2.452J and 22.572J

QUANTUM THERMODYNAMICS

Instructors:	Gian Paolo Beretta, Room 3-339, Ext. 3-7921 Elias P. Gyftopoulos, Room 24-109, Ext. 3-3804
Class Hours:	Tuesday and Thursday, 1:30 - 3:00, Room 24-502
Course Description:	Non-statistical unified quantum theory of mechanics and thermodynamics for all systems, including a single particle, and all states, including nonequilibrium. Equation of motion for reversible and irreversible processes. Self-contained review of necessary background. Stability of equilibrium states. Applications to fermions, bosons, black-body radiation, electrons in metals, and crystals. Nonequilibrium states. Applications to rate processes, and relaxation phenomena.
Final grade:	40% homeworks 20% mid-term take-home examination 40% final take-home examination

References that will be supplied:

(1) Article by Hatsopoulos and Gyftopoulos on "A Unified Quantum Theory of Mechanics and Thermodynamics."

(2) Article by Park on the "Nature of Quantum States."

(3) Chapter by Beretta on the "Concept of State of an Individual System."

(4) Article by Beretta, Gyftopoulos, Park and Hatsopoulos on "Quantum Thermodynamics. A New Equation of Motion for a Single Constituent of Matter."

(5) Article by Beretta on "Entropy and Irreversibility for a Single Isolated Two-Level System. New Individual Quantum States and New Nonlinear Equation of Motion."

(6) Article by Beretta on the "Proof and Generalization of Onsager's Reciprocal Relations."

Additional references for suggested readings:

(7) "Quantum Mechanics" by Messiah, Wiley.

(8) "The Nature of Physical Reality" by Margenau, Ox Bow.

(9) "Foundations of Physics" by Linsday and Margenau, Ox Bow.

(10) "The Principles of Statistical Mechanics" by Tolman, Dover.

(11) "Some Modern Mathematics for Physicists and Other Outsiders" by Roman, Pergamon.

(12) "The Structure of Scientific Revolutions" by Kuhn, Chicago.

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Quantum Thermodynamics

Outline

Note: No previous exposure to the ideas and mathematics of quantum theory is assumed. All the necessary background will be given in self-contained reviews as and when necessary.

- Brief qualitative review of differences and similarities between various theories of physical phenomena.

- Shortcomings of statistical interpretations of classical thermodynamics.

- Hypotheses regarding the fundamental nature of general thermodynamics, and outline of approach to develop a theory that is consistent with these hypotheses.

- Informal review of classical mechanics.

- Definitions of concepts common to all theories of physical phenomena ("so called" theories of Nature):

  STATICS

    - system
    - physical observable
    - preparation
    - act of measurement of an observable
    - ensemble of identically prepared identical systems
    - value of an observable for a preparation
    - complete characterization of a preparation
    - identical preparations
    - statistical composition of preparations
    - homogeneous preparation
    - homogeneous ensemble
    - heterogeneous preparation
    - heterogeneous ensemble
    - individual state of a system

  DYNAMICS

    - equation of motion

STATISTICS

  - statistical description of incomplete information

- Formal review of classical theory
  - classical mechanics
  - classical statistical mechanics
  - inadequacy and incompleteness of classical mechanics

- Formal review of quantum theory of Nature
  - quantum mechanics
  - quantum statistical mechanics

- Applications of quantum mechanics to
  - one-dimensional harmonic oscillator
  - two-level spin system
  - Bose-Einstein assembly of identical particles: boson field
  - Fermi-Dirac assembly of identical particles: fermion field

- Inadequacy and incompleteness of the quantum mechanical description:
  - adiabatic availability
  - reversibility

- A Quantum Thermodynamic Theory of Nature:
  - generalized, non-statistical individual quantum states
  - entropy of a single system in a generalized individual quantum state
  - dynamics
  - conservation of energy
  - rate of entropy production
  - equilibrium states
  - unstable periodic solutions or limit cycles
  - stable equilibrium states and their uniqueness

- Applications of quantum thermodynamics to individual stable equilibrium states of single isolated elementary systems:
  - Onsager's reciprocal relations
  - Bloch's approximation
  - time evolution of a single two-level system
  - interaction between light and a two-level atom:
    - spontaneous emission
    - resonance fluorescence
    - stimulated absorption and emission
- Application of quantum thermodynamics to nonequilibrium states of isolated composite systems:
  - creation and destruction of "correlations" between interacting elementary constituents
  - "heat interaction" limit
  - Boltzmann's limit
  - Boltzmann's equation

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QUANTUM THERMODYNAMICS

Problem Set #1 Due: March 1, 1984

In a short, schematic and concise summary, review the experimental facts that classical mechanics fails to explain. A list of suggested readings for this purpose is given below.

Your next and main task in this problem is a very difficult one. You should try to identify the essential reasons why classical mechanics cannot contemplate such experimental facts. The experimental evidence should lead you to conclude that some of the fundamental premises of the classical theory of Nature are to be abandoned. Which ones? The experimental evidence should force you to abandon some of the key axioms of your "physical intuition" that are so rooted in your way of thinking only because you have always been given "explanations" based on the classical theory of Nature. What are the axioms that should be abandoned?

This problem requires a great deal of thinking! This is the reason why we give you so much time. Do not expect to find the answers written explicitly in the literature. Do the reading immediately. You will need a couple of weeks to rummage your mind for the answers.

Suggested readings:

Messiah, pp. 3 - 27

Tolman, pp. 180 - 189

Margenau, pp. 307 - 328

Lindsay and Margenau, pp. 387 - 394

CHAPTER 3

CONCEPT OF STATE OF AN INDIVIDUAL SYSTEM

This Chapter presents a general discussion on the concept of state of an individual physical system. In classical theory, this concept is well understood and established, and it plays a fundamental role, since every system is thought of as always being in some definite individual state. We will hypothesize that the concept can play a fundamental role even in quantum theory. We will see that within the formulation of conventional Quantum Statistical Mechanics, the concept of state of an individual system is ambiguously represented. Therefore, we shall conclude that conventional quantum theory is incomplete, since it lacks of a statistical quantum theory representing unambiguously this fundamental concept.

That in conventional Quantum Statistical Mechanics the concept of individual state is ambiguously represented, has been clearly shown by J.L. Park (1968a) (cf. Section 3.2.2). However, Park concluded: "Thus the concept of individual quantum state is fraught with ambiguity and should therefore be avoided in serious philosophical inquiries concerning the nature of quantum theory ... A quantum system should be regarded as never being in any physical state." On the contrary, here we take the position that the concept of individual physical state is fundamental. From this premise, we conclude that what is fraught with ambiguity is not the concept of individual state, but rather the current mathematical formulation of Quantum Statistical Mechanics. Therefore, a serious reformulation of quantum theory is in order.

To pursue this objective, we proceed as follows. We re-examine the concept of state of an individual system independently of the formulations of either conventional quantum theory or the Hatsopoulos-Gyftopoulos unified quantum theory. In the light of this re-examination, we study the physical and statistical formulations of both classical theory and conventional quantum theory and review the ambiguity of conventional Quantum Statistical Mechanics. Finally, we identify necessary conditions that a statistical theory must satisfy in order to achieve an unambiguous representation of the concept of state of an individual system. Using these conditions, we shall be able to show (Chapter 4) that the statistical part of the general quantum theory that we propose is unambiguous.

