の物理学生間の交流を目指した略称「都物懇」として知られた有志学生の動きがあり，加藤さんのお名前を知ったのもこのようなアクティヴィティーと無関係ではなかったように記憶している．学部上級生から大学院学生クラスの共通の関心たりえた問題の１つが他ならぬ量子力学であり，とりわけ観測問題などに見られるその哲学的・認識論的側面であった．東大駒場には関根克彦さん（現明星大学）や板倉聖宣さん（現国立教育研究所）達を中心としたグループがガリ版刷りの機関誌を発行し，こうした問題についても鋭利な論文を発表していた．加藤さんは（私の記憶では）むしろ独立の立場から例えばソ連のブロフィンツェフの流れを汲むアメリヤノフスキーの論文をロシア語から訳出しておられたように思う．量子力学の基礎についての彼の深い関心はその頃からのものであり，私をふくめて同世代の理論屋の多くが素粒子や原子核の具体的問題に向かったのに対し，むしろこうした流行から身を傍に置いて，あくまで数理物理的に厳格な手法をもって量子力学の体系に内在する諸問題の追求を目指されたのである．

他方私はといえば，量子力学の基礎的問題への関心は持ちながらもこれに踏み込む自信もないままその後東京を離れ，名古屋大学を経て京都に移って今日に到っており，加藤さんの逆散乱問題等に関するすぐれたお仕事については，人づてに教わってはいたが，学会の折りなどにお会いする機会はあっても話題が量子力学の問題にまで及ぶことはなかった．

ところが，数年前から私は観測理論等について論文を発表する次第となり，それが加藤さんの目に止まり，昨年６月１５日付で論文別刷を送ってほしいとの手紙をいただいた．私は旧友との学問的再会を喜び早速に返事を差し上げたところ，１２月になり彼から一篇の手書き論文が送られてきた．表題はここに

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Abstract

Statistical operators of von Neumann are examined in the wave operator formation. A whole feature of the "state reduction", which occurs in subspaces during the evolution of the total system according to the Schrödinger equation, is presented explicitely. Thus both processes are compatible and inherent in quantum systems.

Let S be the quantums mechanical system which is composed of subystems S^{I} and S^{II}. States of statistical ensembles of systems S^{I}, S^{II} and S are represented by normalized vectors of the Hilbert space $\mathcal{H}^{I}$, $\mathcal{H}^{II}$ and $\mathcal{H}=\mathcal{H}^{I}\otimes\mathcal{H}^{II}$, respectively, and time development of state vectors is determined by unitary operator $U^{I}(t) = \exp[-iH^{I}t]$, $U^{II}(t) = \exp[-iH^{II}t]$ and $U(t) = [-iHt]$ generated by Hamiltonian H^{I} in $\mathcal{H}^{I}$, H^{II} in $\mathcal{H}^{II}$ and $H=H_0+H'(H_0=H^{I}\otimes I+I\otimes H^{II})$ in $\mathcal{H}$, respectively. Here H' is the interaction Hamiltonian between S^{I} and S^{II} and I denotes the unit operator in the Hilbert space under consideration. S^{I} is scattered by S^{II} and S^{I} and S^{II} are considered as the object system and the measuring apparatus in the measurement. Throughout the scattering both sets of constituent particles of S^{I} and S^{II} are invariant, S^{I} is always in some of bound states of Hamiltonian H^{I}, and S^{I} is not absorbed by S^{II}.

