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Held 31 August through 4 September 1977

Per-Olov Löwdin / Jean-Louis Calais / Osvaldo Goscinski

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Preface

The 500th anniversary of the University of Uppsala was celebrated throughout the year 1977 primarily by conducting a large number of symposia in various disciplines. The contribution of the Uppsala Quantum Chemistry Group to this program was a symposium held from August 31 to September 4, 1977 with the theme, "Quantum Chemistry—A Scientific Melting Pot."

This symposium attracted both quantum chemists and a number of specialists in neighboring fields such as astronomy, molecular spectroscopy, solid state physics, surface physics, quantum biology; and, last but not least, it included a number of philosophers who have made important contributions to the epistemology of quantum mechanics. This was particularly fitting for a scientific program commemorating another anniversary: Quantum Chemistry's first 50 years.

The present supplement to the *International Journal of Quantum Chemistry* contains papers submitted in connection with the symposium. They have been arranged essentially according to the order of the sessions, which was as follows: Philosophical Aspects of Quantum Chemistry; Some Current Methods of Quantum Chemistry; Time Dependence; Some Basic Concepts in Quantum Chemistry; Interaction between Quantum Chemistry and Neighboring Fields; and Biology and Quantum Chemistry.

We would like to express our deep gratitude to the Nobel Institute in Physics, The Swedish Natural Sciences Research Council, and the University of Uppsala for the financial support that made this symposium possible.

PER-OLOV LÖWDIN
JEAN-LOUIS CALAIS
OSVALDO GOSCINSKI

List of Participants

Jacob Aboagye
Department of Physics
University of Cape Coast
Cape Coast, Ghana

Noor Ahmad
Institute of Physical Chemistry
University of Peshawar
Peshawar, Pakistan

José Luiz Alves
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Muhammad Anwar
International Seminars in Physics
and Chemistry
Uppsala University, Box 530
S-751 21 Uppsala, Sweden

Ad van der Avoird
Institute of Theoretical Chemistry
University of Nijmegen
Toernooiveld
Nijmegen, The Netherlands

Børge Bak
Kemisk Laboratorium V
H. C. Ørsted Institutet
Universitetsparken 5
DK-2100 København Ø, Denmark

Gian Luigi Bendazzoli
Istituto di Chimica Fisica e
Spettroscopia
Università degli Studi
Viale Risorgimento 4
I-40136 Bologna, Italy

Manuel Berrondo
Instituto de Física
Universidad Nacional Autonoma de
Mexico
Apartado Postal 20-364
Mexico 20, D.F., Mexico

André Bieber
Centre de Recherches sur les
Macromolécules
6, rue Boussingault
F-67083 Strasbourg Cedex, France

Gerhard Bieri
Fysik I
Kungliga Tekniska Högskolan
Fack
S-100 44 Stockholm 70, Sweden

Laurence Boyle
University Chemical Laboratory
University of Kent at Canterbury
Canterbury, Kent CT2 7NH,
England

Manuel Braga
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Erkki Brändas
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Mario Bunge
Foundations and Philosophy of
Science Unit
McGill University
3479 Peel Street
Montreal, Quebec H3A 1W7,
Canada

Edward Burke
Department of Physics
Adelphi University
Garden City, NY 11530, U.S.A.

Jean-Louis Calais
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Jacques Calazans
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Sylvio Canuto
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

Ana M. Cetto
Instituto de Física

U.N.A.M.
Apartado Postal 20-364
Mexico 20, D.F., Mexico

ARNE CLAESSON
Department of Theoretical Physics
University of Umeå
S-901 87 Umeå, Sweden

PIERRE CLAVERIE
Laboratoire de Chimie Quantique
Institut de Biologie Physico-Chimique
13, rue Pierre et Marie Curie
F-75005 Paris, France

LEON COMBS
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

SIMON DINER
Laboratoire de Chimie Quantique
Institut de Biologie Physico-Chimique
13, rue Pierre et Marie Curie
F-75005 Paris, France

GUIDO FANO
Istituto di Fisica "A. Righi"
Via Irnerio 46
I-40100 Bologna, Italy

INGA FISCHER-HJALMARS
Institute of Theoretical Physics
University of Stockholm
Vanadisvägen 9
S-113 46 Stockholm, Sweden

SERAFIN FRAGA
Division of Theoretical Chemistry
Department of Chemistry
University of Alberta
Edmonton, Alberta T6G 2G2, Canada

PIOTR FROELICH
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

ARTHUR FROST
P.O. Box 1605
Sedona, AZ 86336, U.S.A.