3.1 RULES OF CORRESPONDENCE AND DEFINITION OF PARADIGM

A scientific theory of nature comprehends three realms:

- the realm of empirical experience (perceptions)
- the realm of theoretical constructs (conceptions)
- the realm of mathematical descriptions (representations).

The essence of the theory resides in the <u>links</u> that it establishes between elements of these three realms.

The links between perceptions and conceptions have been called <u>rules of correspondence</u> by H. Margenau (1950): "The rules of correspondence ... are not eternally grounded in the nature of things, nor are they immediately suggested by sensory experience; they are important parts of every theory of nature and receive their validity from the consistency, the internal neatness and success of the entire explanatory scheme."

The rules of correspondence are normally defined through the mathematical formulation of the theory. Practitioners do not work with perceptions, conceptions and rules of correspondence expressed by verbose locutions. Rather, they work with data, mathematical entities and mathematical relations, i.e. with <u>mathematical descriptions</u> of perceptions, conceptions and rules of correspondence. The mathematical formulation is essential in giving structure to the theory; however, it is not generally unique. A theory might admit of several different, but mathematically equivalent, formulations.

A set of postulates giving (in their unity) structure to a theory, by linking theoretical constructs and rules of correspondence to mathematical descriptors and mathematical relations, can be called the <u>paradigm</u> of the theory. This terminology has been used by T.S. Kuhn (1962), in his book on The Structure of Scientific Revolutions.

The following two Sections are intended to present our general, non-mathematical re-examination of the concept of state of an individual system, based on the definition of the fundamental rules of correspondence between *states*, *homogeneous ensembles* and *homogeneous preparations*.

3.1.1 *States and Homogeneous Ensembles*

As discussed by J.L. Park (1968a), the dominant theme of quantum theory is the necessity to accept that the notion of state involves probabilistic concepts in an essential way. In quantum theory the links between *probabilities* and the empirical world are implicitly defined by established practices of experimental science: the construct probability is linked to the relative frequency in an *ensemble*. Thus the primary connection of a quantum theory of nature to the empirical world is through ensembles.

The purpose of a quantum theory is to regularize purely probabilistic information about the measurement results from a real ensemble of identical systems. A *real ensemble* is either an aggregate of identically prepared systems upon which measurements are performed or a sequence of measurements performed on a single system identically reprepared prior to each measurement, or a combination of both.

An important scheme for the classification of ensembles, expecially emphasized by J. von Neumann (1932), hinges upon the concept of ensemble homogeneity. Given an ensemble it is always possible to conceive of it as subdivided into many subensembles.

Definition: Homogeneous Ensembles

An ensemble is said to be homogeneous if, and only if, every conceivable subdivision results into subensembles all identical to the original.

Here, two ensembles of identical systems are said to be identical if, and only if, the arithmetic mean value of data yielded by measurements of a physical observable on the member systems of one of the two ensembles is equal to the mean value of data yielded by measurements of the same physical observable on the member systems of the other ensemble, for all conceivable physical observables.

Since, by definition, there exist no subdivisions of a homogeneous ensemble into different subensembles, it follows that each individual member system of a homogeneous ensemble has exactly the same intrinsic characteristics as any other member. For, if all member systems did not have the same intrinsic characteristics, then it would be possible to conceive of subdivisions of the ensemble into subensembles that are not identical.

The whole of these intrinsic characteristics, shared by all the individual members systems of a homogeneous ensemble, defines the concept of state of an individual system. In short, a homogeneous ensemble is a real aggregate of identical systems each individually in the same state. Thus, the concept of state acquires physical meaning in its reference to the individual system, though its empirical correspondent is a homogeneous ensemble of identical systems. In fact, we can now express the rule of correspondence linking the physical concept of state to the empirical world:

> The empirical correspondent of the theoretical concept of state of an individual system is a particular kind of ensemble: the homogeneous ensemble.

The power of this rule of correspondence is that it holds with the same fundamental meaning whether the concept of state does or does not involve probabilistic concepts.

3.1.2 Preparations and Ensembles

The act of generating an ensemble consists of the repeated application, on the member systems, of a list of operations called an ensemble preparation scheme or, simply, a preparation. By definition, a preparation must be reproducible in that it must be identically applied to all the members that are to form the ensemble.

It is noteworthy that the act of generating an ensemble, i.e. the concept of preparation, does not necessarily involve an interaction with the member systems of the ensemble itself. It is only the following measurement act which must necessarily involve an interaction. The concepts of preparation and measurement must not be confused (cf. H. Margenau and J.L. Park (1973)). A measurement act is an "operation performed on a system for the purpose of obtaining a numerical value which can, by virtue of the chosen experimental arrangement, be assigned to some definite, nameable observable." A preparation scheme is instead any set of operations selected for the purpose of obtaining a real ensemble of identical systems. Thus a preparation is a scheme to "accept" systems upon which to perform measurements.

Deliberately, the concept of preparation as just defined is quite broad and unrestricted. In general, not all preparations generate homogeneous ensembles. If a preparation generates a homogeneous ensemble, it will be called a homogeneous preparation, otherwise, it will be called a heterogeneous preparation.

It is useful to define a shorthand notation to represent the notion of statistical composition of two, or more, preparation schemes. Let Π_1 and Π_2 represent two preparation schemes for a physical system. If the system is prepared according to scheme Π_1 with statistical weight w_1 or according to scheme Π_2 with statistical weight w_2 (where $w_1 + w_2 = 1$ and $w_1, w_2 > 0$), then we indicate the resulting composite preparation scheme Π by writing

$$\Pi = w_1\Pi_1 + w_2\Pi_2 ,$$

where this expression must be understood exclusively as a shorthand symbolic notation having no other meaning than that just cited. With this notation, and by the definition of homogeneous ensemble, we can give an alternative definition of homogeneous preparation.

Definition: Homogeneous Preparations

> A preparation scheme is said to be homogeneous if, and only if, it cannot result from the statistical composition of different preparation schemes, i.e. if, and only if, any conceivable decomposition of the type

$$\Pi = w_1\Pi_1 + w_2\Pi_2 \quad \text{with} \quad w_1, w_2 > 0$$

implies that $\Pi_1 = \Pi_2 = \Pi$.

As seen in the last Section, to the theoretical concept of state of an individual system is linked the empirical concept of homogeneous ensemble, which, in turn, has been linked here to the theoretical concept of homogeneous preparation. Thus the two theoretical concepts of state and homogeneous preparation are linked through their correspondence with the homogeneous ensemble. If the concept of state of an individual system is fundamental to the particular theory of nature under consideration, then so is the concept of homogeneous preparation. The two concepts are linked one-to-one regardless of the particular mathematical formulation of the theory. This is the conclusion of our re-examination of the concept of state of an individual system. The foregoing analysis has followed closely the analysis of J.L. Park (1968a). However, our conclusion is different, since, as we already discussed, our premise is to consider the concept of individual state as fundamental, regardless of the current formulation of quantum theory.

