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PROBABILISTIC AND STATISTICAL ASPECTS OF QUANTUM THEORY

A. S. HOLEVO

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PREFACE

The mathematical language of modern quantum mechanics is operator theory. Operators play there a role similar to functions in classical mechanics, probability theory and statistics. However, while the use of functions in classical theories is founded on premises which seem intuitively quite clear, in quantum theory the situation with operators is different.

Historically the ‘matrix mechanics’ of Heisenberg and the ‘wave mechanics’ of Schrödinger which gave rise to the contemporary form of quantum theory, originated from ingenious attempts to fit mathematical objects able to reflect some unusual (from the macroscopic point of view) features of microparticle behaviour—in particular, a peculiar combination of continuous and discrete properties. The ‘probabilistic interpretation’ developed later by Born and others elucidated the meaning of operator formalism by postulating rules connecting mathematical objects with observable quantities. However a good deal of arbitrariness remained in these postulates and the most convincing argument for quantum-theoretical explanations was still the ‘striking’ coincidence of theoretical predictions with experimental data. This state of affairs gave rise to numerous attempts, on one hand, to find classical alternatives to quantum theory which would give an equally satisfactory description of the experimental data, and on the other hand, to find out physical and philosophical arguments for justifying the inevitability of the new mechanics.

Notwithstanding the impressive philosophical achievements in this field there was and still is a need for the structural investigation of quantum theory from a more mathematical point of view aimed at elucidating the connections between the entities of the physical world and the elements of operator formalism. The present book is essentially in this line of research opened by the classical von Neumann’s treatise “Mathematical Foundations of Quantum Mechanics”. However it differs from most subsequent investigations by the strong emphasis on the

statistical rather than 'logical' essence of quantum theory; it gives an account of recent progress in the statistical theory of quantum measurement, stimulated by the new applications of quantum mechanics, particularly in quantum optics.

The first three chapters give an introduction to the foundations of quantum mechanics, addressed to the reader interested in the structure of quantum theory and its relations with classical probability. In spite of the mathematical character of the presentation it is not 'axiomatic'. Its purpose is to display the origin of the basic elements of operator formalism resting, as far as possible, upon the classical probabilistic concepts.

The present revision is not an end in itself—it emerged from the solution of concrete problems concerning the quantum limitations to measurement accuracy, arising in applications. So far there has been no general approach to such kind of problems. The methods of mathematical statistics adapted for classical measurements required radical quantum modification. The last chapters of the book are devoted to the recently developed quantum estimation theory, which is an analog of the corresponding branch of mathematical statistics.

We now give a more detailed account of the contents of the book. In Chapter I the general concepts of state and measurement are introduced on the basis of statistical analysis of an experimental situation. From the very beginning this approach leads to a substantial generalization of the Dirac-von Neumann concept of an observable. Mathematically it is reflected by the occurrence of arbitrary resolutions of identity in place of orthogonal ones (spectral measures) and the repudiation of self-adjointness as an indispensable attribute of an observable. In this way nonorthogonal resolutions of identity like the 'overcomplete' system of coherent states known in physics for rather a long time find their proper place in quantum phenomenology. The new concept of quantum measurement is central for the whole book.

The notion of statistical model exploited in Chapter I is quite general and may find applications different from quantum theory. It gives us a new insight into the still controversial 'hidden variables' problem.

In Chapter II the elements of operator theory in Hilbert space are introduced to provide mathematical background for the subsequent material. As compared to standard presentations relatively much attention is paid to nonorthogonal resolutions of identity and related questions. A novel feature is also the introduction of the \mathcal{L}^2 spaces of

observables associated with a quantum state and playing a role similar to the Hilbert space of random variables with finite second moment in probability theory. These \mathcal{L}^2 spaces give the framework for a calculus of unbounded operators.

Of fundamental importance to quantum theory are groups of symmetries. In Chapter III elementary quantum mechanics is considered from this point of view. An important result of this discussion is the isolation of the notion of covariant measurement which ties physical quantities with certain classes of resolutions of identity in the underlying Hilbert space. In this way we construct quantum measurements canonically corresponding to such quantities as time, phase of harmonic oscillator, angle of rotation and joint measurement of coordinate and velocity. Allowing the broader concept of quantum measurement enables us to resolve old troubles of quantum theory connected with the non-existence of self-adjoint operators having the required covariance properties.

Chapter IV is devoted to a more advanced study of covariant measurements and extreme quantum limits for the accuracy of estimation of physical parameters. The latter problem becomes important in view of the progress in experimental physics. We present a unified statistical approach to 'non-standard' uncertainty relations of the 'angle-angular momentum' type. They appear to be related to the quantum analog of the Hunt-Stein theorem in mathematical statistics. A general conclusion which can be drawn from Chapter IV is that the requirements of covariance and optimality, i.e., extremal quantum accuracy, determine the canonical measurement of a 'shift' parameter, such as angle, coordinate, time, uniquely up to a 'gauge' transformation.