KENICHI FUKUI
Department of Hydrocarbon Chemistry
Kyoto University
Kyoto, Japan

SHREEDHAR RAMCHANDRA GADRE
Hall IV/H201
Indian Institute of Technology
Kanpur, 208016, India

CLAUDE GEORGE
Service de Chimie Physique II
Université Libre de Bruxelles
Campus Plaine U.L.B., C.P. 231
B-1050 Bruxelles, Belgium

OSVALDO GOSCINSKI
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

ANTE GRAOVAC
Institute "R. Bosković"
P.O.B. 1016
YU-41001 Zagreb, Croatia, Yugoslavia

EMIL AMITAI HALEVI
Department of Chemistry
Technion—Israel Institute of Technology
Haifa, Israel

MICHAEL HEHENBERBER
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

FRANK HERMAN
IBM Research Laboratory, K33/281
San José, CA 95193, U.S.A.

ZELEK HERMAN
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

E. C. HERRMANN
c/o Schering AB
Fachbereich Physikochemi und Information
Department Spektrometrie und Quantenchemie
Postfach 650311, D-1000 Berlin 65, West Germany

SAMSON HETTIARACHCHI
Department of Chemistry
University of Sri Lanka
Colombo Campus, Box 1490
Colombo 3, Sri Lanka

LATEEF HUSSAIN
Department of Physics

University of Ibadan
Ibadan, Nigeria

SIGERU HUZINAGA
Department of Chemistry
University of Alberta
Edmonton, Alberta, Canada

LAURENS JANSEN
Battelle Memorial Institute
Division Internationale
7, Route de Drize
CH-1227 Carouge Genève, Switzerland

HERBERT JEHLE
Institut f. Theoretische Physik
University of Munich
Theresienstrasse 37, III
Munich 2, West Germany

HERBERT JONES
Florida A&M University
P.O. Box 981
Tallahassee, FL 32307, U.S.A.

ANDRÉS KALNAY
Université de Paris VI
Laboratoire de Physique Théorique
Institute Henri Poincaré
11, rue Pierre et Marie Curie
F-75231 Paris Cedex 05, France

SUNGZONG KANG
Department of Pharmacology
Mount Sinai School of Medicine of the City University of New York
Fifth Avenue and 100th Street
New York, NY 10029, U.S.A.

SVEIN OTTO KANSTAD
Norwegian Defence Research Est.
Division for Electronics
P.O. Box 25
N-2007 Kjeller, Norway

DAVID NJOROGE KARIUKI
Chemistry Department
University of Nairobi
P.O. Box 30197
Nairobi, Kenya

ISABELLA KARLE
Laboratory for the Structure of Matter
Naval Research Laboratory
Code 6030
Washington, DC 20375, U.S.A.

JEROME KARLE
Laboratory for the Structure of Matter
Naval Research Laboratory
Code 6030
Washington, DC 20375, U.S.A.

GÖRAN KARLSSON
Institute of Theoretical Physics
Uppsala University
Trädgårdsgatan 18
S-752 20 Uppsala, Sweden

ARNOLD KARO
Lawrence Livermore Laboratory
University of California
P.O. Box 808
Livermore, CA 94550, U.S.A.