The importance of the notion of homogeneity, especially in the framework of quantum theory, has been emphasized by several authors, starting with J. von Neumann (1932). G. N. Hatsopoulos and E. P. Gyftopoulos (1976) have proposed a unified quantum theory of Mechanics and Thermodynamics requiring such a notion in a fundamental way. Their theory is concerned exclusively with a description of the homogeneous preparations, i.e. the individual states, of a physical system. The class of individual quantum states which are considered in their unified quantum theory is broader than the class of states considered by von Neumann. To underline this distinction, they adopted the term unambiguous preparation instead of homogeneous preparation. In the general quantum theory that we propose in Chapters 4 and 5, the Hatsopoulos-Gyftopoulos broader class of individual quantum states is maintained; however, also the term homogeneous preparation is maintained, since we have shown that the concept of homogeneity stands independently of the particular theory of nature under consideration.

3.2 PHYSICS VERSUS STATISTICAL PHYSICS

Physics is that branch of the theory of nature which is intended to describe within a causal framework the states of any physical system. Equivalently, the objective of physics is a description of the homogeneous preparations of a general physical system. To the concept of state, the physical theory generally associates a mathematical descriptor, usually an element of a set. The same mathematical entity is thus also associated with the corresponding homogeneous preparation and the corresponding homogeneous ensemble.

Statistical physics is that branch of the theory of nature which is intended to describe within a statistical framework the distributions of states in an ensemble of identical systems each of which individually obeys the laws of the physical branch of the theory. Equivalently, the objective of statistical physics is a statistical description of all possible preparations of a physical system. To the concept of preparation, regardless of its homogeneity, the statistical theory generally associates a mathematical descriptor. The same descriptor is thus associated with the corresponding ensemble.

The typical construction pattern is to first formulate physics and then superimpose a statistical theory to it. Thus, first a physical theory of homogeneous preparations (states) is developed and then a statistical theory is superimposed to it for the description of any preparation, regardless of its homogeneity.

This pattern is exemplified in the next Sections, by reviewing classical theory -- composed of the paradigms of Classical Mechanics and Classical Statistical Mechanics -- and conventional quantum theory -- composed of the paradigms of Quantum Mechanics and Quantum Statistical Mechanics.

Throughout this dissertation, the postulates forming the paradigms of different theories are identified by monograms of the type

PnNT: title

where Pn stands for "Postulate number n", NT stands for the "Name of the Theory" and the title indicates the concept which is being given a mathematical description.

3.2.1 Classical Mechanics vs Classical Statistical Mechanics

The following review serves to clarify the role that the notions introduced in the foregoing discussion play in the classical theory of nature. It is presented here because this is the only complete (i.e., physical and statistical) theory of nature which is free of ambiguities. Its failure is not due to logical inconsistencies within the theory itself, but rather to its inability to regularize a class of empirical phenomena.

CLASSICAL MECHANICS

P1CM: Systems

To every physical system there corresponds a real phase-space Ω whose elements are points with coordinates indicated by $(\underline{q},\underline{p})$.

P2CM: Homogeneous Preparations

To every homogeneous preparation scheme Π for a system, there corresponds a point $(\underline{q},\underline{p})$ in the phase-space Ω of the system.

P3CM: Physical Observables

Some real functions g, h, ... defined on Ω correspond to physical observables of the system. Given an ensemble of identical systems prepared according to the homogeneous scheme Π, with corresponding point $(\underline{q},\underline{p})$ in phase-space, the arithmetic <u>mean</u> <u>value</u> $\overline{g}$ of data yielded by measurements of the observable g is given by the value of the function g at the point $(\underline{q},\underline{p})$, namely,

$$\overline{g} = g(\underline{q},\underline{p}) .$$

P4CM: States

Every individual system is always in a <u>state</u> described by some point $(\underline{q},\underline{p})$ in the corresponding phase-space.

P5CM: Causal Evolution

For every physical system there exists a function h (the Hamiltonian function), defined on the phase-space of the system, which determines the <u>causal</u> <u>evolution</u> of the state descriptor $(\underline{q},\underline{p})$ via the following law (Hamilton's equations of motion)

$$\frac{d\underline{q}}{dt} = \frac{\partial h}{\partial \underline{p}} \qquad \frac{d\underline{p}}{dt} = -\frac{\partial h}{\partial \underline{q}} \quad . \tag{3.1}$$

This formulation of Classical Mechanics is non-orthodox, especially as regards postulates P2CM and P3CM. It has been adopted here in order to maintain a parallel structure with the formulations of other theories considered in the dissertation, and to exemplify the role played by the concept of homogeneous preparation in this well established theory of nature.

CLASSICAL STATISTICAL MECHANICS

P1CSM: Systems

Same as P1CM.

P2CSM: Preparations

To every <u>preparation</u> scheme Π for a system, there corresponds a continuous, real, positive function f defined on the phase-space Ω of the system, satisfying the normalization condition

$$\int_{\Omega} f(\underline{q},\underline{p})d\underline{q}d\underline{p} = 1 . \tag{3.2}$$

The function f is called the <u>density-of-phase function</u>.

P3CSM: Physical Observables

Some real functions g, h, ... defined on Ω correspond to <u>physical observables</u> of the system. Given an ensemble of identical systems prepared according to the scheme Π, with corresponding density-of-phase function f, the <u>expected mean value</u> $\langle \overline{g} \rangle$ of measurements of the observable g is given by the following integral functional

$$\langle \overline{g} \rangle = \int_{\Omega} f(\underline{q},\underline{p})g(\underline{q},\underline{p})d\underline{q}d\underline{p} . \tag{3.3}$$

P4CSM: States

Same as P4CM.

P5CSM: Causal Evolution

Same as P5CM. The corresponding evolution of the preparation descriptor (i.e, of the density-of-phase function f) is given by the equation (Liouville's equation)

$$\frac{df}{dt} = \{h,f\} \qquad (3.4)$$

where { , } represents the Poisson bracket.

Some theorems of Classical Statistical Mechanics are as follows. Our conclusion from these theorems will be that Classical Statistical Mechanics provides an <u>unambiguous</u> description of preparations, regardless of their homogeneity.

Th1CSM

Among all the normalized functions definable on the phase-space Ω, only the Dirac delta "functions" $\delta_o(\underline{q},\underline{p}) = \delta(\underline{q}-\underline{q}_o)\,\delta(\underline{p}-\underline{p}_o)$ are <u>irreducible</u>, in the sense that the equality

$$\delta_o(\underline{q},\underline{p}) = w_1 f_1(\underline{q},\underline{p}) + w_2 f_2(\underline{q},\underline{p}) \quad \text{with} \quad w_1,\ w_2 > 0 \qquad (3.5)$$

holds if, and only if, $f_1 = f_2 = \delta_o$.

This follows from the fact that the Dirac delta function has a <u>support</u> (i.e., that part of the phase-space for which the function is nonzero) which is indivisible, being a single point $(\underline{q}_o,\underline{p}_o)$.