Wave operator[1)]

The scattering of S^{I} by S^{II} is assumed to be described in terms of wave operators $W_{\pm}$ and their ajoint

$$W_{\pm} = s-\lim_{t\to\pm\infty}(U(t))^{-1}U_0(t)$$

$$W_{\pm}^{*} = W_{\pm}^{-1} = s-\lim_{t\to\pm\infty}(U(t))^{-1}U_0(t) \qquad (1)$$

where $U_0(t)=\exp[-iH_0t]$, $s-\lim$ means the strong convergence of the operator in $\mathcal{H}$, and the double sign $\pm$ is ordered. $W_{\pm}$ is unitary and satisfies the intertwining property

$$HW_{\pm} = W_{\pm} H_0 \qquad \text{in } \mathcal{H}. \tag{2}$$

We have the one-to-one correspondence between vectors $\{\psi(0)\}$ and $\{\psi'_{\pm}(0)\}$ of $\mathcal{H}$ such that

$$W_{\pm}\ \psi_{\pm}(0) = \psi(0) \tag{3}$$

and (1) means the asymplotic relation in the sense of norm of $\mathcal{H}$;

$$\psi(t) = U(t)\psi(0) \rightarrow \psi_{\pm}(t) = U_0(t)\psi_{\pm}(0) \qquad t \rightarrow \pm\infty \tag{4}$$

We see that (4) implies the replacement of $U(t)$ by the interaction free evolution $U_0(t)$ together with the mapping by Eq.(3). Hereafter we consider only $t \geqq 0$, thus W_+.

von Neumann's statistical operator[2)]

Statistical operator for the statistical ensemble of S, is defined from normalized state vectors $\psi(t), \psi_j(t) \in \mathcal{H}$ $(j=1,2,\cdots)$ as follows,

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)|, \tag{5}$$

$$\rho_m(t) = \Sigma_j w_j\ |\psi_j(t)\rangle\langle\psi_j(t)|\ ,\ \Sigma w_j = 1, w_j \geqq 0. \tag{6}$$

ρ is the statistical operator for a pure state and ρ_m is for a mixture (mixed state) with probability distribution $\{w_j\}$, and we use frequently Dirac's notation of bra and ket, $\langle 1$ and $1\rangle$. Expectation value of physical quantity (observable) O for a pure state ψ or a mixture $\{\psi_j, w_j\}$ is given by $\mathrm{Tr}O\rho$ or $\mathrm{Tr}O\rho_m$, respectively, where Tr denote the trace on the Hilbert space $\mathcal{H}$.

Subspace of $\mathcal{H}$

We denote the complete set of commuting observables in $\mathcal{H}^{\mathrm{I}}$

and $\mathcal{H}^{II}$ by $A=\{A_1,\cdots,A_p\}$ and $B=\{B_1,\cdots,B_q\}$,the set of their eigenvalues as $a=\{a_1,\cdots,a_p\}$ and $b=\{b_1,\cdots,b_q\}$, and the corresponding normalized eigenvector by $|a\rangle=|a_1\rangle\cdots|a_p\rangle$ and $|b\rangle=|b_1\rangle\cdots|b_q\rangle$, respectively. We introduce a special assumption that $H^{I}\in A$ and $H^{II}\in B$, thus each observable from $A\cup B$ is commutable to H^{I} and H^{II} . We divide the set A and B

$$A=A^{M}\cup A^{N} \quad , \quad B=B^{R}\cup B^{S} \tag{7}$$

and construct Hilbert spaces $\mathcal{H}^{M},\mathcal{H}^{N},\mathcal{H}^{R},\mathcal{H}^{S}$ whose bases are constructed from eigenvectors $|a^{M}\rangle$, $|a^{N}\rangle$, $|b^{R}\rangle$, $|b^{S}\rangle$, of A^{M}, A^{N}, B^{R}, B^{S}, respectively. Then we have divisions of $\mathcal{H}^{I}$ and $\mathcal{H}^{II}$ into subspaces;

$$\mathcal{H}^{I}=\mathcal{H}^{M}\otimes\mathcal{H}^{N} \quad , \quad \mathcal{H}^{II}=\mathcal{H}^{R}\otimes\mathcal{H}^{S} \tag{8}$$