JAIME KELLER
Depto. de Química Teórica
División de Estudios Superiores
Facultad de Química
U.N.A.M.
Apartado Postal 70-528
Mexico 20, D.F., Mexico

WLODZIMIERZ KOŁOS
Quantum Chemistry Group
University of Warsaw
ul. Pasteura 1
PL-02-093 Warsaw, Poland

JAROSLAV KOUTECKÝ
Freie Universität Berlin
Fachbereich 21, WE 3
D-1000 Berlin, West Germany

SVEN LARSSON
Department of Quantum Chemistry
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

DAVID LAYZER
Department of Astronomy
Harvard University
60 Garden Street
Cambridge, MA 02138, U.S.A.

J-M. LÉVY-LEBLOND
Université Paris VII
Laboratoire de Physique Théorique et Hautes Energies
Tour 33—1er étage
2, Place Jussieu
F-75221 Paris Cedex 05, France

A. LIMA-DE-FARIA
Institute of Molecular Cytogenetics

University of Lund
Tornavägen 13
S-223 63 Lund, Sweden

JAN LINDERBERG
Department of Chemistry
Aarhus University
DK-8000 Aarhus C, Denmark

EINAR LINDHOLM
Fysik I
Kungliga Tekniska Högskolan
Fack, S-100 44 Stockholm, Sweden

PETER LINDNER
Department of Quantum Chemistry
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

JENS LOTHE
Fysisk Institutt
Universitetet i Oslo
Postboks 1048, Blindern
Oslo 3, Norway

WILLIAM LOW
The Hebrew University
Jerusalem, Israel

STIG LUNDQVIST
Institute of Theoretical Physics
University of Göteborg, Fack
S-402 20 Göteborg 5, Sweden

INGEMAR LUNDSTRÖM
Research Laboratory of Electronics
Chalmers University of Technology, Fack
S-402 20 Göteborg 5, Sweden

STEN LUNELL
Department of Quantum Chemistry
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

PER-OLOV LÖWDIN
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

ROLF MANNE
Department of Chemistry
University of Bergen
N-5014 Bergen, Norway

A. D. MCLACHLAN
MRC Laboratory of Molecular Biology
Hills Road
Cambridge, CB2, 2QH, England

INGRID MORING
Institute of Physical Chemistry
Uppsala University, Box 532
S-751 21 Uppsala, Sweden

ROBERT NESBET
IBM Research Laboratory K34/281
San Jose, CA 95193, U.S.A.

CEFERINO OBCEMEA
Physics Department
De la Salle University, Box 3819
Manilla 2800, Philippines

KIMIO OHNO
Department of Chemistry
Faculty of Science
Hokkaido University
Sapporo 060, Japan

RUBEN PAUNCZ
Department of Chemistry
Technion-Israel Institute of Technology
Haifa, 32000, Israel

T. E. PEACOCK
Chemistry Department
University of Queensland
St. Lucia, Queensland, Australia 4067

L. DE LA PEÑA-AUERBACH
Instituto de Física
U.N.A.M.
Apartado Postal 20-364
Mexico 20, D. F., Mexico

PIET PHARISEAU
Seminarie voor Theoretische Vaste Stof- en Lage Energie Kernfysica
Rijksuniversiteit Gent
Krijgslaan 271, Gebouw S9
B-9000 Gent, Belgium

ALEJANDRO PISANTY
Universidad Nacional Autonoma de México
Mexico, Mexico

ENRIQUE POULAIN
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

ILYA PRIGOGINE
Chimie Physique II

Université Libre de Bruxelles
Campus Plaine U.L.B., C.P. 231
B-1050 Bruxelles, Belgium

EDUARDO SANHUEZA
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

LUT SCHEIRE
Seminarie voor Theoretische Vaste Stof- en Lage Energie Kernfysica
Rijksuniversiteit Gent
Krijgslaan 271/S9
B-9000 Gent, Belgium

J. ROBERT SCHRIEFFER
Department of Physics
University of Pennsylvania
Philadelphia, PA 19174, U.S.A.

JACK SIMON
Chemistry Department
University of Utah
Salt Lake City, UT 84112, U.S.A.