Th2CSM

To every distinct point $(\underline{q}_0,\underline{p}_0)$ in Ω there corresponds a distinct Dirac delta function $\delta(\underline{q}-\underline{q}_0)\delta(\underline{p}-\underline{p}_0)$ defined on Ω.

This theorem establishes a one-to-one correspondence between Dirac delta functions on phase-space and the state descriptors of Classical Mechanics, i.e. the points in phase-space.

Definition: Homogeneous Preparations within CSM

A preparation is said to be homogeneous if, and only if, it is represented by a Dirac delta function.

Th3CSM

Among all the preparation schemes for a physical system, only the <u>homogeneous</u> preparations cannot be conceived of as the result of a statistical composition of <u>different</u> preparation schemes. Moreover, each homogeneous preparation corresponds to one and only one <u>state</u> of an individual system, and vice versa.

This theorem discloses that the <u>rule of correspondence</u> linking the concept of state of an individual system to the concept of homogeneous preparation is indeed reproduced within the paradigm of Classical Statistical Mechanics.

Th4CSM

Every normalized function f defined on Ω can be uniquely expressed as a "weighted sum" of Dirac delta functions, i.e.

$$f(\underline{q},\underline{p}) = \int_{\Omega} \delta(\underline{q}-\underline{q}_0)\,\delta(\underline{p}-\underline{p}_0)\,f(\underline{q}_0,\underline{p}_0)\,d\underline{q}_0\,d\underline{p}_0 \qquad (3.6)$$

where the function $f(\underline{q}_0,\underline{p}_0)$ itself represents the "weight" of the corresponding Dirac delta function. Consequently, every heterogeneous preparation can be <u>uniquely</u> <u>resolved</u> into its homogeneous component preparations.

This last theorem states explicitly that the mathematical descriptor of a heterogeneous preparation is <u>uniquely</u> indicative of the statistical structure of the preparation itself, i.e. of its homogeneous component preparations and the associated statistical weights. It is therefore correct, within the framework of this theory, to conceive of an individual system, which has been prepared according to a heterogeneous preparation, as being "in" a <u>state</u> corresponding to one of the homogeneous component preparations, with a probability given by the associated statistical weight.

To summarize, we have exemplified the key role played by the distinction between homogeneous and heterogeneous preparations within the framework of the classical theory of nature. The <u>link</u> between homogeneous preparations and states of an individual system is indeed reproduced in the theory. Moreover, the <u>concept</u> of state of an individual system is unambiguously represented even when the preparation scheme is heterogeneous.

3.2.2 Quantum Mechanics vs Quantum Statistical Mechanics

We now turn to the currently accepted version of conventional quantum theory -- composed of the paradigms of Quantum Mechanics and Quantum Statistical Mechanics -- and show that, within this formulation, the notion of state of an individual system is ambiguously represented. The structure of the paradigms is mathematically equivalent to the general structure outlined by J.L. Park (1968b).

QUANTUM MECHANICS

P1QM: Systems

To every physical system there corresponds a separable, complex Hilbert space $\mathscr{H}$ whose elements are vectors ψ. The Hilbert space of a system composed of two distinguishable subsystems 1 and 2, with corresponding Hilbert spaces $\mathscr{H}(1)$ and $\mathscr{H}(2)$, is the direct product Hilbert space $\mathscr{H}(1)\otimes\mathscr{H}(2)$.

P2QM: Homogeneous Preparations

To every homogeneous preparation scheme Π for a system, there corresponds a unit-norm vector ψ in the Hilbert space of the system. The vector ψ is called the state vector.

P3QM: Physical Observables

Some linear, Hermitian operators G, H, ... defined on $\mathscr{H}$ correspond to physical observables of the system. Given an ensemble of identical systems prepared according to the homogeneous scheme Π, with corresponding state vector ψ, the arithmetic mean value $\overline{g}$ of data yielded by measurements of the observable G is given by the value of the following scalar product

$$\overline{g} = \langle\psi, G\psi\rangle \quad . \tag{3.7}$$

P4QM: States

Every individual system is always in a state described by some vector ψ in the corresponding Hilbert space.

P5QM: Causal Evolution

For every physical system there exists an operator H (the Hamiltonian operator), defined on the Hilbert space of the system, which determines the causal evolution of the state descriptor ψ via the following law (Schrödinger's equation of motion)

$$\frac{d\psi}{dt} = -\frac{i}{\hbar} H\psi \quad . \tag{3.8}$$

The above paradigm has been constructed so as to entail the famous uncertainty theorem (W. Heisenberg (1927)). Mathematically, the theorem follows immediately from the Cauchy-Schwarz inequality applied to the scalar product $\langle\ ,\ \rangle$. Let the variance of measurement results for the physical observable G be defined by

$$\mathrm{var}(G) = \overline{(g - \bar{g})^2} = \langle\psi, G^2\psi\rangle - (\langle\psi, G\psi\rangle)^2 \quad . \tag{3.9}$$

The uncertainty theorem consists of the following well known general inequality valid for any two Hermitian operators G and F and therefore for two physical observables of the system

$$\mathrm{var}(G)\mathrm{var}(F) \geqslant |\langle\psi,[F,G]\psi\rangle|^2 \tag{3.10}$$

where [,] is the standard commutator symbol ([F,G] = FG - GF). Coversely, the theory reflects the <u>fundamental Heisenberg hypothesis</u>, namely, that <u>inherent in the nature of the state</u> of any individual physical system there exist <u>uncertainties</u>. These uncertainties induce irreducible dispersions in the results of measurements performed on any <u>homogeneous</u> ensemble. No dispersionless ensemble can even be <u>conceived</u> within the framework of Quantum Mechanics. This striking conclusion constitutes one of the essential aspects of the departure of Quantum Mechanics from Classical Mechanics. The existence of uncertainties intimately connected with the nature of the state of any individual material system is a universally accepted aspect of today's physics.

QUANTUM STATISTICAL MECHANICS

P1QSM: Systems

Same as P1QM.

P2QSM: Preparations

To every <u>preparation</u> scheme Π for a system, there corresponds a linear, Hermitian, nonnegative-definite, unit-trace operator

W defined on the Hilbert space of the system. The operator W is called the statistical operator.

P3QSM: Physical Observables

Some linear, Hermitian operators G, H, ... defined on $\mathcal{H}$ correspond to physical observables of the system. Given an ensemble of identical systems prepared according to the scheme Π, with corresponding statistical operator W, the expected mean value $\langle\bar{g}\rangle$ of measurements of the observable G is given by the value of the following trace functional

$$\langle\bar{g}\rangle = \mathrm{Tr}(WG) \ . \tag{3.11}$$

P4QSM: States

There can be no "P4" postulate. Saying that every individual system is always in a state, described by some vector ψ in $\mathcal{H}$, leads to inconsistencies and paradoxes (see the discussion at the end of this Section).

P5QSM: Causal Evolution

Same as P5QM. The corresponding evolution of the preparation descriptor (i.e., of the statistical operator W) is given by the equation (von Neumann's equation)

$$\frac{dW}{dt} = -\frac{i}{\hbar}[H,W] \ . \tag{3.12}$$

It is noteworthy that the statistical operator W (which is also usually called the density operator and indicated by the symbol ρ) has an essentially different physical meaning than the state operator defined within the paradigm of Quantum Thermodynamics. This distinction will be clarified in Section 4.1.1.