<u>Projections of the statistical operator into subspaces of $\mathcal{H}$</u>

We construct traces of $\rho(t)$ on subspaces $\mathcal{H}^{N,II}=\mathcal{H}^{N}\otimes\mathcal{H}^{II}$ and $\mathcal{H}^{I,S}=\mathcal{H}^{I}\otimes\mathcal{H}^{S}$;

$$\rho^{M}(t)=\mathrm{Tr}_{(N,II)}\rho(t) \tag{9}$$

$$\rho^{R}(t)=\mathrm{Tr}_{(I,S)}\rho(t). \tag{10}$$

Then $\rho^{M}(t)$ or $\rho^{R}(t)$ becomes operator on $\mathcal{H}^{M}$ or $\mathcal{H}^{R}$ and is regarded as projection of ρ into the subspace $\mathcal{H}^{M}$ or $\mathcal{H}^{R}$, respectively. Here $\mathrm{Tr}_{(N,II)}$ or $\mathrm{Tr}_{(I,S)}$ means to construct trace with respect to the complete orthonormal set of $\mathcal{H}^{N,II}$ or $\mathcal{H}^{I,S}$, respectively. Expectation value of observable O in $\mathcal{H}^{M}$ or $\mathcal{H}^{R}$ is given by $\mathrm{Tr}_{(M)}O\rho^{M}$ or $\mathrm{Tr}_{(R)}O\rho^{R}$ by constructing trace in

terms of the complete set of $\mathcal{H}^M$ or $\mathcal{H}^R$, respectively.

Initial values and asymptotic forms of $\rho(t), \rho^M(t)$ and $\rho^R(t)$

Let us put

$$\psi(0) = \sum_{a,b} c(a, b) \mid a> \mid b> \quad \in \mathcal{H}, \tag{11}$$

$$\psi_+(0) = \sum_{a,b} d(a, b) \mid a> \mid b> \quad \in \mathcal{H}, \tag{12}$$

then we have from Eq.(3)

$$d(a,b) = \sum_{a',b'} W_+^*(a,b\,;a',b')\,c(a',b'), \tag{13}$$

where $W_+^*(a,b\,;a',b')$ denotes matrix element of $W_+^* = W_+^{-1}$ with basis $\mid a> \mid b>$ and $\mid d(a,b)\mid^2$ gives a transition probability from the state $\psi(0)$ at $t=0$ to the state $\mid a> \mid b>$ for $t\to\infty$ after scattering.

Since W_+ is unitary, we have the relation, for $\| \psi(0) \| = 1$,

$$\| d \|^2 = \| c \|^2 = 1. \tag{14}$$

Let us assume that $H^{\mathrm{I}} \in A^N$ and $H^{\mathrm{II}} \in B^S$, and set the initial state as

$$\begin{aligned} \mid \psi(0) > &= \sum_{a,b} c(a,b) \mid a> \mid b> \\ &= \mid \psi^M(0)> \mid \psi^{NS}(0) > \mid \psi^R(0)> \end{aligned} \tag{15}$$

$$\mid \psi^M(0)> = \sum_{a^M} f(a^M) \mid a^M>,$$

$$\mid \psi^{NS}(0) > = \sum_{a^N, b^S} g(a^N, b^S) \mid a^N> \mid b^S>,$$

$$\mid \psi^R(0)> = \sum_{b^R} h(b^R) \mid b^R>, \tag{16}$$

$$\| f \|^2 = \| g \|^2 = \| h \|^2 = 1,$$

then we have from Eqs.(3)~(5),(9)~(12),(15),(16)

$$\rho(0) = | \psi(0) \rangle \langle \psi(0) | \quad \text{on} \quad \mathcal{H} \tag{17}$$

$$\rho(t) \to \rho_\infty(t) = | \psi_+(t) \rangle \langle \psi_+(t) | \quad \text{on} \quad \mathcal{H}, t \to \infty \tag{18}$$

$$\rho^M(0) = \{ \sum_{a^M} f(a^M) \, | a^M \rangle \} \; \{ \sum_{a^{M'}} \overline{f}(a^{M'}) \langle a^{M'} | \} \quad \text{on} \quad \mathcal{H}^M \tag{19}$$