An example of a situation where quantum limitations are important is provided by optical communication. As is known "quantum noise" distorting the signal in the optical range can be much more significant than the thermal background radiation. As in ordinary communication theory the problem of signal estimation arises, but now it requires a specifically quantum-theoretic formulation and solution.

Chapter V is devoted to the so called Gaussian states which, in particular, describe radiation fields in optical communication theory. The presentation is intended to make maximal use of the remarkable parallel with the Gaussian probability distributions. An important role is played here by quantum characteristic functions.

In Chapter VI the general inequalities for the measurement mean-

square errors are derived, which are quantum analogs of the well-known Cramer–Rao inequality in mathematical statistics. The best unbiased measurements of the mean-value parameters of a Gaussian state are described.

Needless to say, the present book cannot (and is not intended to) replace the standard textbooks on quantum mechanics. Most of the important topics, such as perturbation theory, are apparently out of its scope. Nor does it pretend to give a full account of quantum measurements. We have discussed only those problems which concern measurement statistics and do not require consideration of state changes after measurements. The references to the relevant work on ‘open’ quantum systems and quantum stochastic processes can be found in the comments.

The author’s intention was to write a book accessible to a wide circle of readers, both mathematicians and physicists. As a result, the presentation, being in general mathematical, is rather informal and certainly not ‘the most economic’ from a mathematical point of view. On the other hand, it neglects some subtleties concerning measurability etc. As a rule a rigorous treatment can be found in the special papers referred to. The necessary background for the whole material is knowledge of fundamentals of the probability theory. Mathematically the most elementary is Chapter I which uses mainly finite-dimensional linear analysis. The functional analytic minimum is given in Sections 1–6 of Chapter II, and a mathematically educated reader may just glance over it. On the other hand, a reader familiar with quantum mechanics can omit the detailed discussion of such topics as harmonic oscillators and spin in Chapter III, included to make the presentation self-contained, and concentrate on less familiar things.

The Dirac notation is used intensively throughout the book but with round brackets for the inner product as accepted in mathematical literature. The angle brackets, associated with the averaging symbol in statistical mechanics, are reserved for the different inner product defining the correlation of a pair of observables. To denote a quantum state as well as its density operator we use the letter S (not the usual ρ) allied to the notation P for the classical state (probability distribution). The double numeration for formulas and theorems is accepted within each chapter; references to items from other chapters also contain the number of the chapter.

The author’s thanks are due to Prof. D.P. Želobenko and the late Prof.

Yu.M. Shirokov who read the manuscript and made useful comments.

In translating the book the author took the opportunity of improving the presentation which concerned mainly Chapters III, IV. Few references were added. The author is grateful to Prof. Yu.A. Rozanov and Prof. P.R. Krishnaiah for providing the opportunity of translating this book for *North-Holland Series in Statistics and Probability*.

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STATISTICAL MODELS

1. States and measurements

Any theoretical model ultimately relies upon experience—the framework for a model is constituted by the array of experimental data relevant to the study of the object or phenomenon. Let us consider a very schematic and general description of an experimental situation and try to trace back the emergence of the principal components of a theoretical model.

The fundamental reproducibility condition requires at least in principle the unrestricted possibility of repetition of an experiment. Considering a sequence of identical and independent realizations of some experimental situation one always sees that practically the data obtained are not identically the same but subject to random fluctuations, the magnitude of which depends on the nature of the experiment and of the object under investigation.

There exist large classes of phenomena, for example, planetary motion or constant electric currents, in which these random fluctuations can be both practically and theoretically ignored. The corresponding theories—classical celestial mechanics and circuit theory—proceed from the assumption that the parameters describing the object can be measured with arbitrary accuracy, or, ultimately, with absolute precision. In such cases the object is said to admit deterministic description. Such a description, however self-contained it seems to be, is usually only an approximation to reality, valid in so far as it agrees with the experience.

The fruitfulness of the deterministic point of view in the classical physics of the 18–19th centuries gave rise to the illusion of its universality. However, with the penetration of experimental physics into the atomic domain the inapplicability of the classical deterministic approach and the relevance of statistical concepts in this domain became

more and more evident. The behaviour of atomic and subatomic objects is essentially probabilistic; an ordinary way to extract information about them is to observe a large number of identical objects to obtain statistical data. The interested reader can find about the experimental evidence for statistical description in microphysics, which is now generally accepted, in any contemporary tract on quantum physics.

The possibility of statistical description presumes the fulfilment of the following statistical postulate, incorporating the previous requirement of reproducibility: *the individual results in a sequence of identical, independent realizations of an experiment may vary, but the occurrence of one or another result in a long enough sequence of realizations can be characterized by a definite stable frequency*. Then, abstracting from the practical impossibility of performing an infinite sequence of realizations, one can adopt that the results of the experiment are theoretically described by the *probabilities* of various possible outcomes. More precisely, we must distinguish an individual realization of the experiment which results in some concrete outcome from the experiment as a collection of all its possible individual realizations. In this latter sense, the final results of the experiment are theoretically described by probability distributions. The deterministic dependence of the experimental results on the initial conditions is replaced by the statistical one: the function of the initial data is now the output probability distribution.