Some of the theorems of Quantum Statistical Mechanics are as follows.

Th1QSM (J. von Neumann (1932))

> Among the linear, Hermitian, nonnegative-definite, unit-trace operators W definable on the Hilbert space $\mathcal{H}$, only the projection operators P_ψ onto the one-dimensional subspaces of $\mathcal{H}$ are irreducible, in the sense that the equality
>
> $$P_\psi = a_1 W_1 + a_2 W_2 \qquad \text{with} \qquad a_1, a_2 > 0 \tag{3.13}$$
>
> holds if, and only if, $W_1 = W_2 = P_\psi$.

This follows from the fact that the projection operators P_ψ onto the one-dimensional subspaces of $\mathcal{H}$ are the extreme elements of the convex set of statistical operators on $\mathcal{H}$.

Th2QSM

> To every distinct unit-norm vector ψ in $\mathcal{H}$ there corresponds a distinct projection operator P_ψ onto the one-dimensional subspace of $\mathcal{H}$ spanned by ψ.

This theorem establishes a one-to-one correspondence between projection operators onto one-dimensional subspaces of the Hilbert space and the state descriptors of Quantum Mechanics, i.e. the state vectors in Hilbert space.

Definition: Homogeneous Preparations within QSM

A preparation is said to be homogeneous if, and only if, it is described by a projection operator P_ψ onto a one-dimensional subspace of $\mathscr{H}$.

Th3QSM

Among all the preparation schemes for a physical system, only the homogeneous preparations cannot be conceived as the result of a statistical composition of different preparation schemes. Moreover, each homogeneous preparation corresponds to one and only one state of an individual system, and vice versa.

This theorem discloses that the rule of correspondence linking the concept of state of an individual system to the concept of homogeneous preparation is indeed reproduced within the paradigm of Quantum Statistical Mechanics.

Th4QSM (E. Schrödinger (1936))

Every non-idempotent statistical operator W on $\mathscr{H}$ (i.e., the statistical operators that are not projection operators onto one-dimensional subspaces of $\mathscr{H}$) can be expressed as a weighted sum of projection operators (onto one-dimensional subspaces of $\mathscr{H}$) in at least two different ways (generally, an infinity of ways), such as

$$W = \sum_n w_n P_{\psi_n} = \sum_q w'_q P_{\phi_q} = \ldots \qquad (3.14)$$

Consequence of this theorem is that the concept of state of an individual system is not unambiguously represented within Quantum Statistical Mechanics and, therefore, there can be no state postulate (P4QSM). In fact, if we insisted that such a postulate be included in the paradigm of the theory, a logical consequence of the last theorem would be that an individual system prepared according to the heterogeneous preparation scheme Π, with corresponding statistical operator W, is, for example, in state ψ_n with probability w_n and, at the same time, in state ϕ_q with probability w'_q. Such a system is what J.L. Park (1968a) called a quantum monster: a single system which is concurrently "in" two different states.

This is the observation that led Park to the conclusion quoted at the beginning of this Chapter. We have already objected that the above ambiguity about the concept of state of an individual system should be charged to the underlying mathematical description rather than to the concept itself.

To summarize, this Section has exemplified the key role played by the distinction between homogeneous and heterogeneous preparations within the framework of the conventional quantum theory of nature. The link between homogeneous preparations and states of an individual system is reproduced. However, the concept of state of an individual system is ambiguously represented when the preparation scheme is heterogeneous.

To this point, we have established the scientific need to formulate a quantum statistical theory that includes the concept of state of an individual system without ambiguities.

3.2.3 Unambiguous Description of Heterogeneous Preparations

By examining the paradigms of Classical Statistical Mechanics and Quantum Statistical Mechanics, we have learned that a mathematical description of heterogeneous preparations must satisfy certain conditions in order to be considered unambiguous. We summarize the results by stating three necessary conditions which define explicitly the notion of unambiguous mathematical description of heterogeneous preparations.

A mathematical description of preparations is defined as follows:

(o) To any preparation scheme there corresponds an element of the set of mathematical descriptors.

The three necessary conditions are as follows. Each condition is exemplified by indicating its realization within the paradigm of CSM, where the set of mathematical descriptors is the set of density-of-phase functions defined on the phase-space of the system.

(i) To the concept of statistical composition of different preparation schemes there must correspond a mathematical <u>rule</u> to combine their mathematical descriptors so as to obtain the mathematical descriptor of the composite preparation. This rule of combination must be such that, for every physical observable, the expected mean value corresponding to the composite preparation equals the statistically weighted sum of the expected mean values corresponding to the component preparations.

Within CSM, to the statistical composition (with weights w_1 and w_2) of two preparations with corresponding density-of-phase functions f_1 and f_2, there corresponds the following rule of combination yielding the density-of-phase function f_c of the composite preparation:

$$f_c = w_1 f_1 + w_2 f_2 \quad .$$

It is immediate to verify that the requirement about the expected mean values is satisfied, i.e. that

$$\langle \bar{g} \rangle_c = w_1 \langle \bar{g} \rangle_1 + w_2 \langle \bar{g} \rangle_2 \quad .$$

(ii) To every homogeneous preparation there must correspond an <u>irreducible</u> mathematical descriptor, i.e. an element of the set of mathematical descriptors which cannot be obtained from the combination of <u>different</u> elements of the set. This implies not only that such irreducible elements must exist, but also that they must be at least as "numerous" as the different homogeneous preparations.

Within CSM, to every homogeneous preparation there corresponds a Dirac delta "function" which is indeed irreducible, since its support is a single point in phase-space. Moreover, a Dirac delta function can be defined in correspondence to every point in phase space (cf. theorem Th2CSM).

(iii) To the uniqueness of resolution of any preparation into its homogeneous component preparations there must correspond the uniqueness of resolution of each mathematical descriptor into a combination of its irreducible components.

Within CSM, every density-of-phase function can be uniquely resolved into a "weighted sum" of irreducible Dirac delta functions (cf. theorem Th4CSM).

The most demanding conditions are (ii) and (iii). Condition (ii) reflects the need for a correct mathematical correspondent to the concept of homogeneous preparation. The irreducibility of this class of preparations is essential and must therefore be reflected in the mathematical description. In addition, the description must be mathematically rich enough so that with every distinct homogeneous preparation is associated at least one distinct mathematical descriptor, thus reproducing the rule of correspondence between states and homogeneous preparations. Condition (iii) reflects the need for an unambiguous representation of the concept of state of an individual system prepared according to a heterogeneous preparation. The uniqueness of resolution of a heterogeneous preparation into its homogeneous component preparations is essential to avoid paradoxical conclusions of the type discussed in last Section, and must therefore be reflected in the mathematical description.

In our search for an unambiguous formulation of a statistical theory to be superimposed to Quantum Thermodynamics (cf. Section 4.1), three different mathematical descriptions of heterogeneous preparations were considered. When analysed in the light of the conditions just defined, two were found unsatisfactory (these attempts are instructive and are outlined in appendix A), but the third satisfied all three conditions. This new description of preparations is proposed in Section 4.2.1 and then adopted in Section 4.2.2 to formulate the paradigm of Quantum Statistical Thermodynamics.