VIPIN SRIVASTAVA
Department of Physics
Heriot-Watt University
Riccarton, Currie
Edinburgh EH14 4AS, Scotland

SHOU-SIN SUNG
Centre National de la Recherche Scientifique
7, Parc des Marronniers
F-91600 Savigny-sur-Orge, France

ABDUS SATTAR SYED
Industrial Physics Division
GCSIR Laboratories
Dhanmondi
Dacca-5, Bangladesh

ALBERT SZENT-GYÖRGYI
National Foundation for Cancer Research
P.O. Box 187
Woods Hole, MA 02543, U.S.A.

ORLANDO TAPIA
Centre de Mécanique Ondulatoire Appliquée
23, rue du Maroc
F-75019 Paris, France

COLIN THOMSON
Chemistry Department
University of St. Andrews
Purdie Building
St. Andrews KY16 9ST, Scotland

ERIK THULSTRUP
Department of Chemistry
Aarhus University
DK-8000 Aarhus C, Denmark

ULF WAHLGREN
Inst. för vatten-och luftvårdsforskning
Box 21060
S-100 31 Stockholm, Sweden

BRIAN WEINER
Quantum Chemistry Group
Uppsala University, Box 518
S-751 20 Uppsala, Sweden

GUY WOOLLEY
Department of Physics
Theory of Condensed Matter
Cavendish Laboratory
University of Cambridge
Madingley Road
Cambridge CB3 0HE, England

SHI-YU WU
Department of Physics
University of Louisville
Louisville, KY 40208, U.S.A.

WOLFGANG YOURGRAU
University of Denver
2329 South High Street
Denver, CO 80210, U.S.A.

LEIF ÅSBRINK
Fysik I
Kungliga Tekniska Högskolan, Fack
S-100 44 Stockholm, Sweden

YNGVE ÖHRN
Quantum Theory Project, Williamson Hall
University of Florida
Gainesville, FL 32611, U.S.A.

Contents

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Quantum Mechanics and Measurement

MARIO BUNGE
Foundations and Philosophy of Science Unit, McGill University, Montreal H3A 1W7, Canada

Abstract

The role of the apparatus and the observer in the foundations of elementary quantum mechanics is examined. To this end some of the typical formulas of existing theory are analyzed: the Schrödinger equation, the eigenvalues equation, the Born principle, and the Heisenberg inequalities. No variables representing either instruments or observers are found in the above formulas; they are completely general and concern exclusively a microentity in an unspecified external field.

Next the quantum theories of measurement and their relevance to the question of determinism are analyzed. It is shown that there can be no purely quantum-mechanical theory of measurement because of the macroscopic nature of measuring instruments. It is also shown that the existing theories are not testable, hence not scientific in the usual sense.

The general conclusion is that the interpretation of quantum mechanics in terms of measurement operations, i.e., the Copenhagen interpretation, is inconsistent with the mathematical formalism of the theory. An alternative interpretation, in terms of exclusively physical entities and properties, is advanced and discussed. Unlike the former interpretation, the alternative one complies with the requirement of objectivity.

1. Introduction

Quantum mechanics and quantum electrodynamics were created during the heyday of logical empiricism (or positivism). This philosophy is phenomenalist and operationalist: it holds that it makes sense to speak of observations or measurements only; that science does not study things in themselves but phenomena, i.e., whatever facts appear to some human observer; and that every scientific concept ought to be defined in terms of scientific operations such as weighing and computing. The holy writ of the new credo was Bridgman's popular book [1].

Logical empiricism was not just one more philosophical doctrine, it was the scientist's philosophy between the two world wars. Therefore it was inevitable that this philosophy should find its way into the very foundations of the quantum theories. One result of this symbiosis is that we are still debating such foundations with ideological fervor. Another is that the philosophically naive physicist, as well as the scientifically naive philosopher, tend to accept the positivist philosophy inherent in the textbook formulations of the quantum theories more gullibly than anything else. And yet that philosophy goes against the grain of physics, which is supposed to account for the physical world in strictly physical terms rather than in terms of human operations.