As an example consider a beam of identical independent particles which are scattered by an obstacle and then registered by a photographic plate, so that an individual particle hitting the plate causes a blackening of the emulsion at the place of the collision. Exposing a beam which consists of a large enough number of particles will result in a photographic picture giving the visual image of the probability density for the point at which an individual particle hits the plate. The natural light is the chaotic flow of an immense number of specific corpuscles—the photons. The well-known optical diffraction pictures present the images of the probability density of an individual photon scattered by an aperture.

Of course, the statistical description is by no means subject to atomic or subatomic phenomena. When investigating a system which consists of a large number of components (e.g., a gas or a liquid) the experimenter has at his disposal only a very restricted set of parameters to vary (say, pressure, volume or temperature). An immense number of parameters, giving a detailed description for the behaviour of subsystems of the system

are out of control; their uncontrolled changes may substantially influence the results of measurements. A study of these fluctuations is essential for understanding the mechanisms of phenomena occurring in large systems. The statistics of observations is most important in problems of information transmission, where the fluctuations in the physical carriers of information are the source of various 'noises' distorting the signal.

The statistical approach is often appropriate in biometrical research. In studying the effect of a medicine, a physician can take into account a limited number of parameters characterizing his patients such as age, blood group etc. However the effect of the treatment in each individual case will depend not only on these 'integral' parameters, but also on a number of other internal factors which were not, or could not be taken into account. In such cases the dependence of the effect on the 'input parameters' is not deterministic and often can be successfully described statistically.

These two examples show that the origin of fluctuations in results of measurement may be uncertainty in the values of some 'hidden variables' which are beyond the control of the experimenter. The nature of randomness in atomic and subatomic phenomena is still not so clear, though the relevance of the statistical approach is confirmed here by more than half a century experience of applications of quantum theory. We shall not touch here the issues concerning the nature of randomness in microscopic phenomena, but we shall comment on some mathematical aspects of the relevant 'problem of hidden variables' in Section 7. The main attention we shall pay here to the consequences of the statistical postulate irrespective of the nature of the object under consideration. We shall see that already on this very general level the notions of the state and the measurement arise, which play a basic role, in particular, in quantum theory.

In any experiment one can distinguish the two main stages. At the first stage of *preparation* a definite experimental set-up is settled, some initial conditions or 'input data' of the experiment are established. At the following stage of the experiment the 'prepared' object is coupled to a measuring device, resulting in these or the other output data (Fig. 1).

Conventionally, one may conceive the object as a 'black box', at the 'input' of which one can impose some initial conditions \tilde{S} . After the object has been definitely prepared, some measurement is performed, resulting in the output data u . These data may be of arbitrary nature; they may be discrete if the measuring device registers the

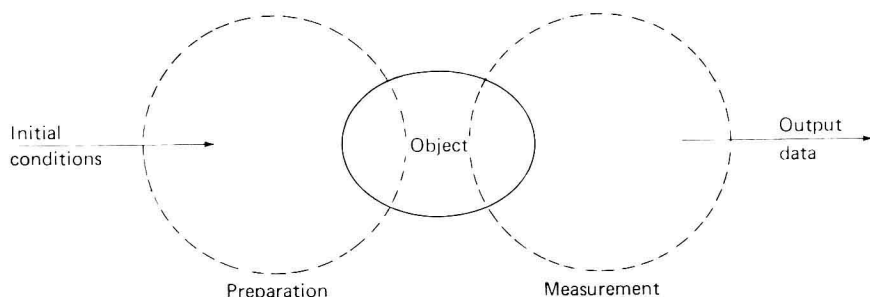


Fig. 1.

occurrence of some events, e.g., the presence or absence of some particles; they may be represented by a scalar or vector quantity, if the measuring device has one or several scales; at last the result of a measurement may be a picture of a whole trajectory, as in a bubble chamber. To give a uniform treatment for all these possibilities we assume that the outcomes of measurement form a measurable space U with the σ -field of measurable subsets $\mathcal{A}(U)$. In the concrete cases we shall deal with, U will be usually a domain in the real n -dimensional space \mathbb{R}^n with the Borel σ -field generated by open sets (or by multi-dimensional intervals). A measurable subset $B \subset U$ corresponds to the event: the result of the measurement u lies in B .

According to the statistical postulate, a result of an individual measurement can be considered as a realization of a random variable taking values in U . Let $\mu_{\tilde{S}}(du)$ be the probability distribution of this random variable. The subscript \tilde{S} reflects the dependence of the statistics of the measurement upon the preparation procedure, i.e., the initial conditions of the experiment, so that

$$\mu_{\tilde{S}}(B) = \Pr\{u \in B \mid \tilde{S}\}, \quad B \in \mathcal{A}(U)$$

is the conditional probability of obtaining a result $u \in B$ under the initial