ENTROPY AND IRREVERSIBILITY FOR A SINGLE ISOLATED TWO-LEVEL SYSTEM. NEW INDIVIDUAL QUANTUM STATES AND NEW NONLINEAR EQUATION OF MOTION

by

Gian Paolo Beretta
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139
(Received 24 October 1983)

ABSTRACT

We propose a new nonlinear equation of motion for a single isolated two-level quantum system. The resulting generalized two-level quantum dynamical theory entails a new alternative resolution of the long-standing dilemma on the nature of entropy and irreversibility. Even for a single isolated degree of freedom, in addition to the individual mechanical states for which all the results of conventional quantum mechanics remain valid, our theory implies the existence of new non-mechanical individual quantum states. These states have nonzero individual entropy and, by virtue of a constant-energy, internal redistribution mechanism, relax irreversibly towards stable equilibrium. We discuss the possibility of an experimental verification of these conclusions by means of a high-resolution, essentially single-particle, magnetic-resonance experiment.

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Address: G.P. Beretta, M.I.T., Room 3-339, Cambridge, MA 02139

1. INTRODUCTION

The long-standing dilemma on the nature of entropy and irreversibility still lacks a universally accepted resolution,[1] in spite of a century of scientific efforts. As stated in a recent review by Wehrl:[2] "There are many opinions and proposals for a solution to this problem; however, none of them seems to be completely satisfactory." The purpose of this paper is to present a novel nonlinear equation of motion for a single two-level quantum system that was proposed by the author[3] in an effort to attempt a satisfactory resolution of the irreversibility dilemma.

Our approach differs essentially from the traditional where entropy, irreversibility and the laws of thermodynamics are invariably regarded as statistical, macroscopic or phenomenological concepts with no fundamental counterpart in the microscopic reality. Indeed, our underlying premise is that the gap between mechanics and thermodynamics can be conceivably bridged without resorting to any statistical or information-theoretic reasoning, without hinging on the distinction between microscopic and macroscopic reality, and without regarding the laws of thermodynamics as simply "phenomenological."[1]

For definiteness, we discuss only the simplest case of a single two-level quantum system. Our proposal, based on the two fundamental hypotheses presented in Section 2, provides a quite unconventional, but logically coherent, new resolution of the irreversibility dilemma consistent with the declared premise. Irreversibility emerges as a manifestation of an inherent energy-conserving relaxation mechanism implied by the postulated new equation of motion, even in the absence of any form of interaction of the system with any other system, lattice or "heat bath," i.e., even for a strictly isolated two-level system.

In addition to all the results of conventional quantum mechanics which hold as special cases of our theory, the new equation of motion implies the existence of inherent relaxation effects that should be in principle experimentally verifiable. For this purpose, we study the dynamics of a single spin-1/2 system in an external time-dependent magnetic field and propose that the predicted single-particle relaxation effect may be verified with a high-resolution magnetic-resonance experiment on a beam of spin-1/2 particles of very low intensity (essentially single-particle).

The paper is organized as follows. Section 2 presents the two new fundamental postulates of our theory. Section 3 discusses the general properties of the new nonlinear equation of motion that we propose for a single isolated two-level system. Section 4 presents special classes of exact and approximate solutions of the equation of motion. Section 5 proposes one method to verify experimentally the validity of our two postulates and Section 6 gives conclusions.

2. NON-IDEMPOTENT QUANTUM STATES AND NONLINEAR EQUATION OF MOTION

Our first fundamental hypothesis is due to Hatsopoulos and Gyftopoulos.[4] They proposed that, in addition to the individual quantum states conceived of within conventional quantum mechanics and represented mathematically in terms of idempotent state operators,[5] a single strictly isolated (i.e., noninteracting and uncorrelated) system admits also of individual quantum states that must be represented by non-idempotent state operators. State operators ρ have the same mathematical properties[5] as the statistical or density operators considered in traditional (von Neumann) quantum statistical mechanics,[6] but acquire in our theory an entirely different physical meaning. A state operator ρ represents an individual quantum state of the single strictly isolated system. It does not represent the index of statistics from a generally heterogeneous ensemble of identical systems.

As shown in Reference 4, the only trace functional of the state operator ρ that can represent the physical observable entropy is $s(\rho) = -k\mathrm{Tr}\rho\ln\rho$. The nonlinear state functional $s(\rho)$ is defined for all state operators, idempotent and non-idempotent. It represents the individual entropy of the single strictly isolated and uncorrelated system. It does not represent a measure of statistical or information-theoretic uncertainty.

In summary, with the Hatsopoulos-Gyftopoulos fundamental hypothesis, we conceive of a larger set of individual quantum states of uncorrelated systems than in conventional quantum mechanics. A single isolated system may be found not only in a quantum mechanical state ($\rho^2 = \rho$, $s(\rho) = 0$) but also in a non-mechanical quantum state described by a non-idempotent state operator ρ for which the entropy functional is nonzero.

Our next step is to describe the time evolution of all the individual quantum states of a single isolated two-level system. For quantum mechanical individual states, the dynamical law is the Schroedinger equation of motion or, in terms of state operators, the von Neumann equation of motion. But, for the additional non-mechanical individual quantum states that we have postulated, the dynamical law cannot be "derived" from conventional quantum mechanics, simply because that theory cannot even conceive of such individual states. We must therefore augument the dynamical postulate with a new equation of motion, consistent with the Schroedinger equation for idempotent state operators.

Our second fundamental hypothesis is the following equation of motion[3] that we propose for a single isolated two-level system

$$\frac{d\rho}{dt} + \frac{i}{\hbar}[H,\rho] = \begin{cases} -\dfrac{1}{\tau}\,\dfrac{\begin{vmatrix} \rho\ln\rho & \rho & \frac{1}{2}\{H,\rho\} \\ \mathrm{Tr}\,\rho\ln\rho & 1 & \mathrm{Tr}\,\rho H \\ \mathrm{Tr}\,\rho H\ln\rho & \mathrm{Tr}\,\rho H & \mathrm{Tr}\,\rho H^2 \end{vmatrix}}{\mathrm{Tr}\,\rho H^2 - (\mathrm{Tr}\,\rho H)^2} & \text{if } \rho^2 \neq \rho \qquad (1a) \\ 0 & \text{if } \rho^2 = \rho \qquad (1b) \end{cases}$$

where H is the Hamiltonian operator and τ is an inherent internal-redistribution time constant of the system. For the same reason why the dynamical law for non-mechanical states cannot be "derived" from mechanics, the value of the time constant τ cannot be obtained other than by analysis of experimental data. Equation 1 has been "invented," not "derived." Its adoption is justified only insofar as its consequences are consistent with our declared premises, in particular, with the laws of mechanics for idempotent individual states and with the laws of thermodynamics for all individual states.