$$\rho^M(t) \to \rho^M_\infty = \sum_{a^M, a^{M'}} \xi(a^M, a^{M'}) \, | a^M \rangle \langle a^{M'} | \quad \text{on} \quad \mathcal{H}^M, t \to \infty \tag{20}$$

$$\xi(a^M, a^{M'}) = \sum_{a^N, b} d(a^M, a^N, b) \overline{d}(a^{M'}, a^N, b) \tag{20ξ}$$

$$\rho^R(0) = \{ \sum_{b^R} h(b^R) \, | b^R \rangle \} \; \{ \sum_{b^{R'}} \overline{h}(b^{R'}) \langle b^{R'} | \} \quad \text{on} \quad \mathcal{H}^R \tag{21}$$

$$\rho^R(t) \to \rho^R_\infty = \sum_{b^R, b^{R'}} \eta(b^R, b^{R'}) \, | b^R \rangle \langle b^{R'} | \quad \text{on} \quad \mathcal{H}^R, t \to \infty \tag{22}$$

$$\eta(b^R, b^{R'}) = \sum_{a, b^S} d(a, b^R, b^S) \overline{d}(a, b^{R'}, b^S), \tag{22η}$$

where $\overline{\alpha}$ denotes complex conjugate of α.

<u>Diagonal representation of the asymptotic forms ρ^M_∞ and ρ^R_∞</u>

Since the matrix $\{ \xi(a^M, a^{M'}) \}$ and $\{ \eta(b^R, b^{R'}) \}$ is Hermite symmetric on $\mathcal{H}^M$ and $\mathcal{H}^R$, it can be diagonalized by applying a unitary operator U^M in $\mathcal{H}^I$ and U^R in $\mathcal{H}^{II}$, respectively, in the following way.

$$\hat{\xi} = U^M \xi U^{M*} \quad | \hat{a}^M \rangle = U^M | a^M \rangle \quad | \hat{a}^N \rangle = U^M | a^N \rangle = | a^N \rangle$$

$$\hat{\eta} = U^R \eta U^{R*} \quad | \hat{b}^R \rangle = U^R | b^R \rangle \quad | \hat{b}^S \rangle = U^R | b^S \rangle = | b^S \rangle,$$

$$\rho^{M}_{\infty} = \sum_{\hat{a}^M} \hat{\xi}(\hat{a}^M) |\hat{a}^M\rangle\langle\hat{a}^M| \ , \quad \rho^{R}_{\infty} = \sum_{\hat{b}^R} \hat{\eta}(\hat{b}^R) |\hat{b}^R\rangle\langle\hat{b}^R| \qquad (23)$$

Here we choosed U^M and U^R, respectively, in such a way that it transforms quantities in $\mathcal{H}^M$ and $\mathcal{H}^R$ but is identity in $\mathcal{H}^N$ and $\mathcal{H}^S$. We obtained diagonal representation of ρ^{M}_{∞} and ρ^{R}_{∞} of Eq.(23), but we may construct ρ initially by using transformed vectors $|\hat{a}^M\rangle$ and $|\hat{b}^R\rangle$ etc. in place of $|a^M\rangle$ and $|b^R\rangle$ etc. and get Eq.(23) directly, and in this sense we are allowed to omit the symbol $\hat{}$ everywhere, without loss of generality. Thus we use in the sequel the following relations in place of Eqs.(20),(20 ξ), (22), (22η), respectively;

$$\rho^{M}(t) \to \rho^{M}_{\infty} = \sum_{a^M} \xi(a^M) \, |a^M\rangle\langle a^M| \qquad \text{on } \mathcal{H}^M, t \to \infty \qquad (20')$$

$$\xi(a^M) = \sum_{a^N, b} |d(a^M, a^N, b)|^2, \quad \sum_{a^M} \xi(a^M) = 1 \qquad (20\xi')$$

$$\rho^{R}(t) \to \rho^{R}_{\infty} = \sum_{b^R} \eta(b^R) \, |b^R\rangle\langle b^R| \qquad \text{on } \mathcal{H}^R, t \to \infty \qquad (22\eta')$$

$$\eta(b^R) = \sum_{a, b^S} |d(a, b^R, b^S)|^2, \quad \sum_{b^R} \eta(b^R) = 1 \qquad (20\eta')$$