It is of course possible to dissociate the quantum theories from logical empiricism. The advantage of such a divorce is that it frees physics from the subjectivist, hence nonphysical, traits of logical empiricism [2–3]. The most general and rigorous way of separating the scientific grain from the philosophical

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chaff of a theory is to axiomatize it in the most parsimonious possible way, i.e., without reference to things, events or procedures that have no counterpart in the mathematical formalism. For example, if a certain property of a physical system is the same relative to all reference frames of a certain kind, we just say so, instead of stating that the property looks the same to all observers, first, because a physical theory is not about observers; second, because the property in question may not be observable; third, because—as any psychologist will attest—one and the same stimulus may be perceived differently by different observers and even by one and the same observer when in different internal states. In short, if we wish to uncover the genuine referents of a scientific theory without being misled by any preconceived philosophy, we had better axiomatize the theory.

The axiomatize-and-cleanse operation has been performed on a number of physical theories, among them the two relativities and elementary quantum mechanics [3]. However, the quickest and pedagogically most effective way of eliminating nonphysical elements from a physical theory is to analyze the structure of some typical concepts and formulas of the theory and show that they warrant no reference to extraphysical entities. This I propose to do in the present paper in the case of elementary quantum mechanics.

2. The Phenomenalist Thesis

Most textbooks on quantum mechanics adopt, and most physicists pay at least lip service to, the so-called Copenhagen interpretation, proposed by Bohr and others [4–9]. The nucleus of this doctrine is the following

Phenomenalist Thesis

The physical object has no existence independent from the subject of knowledge or observer. What does exist is a sort of sealed unit composed by the observer, his means of observation, and the observed object. The distinction between the three components of this system is not unambiguous and objective but is left to the observer, who may merge object and apparatus or else regard the latter as a continuation of himself. Consequently every statement about an object must also refer to the way of observing it. Quantum mechanics complies by design with this requirement: every formula of it concerns some experimental situation.

The phenomenalist thesis looks plausible in the case of experimental physics, since every experimentalist deals, in fact, with some object assisted by observation or instruments of measurement. However, the experimenter strives to find out what part of the behavior of his object is an artifact, i.e., a result of his intervention. For example, he will avoid direct contact between his own body and the object when measuring the temperature of the latter.

Of course every statement made by the experimental physicist will make some reference to the means and the technique of observation or measurement. However this is not because the physicist conjures up all the events he observes. On the contrary, his reference to the mode of observation is intended to reassure his readers, persuading them that things are really thus and not simply appearances or phenomena that would disappear with a different observer or a different technique. In sum, the experimenter knows that his actions could disturb the object and precisely because of this he tries to minimize such a perturbation or at least to correct for it with the help of theory in order to supply objective results, i.e., results that are observer-invariant. In other words, the experimenter, regardless of his explicit philosophy, behaves as an objectivist. If he did not he would be regarded as incompetent.

Consequently phenomenalism is false in the domain of experimental physics. However, the defenders of the Copenhagen interpretation claim that it holds not only in that domain but also in theoretical physics: in fact they demand that every theoretical formula be read in terms of observation or measurement operations. Let us see whether this is possible. To this end we shall examine a few typical and basic formulas of elementary quantum mechanics.

3. The Schrödinger Equation

The Schrödinger equation, in some form or other, is one of the two basic law statements of quantum mechanics. Hence it is employed in the study of the constitution and evolution of any microphysical entity. Let us examine it in the simplest case, which is that of a structureless thing of mass m and electric charge e in an external macroscopic field represented by a four vector potential $\langle A_0, A\rangle$. In this case the equation is

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi \tag{1}$$

where

$$H=\frac{1}{2m}\left(p-\frac{e}{c}A\right)^2+eA_0, \qquad p=\frac{\hbar}{i}\nabla \tag{2}$$

In the absence of an external field, $A_0=A=0$, and the equation reduces to

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi \tag{3}$$

whose elementary solution is of the form

$$\psi(x,t)=u(x)\cdot e^{-iEt/\hbar}, \qquad E\in\mathbb{R} \tag{4}$$

where the amplitude u satisfies the time-independent equation

$$Eu=-(\hbar^2/2m)\nabla^2 u \tag{5}$$

A particular solution of this last equation is

$$u(x)=a\cos(kx+b) \tag{6}$$

where a, b, and k are real numbers. The corresponding value of the energy is $E=\hbar^2k^2/2m$.