For example, we will see that a consequence of Equation 1 is a statement that the entropy of the strictly isolated two-level system is constant for all the mechanical states ($s(\rho) = 0$) and for all the equilibrium states (there is one equilibrium state for each initial value of the mean energy), but it is strictly increasing in time for all other non-mechanical states. Again, consistently with the fact that it describes the time evolution of an isolated system, Equation 1 conserves the mean energy.

3. PROPERTIES OF THE NEW EQUATION

On the two-dimensional Hilbert space of the two-level system, we introduce the 3-vector $\underline{R} = (R_1,R_2,R_3)$ of spin operators which obey the commutation rule $[R_j,R_m] = i\varepsilon_{jmn}R_n$ and may be expressed in terms of the lowering and raising operators $b = R_1 - iR_2$ and $b^\dagger = R_1 + iR_2$. A state operator $\rho(t)$ may then be represented as

$$\rho(t) = \frac{1}{2}I + r_1(t)R_1 + r_2(t)R_2 + r_3(t)R_3 = \frac{1}{2}I + \underline{r}(t)\cdot\underline{R} \tag{2a}$$

$$= \frac{1}{2}I + \alpha^*(t)b^\dagger + \alpha(t)b + r_3(t)R_3 \tag{2b}$$

where the 3-vector $\underline{r} = (r_1,r_2,r_3)$ of real scalars and the complex scalar α satisfy the condition

$$r = |\underline{r}| = (r_1{}^2+r_2{}^2+r_3{}^2)^{1/2} = (4\alpha^*\alpha + r_3{}^2)^{1/2} \leq 1 \tag{2c}$$

Geometrically, the set of state operators is isomorphic with a closed spherical domain of unit radius (the Bloch sphere) in an auxiliary three-dimensional space with orthogonal coordinates r_1, r_2 and r_3. Each point $\underline{r}$ in the Bloch sphere represents, via Relation 2a, a state operator. A state operator is idempotent ($\rho^2 = \rho$) if and only if $r = 1$. Thus, all the state operators conceived of within conventional quantum mechanics (for a single strictly isolated two-level system) lie on the surface of the Bloch sphere. The Hatsopoulos-Gyftopoulos hypothesis extends the domain of conceivable individual states of uncorrelated two-level systems to the whole volume inside the Bloch sphere, including state operators for which $\rho \neq \rho^2$ and $r < 1$.

A general Hamiltonian operator corresponding to the energy relative to a point midway between the two energy levels of the isolated two-level system may be represented as

$$H = \hbar\Omega_o(\Lambda_1R_1 + \Lambda_2R_2 + \Lambda_3R_3) = \hbar\Omega_o\underline{\Lambda}\cdot\underline{R} \tag{3a}$$

$$= -\frac{1}{2}\hbar\Omega(\varepsilon b^\dagger + \varepsilon^* b) + \hbar\omega_o R_3 \tag{3b}$$

where $\hbar$ is the reduced Planck constant, $\underline{\Lambda} = (\Lambda_1,\Lambda_2,\Lambda_3)$ is a unit-norm 3-vector of real scalars ($|\underline{\Lambda}| = \underline{\Lambda}\cdot\underline{\Lambda} = 1$), ε is a complex scalar with $\varepsilon^*\varepsilon = 1$, $\omega_o = \Omega_o\Lambda_3$ is the transition frequency between the two levels and $\Omega_o{}^2 = \Omega^2 + \omega_o{}^2$.

If $\underline{r} = \pm\underline{\Lambda}$, then $\rho_\pm = \rho_\pm{}^2 = P_{\psi_\pm}$ where $\psi_\pm$ are the eigenvectors of the Hamiltonian operator H. According to Equation 1, and consistently with conventional quantum mechanics, the two pure mechanical states $\rho_\pm$ are equilibrium states. Assuming from now on that $\underline{r} \neq \pm\underline{\Lambda}$, after lengthy but straightforward manipulations (outlined in Appendix A), using Relations 2 and 3 for operators ρ and H in Equation 1 with $\underline{r} \neq \pm\underline{\Lambda}$, we find the following forms of the new equation of motion

$$\frac{d\underline{r}}{dt} - \Omega_o\,\underline{\Lambda}\times\underline{r} = -\frac{1}{\tau}K(\underline{r})[\underline{r} - (\underline{\Lambda}\cdot\underline{r})\underline{\Lambda}] \tag{4a}$$

$$= -\frac{1}{\tau}K(\underline{r})[\underline{\Lambda}\times\underline{r}\times\underline{\Lambda}] \tag{4b}$$

or

$$\frac{d\alpha}{dt} + i\omega_o\alpha + i\Omega\varepsilon r_3/2 = -\frac{K(\alpha,r_3)}{\tau\Omega_o{}^2}[\omega_o{}^2\alpha + \omega_o\Omega\varepsilon r_3/2 + \Omega^2\varepsilon(\varepsilon^*\alpha - \varepsilon\alpha^*)/2] \tag{5a}$$

$$\frac{dr_3}{dt} + i\Omega(\varepsilon^*\alpha - \varepsilon\alpha^*) = -\frac{K(\alpha,r_3)}{\tau\Omega_o{}^2}[\Omega^2 r_3 + \omega_o\Omega(\varepsilon^*\alpha + \varepsilon\alpha^*)] \tag{5b}$$

where

$$K(\underline{r}) = \frac{f(r)}{1 - (\underline{\Lambda}\cdot\underline{r})^2} = K(\alpha, r_3) = \frac{f(r)}{1 - [\omega_o r_3 - \Omega(\varepsilon\alpha + \varepsilon^* \alpha^*)]^2/\Omega_o^2} \qquad (6)$$

$r = |\underline{r}|$, and

$$f(r) = \begin{cases} 1 & \text{if } r = 0 \\ \dfrac{1 - r^2}{2r} \ln\dfrac{1 + r}{1 - r} & \text{if } 0 < r < 1 \\ 0 & \text{if } r = 1 \end{cases} \qquad (7)$$

As shown in Appendix B, for every initial state $\underline{r}_o$ in the Bloch sphere ($r_o \leq 1$), the new equation of motion admits of one and only one solution $\underline{r}(t)$ with $\underline{r}(0) = \underline{r}_o$ which lies entirely in the Bloch sphere for $-\infty < t < +\infty$. Thus, let $\underline{r}(t)$ be a solution with $\underline{r}(0)$ in the Bloch sphere, i.e., with $r(0) \leq 1$. From Equation 4, we find that

$$\frac{d}{dt}\mathrm{Tr}H\rho(t) = \frac{d}{dt}\,\frac{1}{2}\hbar\Omega_o\underline{\Lambda}\cdot\underline{r}(t) = \frac{1}{2}\hbar\Omega_o\underline{\Lambda}\cdot\frac{d\underline{r}(t)}{dt} = 0 \qquad (8)$$

and, therefore, we conclude that $r_e = \underline{\Lambda}\cdot\underline{r}(t) = \underline{\Lambda}\cdot\underline{r}(0)$ is constant and the mean energy $\mathrm{Tr}H\rho$ is a constant of the motion for the isolated two-level system, consistently with the first law of thermodynamics. Every solution, i.e., the one-parameter family of points $\underline{r}(t)$, lies entirely on a plane of constant mean energy orthogonal to the vector $\underline{\Lambda}$. Again, from Equations 4, 6 and 7, we find that

$$\frac{dr}{dt} = -\frac{1}{\tau}\,\frac{r^2 - r_e^2}{1 - r_e^2}\,\frac{1 - r^2}{2r^2}\ln\frac{1 + r}{1 - r} \begin{cases} = 0 & \text{if } |r_e| < r = 1 \\ < 0 & \text{if } |r_e| < r < 1 \\ = 0 & \text{if } |r_e| = r < 1 \end{cases} \qquad (9)$$

where $r_e = \underline{\Lambda}\cdot\underline{r}$. As shown in Appendix B, a consequence of Relation 9 is that the solution $\underline{r}(t)$ remains within the Bloch sphere at all times. In terms of state operators, this implies that the solution $\rho(t)$ remains at all times within the set of state operators and, therefore, Equation 1 is a valid evolution equation.