<u>Characteristics of the development of $\rho(t)$, $\rho^M(t)$ and $\rho^R(t)$ from $t=0$ to $t \to \infty$</u>

We examine the characteristic feature of the time development of $\rho(t)$ on $\mathcal{H}$, $\rho^M(t)$ on $\mathcal{H}^M$ and $\rho^R(t)$ on $\mathcal{H}^R$ along the general theory of von Neumann[2].

First, we get from Eqs.(3) and (4)

$$\psi_+(t) = U_0(t) W_+^* \psi(0), \tag{24}$$

Hence, in our case where $\rho(0)$ of Eq.(17) is a statistical operator for a pure state $\psi(0) \in \mathcal{H}$, operators $\rho(t) = |\psi(t)\rangle\langle\psi(t)| = |U(t)\psi(0)\rangle\langle U(t)\psi(0)|$ and $\rho_\infty(t) = |\psi_+(t)\rangle\langle\psi_+(t)|$ represent pure states in $\mathcal{H}$, since $\psi(t)$ and $\psi_+(t)$ are obtained always by unitary transformation in $\mathcal{H}$ of $\psi(0)$. On the other hand, although $\rho^M(0)$ and $\rho^R(0)$ of Eqs.(19) and (21) is a statistical operator for pure state $\psi^M(0) \in \mathcal{H}^M$ and $\psi^R(0) \in \mathcal{H}^R$, respectively, it approachs the constant operator ρ^M_∞ and ρ^R_∞ asymptotically as $t \to \infty$, which is nothing but a statistical operator for mixture in $\mathcal{H}^M$ and $\mathcal{H}^R$, respectively, as clearly seen in Eqs.(20')~(22η'). Exceptions are special cases where ξ and η vanish except at only one values of a^M and b^R, respectively. Such a phenomenon that, while $\rho(t)$ in $\mathcal{H}$ continues to represent the pure state in $\mathcal{H}$, its projection into the subspaces $\mathcal{H}^M$ or $\mathcal{H}^R$ represents the pure state or the mixture, generally the mixture, is already described in the general theory of the statistical operator by von Neumann[2]. Thus it is possible and completely rational that, when, in the total system S, the causal and quantum mechanical development proceeds according to the Schrödinger equation, in its subsystems S^I, S^{II} or in the subspaces $\mathcal{H}^R, \mathcal{H}^M$, the transition from the pure state to the mixture, which is apparently acausal and not describable in the Schrödinger's law. We have analyzed the scattering system S composed of S^I and

S^{II} concretely and exhibited the above relationship between the total and the subsystems which is inherent in quantum mechanical systems. The situation does not and should not be altered when we consider measurement problem for the same scattering system S, only by nominating S^{I} and S^{II} as object system and measuring apparatus. Of course in the measurement the reduction of pure state to mixture occurs within the system S. The process of the reduction is described above elaborately and obviously the reduction is proper to the system S developing by the Schrödinger equation and is not influenced from the outside of S. Hence it is neither necessary nor possible to introduce into the theory of measurement the action of the subject, or abstract "Ich" of von Neumann, where the terms are used in the sense of philosophical idealism. Thus the role of the observer in measurement is to recognize the result of the reduction of state as described by statistical operator, and this constitutes a separate problem and is essentially independent of the problem of the reduction of state itself.