No matter how hard and long you stare at the above well known formulas you won't detect any functions concerning measurement apparatus, let alone observers. That is, both H and ψ refer exclusively to the microentity in question (e.g., an electron) immersed in an external field that may well be nil. The mathematical formalism does not tolerate the smuggling in of any apparatus or observers. If still in doubt draw the list of the basic variables and constants occurring in the Schrödinger equation:

Symbol	Concept	Referent
x	Point in space	Space
t	Instant of time	Time
m	Mass of particle	Particle
e	Charge of particle	Particle
p	Momentum of particle	Particle
$\langle A_0, A\rangle$	Four-potential	External field
$\hbar$	Planck's constant	—

Consider next the case of an electron in the electrostatic field of a proton, and model the latter as a classical point particle. In this case, we set $A_0 = e^2/r$, $A = 0$ in Eq. (2), where r is the distance from the proton. The state function ψ is best expressed as a function of the spherical coordinates with center at the proton. And the formula for the discrete energy levels is $E_n = -k/n^2$, where n is a natural number and k the energy of the ground state of the system ($n = 1$).

Nor in this case is it permissible to interpret the results of the calculations in terms of observations, even though the latter are, of course, indispensable to put some of the formulas to the test. In fact, the above formulas contain no features of apparatus or observers: they concern solely an arbitrary hydrogen atom. And this matches the experimental situation, since the spectroscopic measurements that allow us to check the formula for the discrete energy levels of the hydrogen atom do not exert the least influence upon the atoms that emit the light that is being analyzed. For example, the hydrogen atoms in the sun radiate without our permission and without being affected by terrestrial spectrographs. The observer restricts himself to analyzing that light, so that his operations do not influence the emission process. The same holds, of course, for all atoms and molecules: their properties are not explained by the actions of observers. Rather on the contrary, in order to understand the behavior of living beings, in particular physicists, the biologist makes use of physics and, in particular, of quantum mechanics.

Of course one could account for the interaction between a microentity and a measurement apparatus if one wanted to. But then one would have to reformulate the problem *da capo*. In fact the referent would no longer be a free object, as in the case of Eq. (3), nor even an object subjected to a fixed external field that is not influenced by the former, as in the general case of Eq. (2). Instead, the referent would be a system of two interacting components: a microentity and a measurement device. This new system would be represented by a Hamiltonian H that would contain the coordinates and momenta of the two components. We would be facing a different problem altogether. But even in this case it would constitute a physical problem with no reference to observers. We shall come back to this matter in Section 7.

In summary, both the experimentalist and the theorist study things in themselves, such as they exist in nature or in the laboratory; they leave the study of physicists to scientists in other fields, such as biology, psychology, sociology, and operations research. Hence the physicist in his daily work, be it experimental or theoretical, forgets all about the Copenhagen interaction of quantum mechanics. He remembers it only when teaching the general principles of the theory or when philosophizing about them—unless of course his philosophy happens to match his physics.

4. Eigenvalues

A second basic law statement of quantum mechanics is the eigenvalue equation of an arbitrary operator representing a dynamical variable (or rather property)—usually misnamed an "observable." Let A_{op} be an operator representing a property A. It is postulated that A_{op} satisfies an equation of the form

$$A_{op}u_k = a_k u_k \tag{7}$$

where u_k is the kth eigenfunction and a_k the corresponding eigenvalue of A_{op}. (We need not require that A_{op} be Hermitian but, for the sake of simplicity, we assume that the eigenvalues are not degenerate.) The simplest case is that of the linear momentum, represented by $p_{op} = (\hbar/i)\nabla$. Its eigenfunctions are e^{ikx}, where k is an ordered triple of reals and the corresponding momentum eigenvalues are $p_k = \hbar k$. Another example is Eq. (5) which represents the eigenfunctions and eigenvalues of the energy of a free object in a stationary state.

Let us restrict the discussion to the eigenvalues a_k, because it may be argued that the eigenfunctions u_k are only mathematical auxiliaries without any physical meaning. According to the Copenhagen interpretation, a_k is one of the values that an *observer* is bound to find when *measuring* the property A with a suitable instrument—of *any* kind. However, Eq. (7) makes no reference whatever to observers, instruments, measurement techniques, or measurement operations. The only interpretation Eq. (7) tolerates is a strict or literal one, namely, that a_k is *one of the possible values of* A—whether or not we happen to measure it.

Moreover the Copenhagen interpretation of Eq. (7) is at variance with experimental physics, since the results of any precision measurement depend on the measurement method and are rarely exact. (They can be accurate only if the eigenvalues are denumerable and widely separated.) In fact, in general a measured value of A will actually be an interval, namely

$$\text{meas } A = a'_k \pm \varepsilon_k \tag{8}$$

Here a'_k is the arithmetical mean of a set of measured values and ε_k the corresponding relative error, characteristic of the measurement method as well as of k. As a rule the central measured value a'_k differs from the calculated value a_k.

If the Copenhagen interpretation of eigenvalues were taken seriously it would be possible to discontinue all the research projects devoted to the determination of the eigenvalues of dynamical variables, since they would be given *a priori* and accurately by Eq. (7). Fortunately for experimental physicists, that interpretation has no basis in the formulas themselves; it is a philosophical appendix. If still not convinced, take a second look at any eigenvalues equation and try to identify any variables that might be interpreted as representing some features of an experimental device or even of a physicist in charge of such a set up. You won't find them because they are not there: recall that, *by hypothesis*, the A represented by A_{op} is a property of a microentity, not of a macrosystem including experimental equipment and experimentalists.

5. State Function

The third basic principle we shall examine is Born's. It is not a law statement but a semantic postulate, i.e., a hypothesis that assigns a physical interpretation to the state function ψ. (For the concepts of physical interpretation and semantic assumption, see Refs. [10] and [11].) We shall formulate it thus: "Let ψ_a be a solution of the Schrödinger equation for a physical thing a. Then the probability that a be at time t in the region of space comprised between x and $x+\Delta x$ equals $|\psi_a(x, t)|^2 \cdot \Delta x$." The probability in question is a property of thing a; more precisely, it is the probability that a be present in the volume element Δx situated at the tip of the vector x. There is no reference whatsoever to measurements—the more so since the principle is so general that it is stated for arbitrary things with whatever Hamiltonians they may be assigned.

Nevertheless, the Copenhagen version of the principle is different: it states that $|\psi_a(x, t)|^2 \cdot \Delta x$ is the probability of *finding a* in Δx when the position of a is *measured* with *any* position-measurement device whatever. This interpretation is illegitimate because ψ_a does not contain any measuring device coordinates unless the corresponding Hamiltonian H_a contains them. But since the principle is general we do not care what H_a may look like, hence what the corresponding ψ_a may be.

Moreover, it should be obvious that the probability of finding a thing at a given place depends not only on the probability that the thing be there but also on the accuracy of the search instrument and the skill of its operator. If I look for a needle in a haystack without the help of my spectacles, I won't find it. The probability of finding the needle will increase if I put my glasses on, and will be considerably enhanced if I avail myself of a magnet. In sum, the operationalist version of Born's semantic postulate is mathematically illegitimate and empirically false.

If the strict or objectivist version of Born's principle we have proposed is accepted, then the following important point is easier understood. Classical mechanics contains a position coordinate X that assigns each particle, in each