Example of the measurement

We set up a necessary condition such that our scattering constitutes an ideal measurement of some observable of object system S^{I} by means of the measuring apparatus S^{II}. Let $\{a_j^M\} = a^M$ $(j=1,2,\cdots)$ and $\{b_j^R\} = b^R$ $(j=1,2,\cdots)$ be a series of sets of eigenvalues of A^M of S^{I} and B^R of S^{II} respectively,

introduce a one-to-one correspondence in order of j : $a_j^M \longleftrightarrow b_j^R$ ($j=1,2,\cdots$), and assume the following condition for the matrix element of W_+^*;

$$w_+^*(a,b^R,b^S;a^M,a^{N'},b') = (\prod_{j=1}\delta(b_j^R-a_j^M))w(a,b^S;a^{N'},b') \quad (25)$$

As assumed already we have $H^I \in A^N$, $H^{II} \in B^S$ and provide $\psi(0)$ at $t=0$ by Eqs.(15) and (16). From unitarity of W_+, Eqs.(14),

$$\sum_{a^M}\xi(a^M)=\sum_{b^R}\eta(b^R)=1, \quad (26)$$

which shows that $\{\xi(a_j^M)\}$ and $\{\eta(b_j^R)\}$ gives probability distribution of the mixed state $\{|a_j^M\rangle\}$ and $\{|b_j^R\rangle\}$ in $\rho_\infty^M(20')$ and ρ_∞^R of Eqs.(20') and (22'), respectively. Further, we calculate

$$\begin{aligned}\eta(b^R)&=\sum_{a,b^S}|d(a,b_j^R,b^S)|^2\\&=\sum_{a,b^S}|\sum_{a^{N'},b',a^M}W_+^*(a,b^R,b^S;a^M,a^{N'},b')\\&\qquad f(a^M)g(a^{N'},b^{S'})h(b^{R'})|^2\\&=|f(b^R)|^2w_0\ ,\end{aligned}$$

where it should holds that $w_0=1$, since, we have from normalization, Eq.(16), and unitarity, Eq.(26), of W_+^*,

$$\sum_{a^M}|f(a^M)|^2=1, \qquad \sum_{a^M}|f(a^M)|^2w_0=1,$$

and w_0 is independent of a^M, and hence

$$\eta(b^R)=|f(b^R)|^2. \quad (27)$$

We start from $t=0$, where $\rho^M(0)$ and $\rho^R(0)$ is given by pure state of Eqs.(19) and (21) and A^M and B^R takes no definite

value except the case where the state consists of one eigenstate $|a_j^M\rangle$ and $|b_k^M\rangle$, respectively. As $t\to\infty$ $\rho^M(t)$ and $\rho^R(t)$ tends to the asymptotic form ρ^M_∞ and ρ^R_∞ given by mixture, Eqs.(20')~(22η'), with probablity distribution $\{\xi\}$ and $\{\eta\}$, respectively. Specifically the set of eigenvalues b_j^R of B^R is realized in the apparatus S^{II} with probability $\eta = |f(b^R)|^2$ related to the amplitude $f(a^M)$ of the eigenstate $|a^M\rangle$ of observable A^M of S^I. Thus in our scattery of S^I by S^{II} the measurement of A^R is attained by the apparatus S^{II} which records values of B^R corresponding to those of A^M. One see that the whole story is in accordance with Born's ansatz of probability distribution in general quantum mechanical measurement.

Discussion

In the former half of the present letter we give the recognition that the reduction process of state in the subspaces $\mathcal{H}^M$ and $\mathcal{H}^S$ is, as explained elaborately, the inherent property of the total system S. Thus the problem of the reduction of state is separated from the problem to determine $\{\eta(b^R)\}$ of Eq.(27) by the observer in the measurement, which should be discussed in various aspects. The latter part given for the formulation of the measuring process is owing much to works of Maki[3] and Fine[4]. In the present study of measurement only the observables A^M and B^R commutable with H^I and H^{II} are considered, whereas Born's

ansatz covers all observables, and further the relation between W_+ satisfying Eq.(24) and the Hamiltonian H' is not clear. These would be the subject of the future study.

Various studies on measurement are seen using measuring apparatus composed of an infinite number of particles[3),5)] as well as a finite number cases[3),7)]. The relation between them also would be clarified in the future[7)].

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