A special class of solutions of Equation 4 is such that $r(t) = 1$ at all times. In this case, the right-hand side of Equation 4 vanishes for every t ($f(1) = 0$, Equation 7) and thus $\underline{r}(t)$ satisfies the differential equation

$$\frac{d\underline{r}}{dt} = \Omega_o\, \underline{\Lambda} \times \underline{r} \tag{10}$$

Every solution $\underline{r}(t)$ in this class remains on the unit-radius surface of the Bloch sphere and precesses around the vector $\underline{\Lambda}$ at the Larmor angular frequency Ω_o. In terms of state operators, $\rho(t)$ remains idempotent at all times and satisfies the operator form of the Schroedinger equation of motion (Equation 1b). We conclude that all the motions contemplated by conventional quantum dynamics are special solutions of Equation 1.

Next we consider the entropy functional

$$s(\rho) = -k\mathrm{Tr}\rho\ln\rho = -\frac{1}{2}k[(1+r)\ln(1+r) + (1-r)\ln(1-r) - \ln 4] \tag{11}$$

which is a monotonic decreasing function of r ranging from $k\ln 2$ to 0 as r ranges from 0 to 1. In the Bloch sphere, concentric spherical surfaces centered at the origin are constant entropy. A direct consequence of Relation 9 is that $ds(\rho)/dt \geq 0$. More explicitly,

$$\frac{ds}{dt} = \frac{k}{\tau}\,\frac{r^2 - r_e^2}{1 - r_e^2}\,\frac{1 - r^2}{4r}\left(\ln\frac{1+r}{1-r}\right)^2 \geq 0 \tag{12}$$

with strict inequalilty for $|r_e| < r < 1$. We conclude that the entropy of an isolated two-level system is a nondecreasing function of time, consistently with the second law of thermodynamics. Moreover, for solutions with $r(0) < 1$ ($\underline{r}(0) \neq c\underline{\Lambda}$) the entropy is strictly increasing, i.e., Equation 1 implies the existence of irreversible, but energy-conserving relaxation even for a single isolated system. This nonconventional result, which is a consequence of the proposed equation of motion, should be in principle experimentally verifiable (cf. Section 5).

The equilibrium states, for which $d\underline{r}/dt = 0$, are only those with $r = r_e$, i.e., with $\underline{r} = r_e\underline{\Lambda}$ ($|r_e| \leq 1$). It readily follows from Relation 9 that these equilibrium states are stable. Only two equilibrium states are "mechanical" (i.e., idempotent), namely, those with $\underline{r} = \pm\underline{\Lambda}$. All the others, with $\underline{r} = r_e\underline{\Lambda}$ and $-1 < r_e < 1$, are non-idempotent individual equilibrium states not contemplated by conventional mechanics that, in terms of state operators, have the form

$$\rho_e = \frac{\exp(-\beta H)}{\text{Tr}\,\exp(-\beta H)} \tag{13}$$

with

$$\beta = \frac{1}{\hbar\Omega_o} \ln\frac{1 - r_e}{1 + r_e} \tag{14}$$

and, according to the Hatsopoulos-Gyftopoulos hypothesis, represent the thermodynamic equilibrium states of a single isolated two-level system with individual thermodynamic temperature $T = 1/k\beta$ (positive if $r_e < 0$).

To summarize, in the Bloch sphere the solutions of Equation 1 describe constant mean energy trajectories of the state point $\underline{r}$ with velocity given by two orthogonal components. The first component causes a precession of $\underline{r}$ around the vector $\underline{\Lambda}$ and is due to the Hamiltonian, or Schroedinger, term in the equation of motion. The second component, whose intensity is a nonlinear function of $\underline{r}$ vanishing for $r = 1$ and $\underline{r} = c\underline{\Lambda}$, causes an attraction, or relaxation, of $\underline{r}$ towards the stable equilibrium vector $\underline{r}_e = r_e\underline{\Lambda}$ and is due to the non-Hamiltonian nonlinear term in the equation of motion. The resulting motion is a simple precession at the Larmor frequency Ω_o if $r(0) = 1$, whereas it is a spiraling relaxation towards the equilibrium vector if $r(0) < 1$.

By contrast with the phenomenological descriptions based on the Bloch relaxation equation,[7] the relaxation mechanism that we postulate by adopting Equation 1 is not due to any form of coupling between the two-level system and other external degrees of freedom. It is a nonlinear, mean-energy conserving, redistribution mechanism strictly internal and individual to the single strictly isolated system.

4. SOLUTIONS OF THE EQUATION OF MOTION

Equation 4 reduces to the scalar equation

$$\frac{d|\underline{r} - \underline{r}_e|}{dt} = -\frac{1}{\tau}\, f(r)\, \frac{|\underline{r} - \underline{r}_e|}{1 - r_e^2} \tag{15}$$

The nonlinearity of this equation does not allow a general explicit solution. However, for $r_e = 0$, it becomes

$$\frac{dr}{dt} = -\frac{1}{\tau}\, f(r)\, r \tag{16}$$

or, equivalently,

$$\frac{d}{dt}\ln\frac{1 + r}{1 - r} = -\frac{1}{\tau}\, \ln\frac{1 + r}{1 - r} \tag{17}$$

which integrated from 0 to t yields,

$$\frac{1 + r(t)}{1 - r(t)} = \left(\frac{1 + r(0)}{1 - r(0)}\right)^{\exp(-t/\tau)} \tag{18}$$

or, equivalently,

$$r(t) = \tanh\left[\frac{1}{2}\exp\left(-\frac{t}{\tau}\right)\ln\frac{1 + r(0)}{1 - r(0)}\right] \tag{19}$$

Thus, we found a class of special solutions of the new equation of motion which satisfy initial conditions with $r(0) < 1$ and $r_e = 0$, i.e., initial non-idempotent state operators with zero mean energy.

Next, we consider the limit as $\underline{r}(0)$ tends to $\underline{r}_e$. Then, we can use the approximation $f(r) \approx f(r_e)$ and linearize Equation 15 to yield

$$|\underline{r}(t) - \underline{r}_e| = |\underline{r}(0) - \underline{r}_e|\exp(-t/T_R) \tag{20}$$

where, using Equation 14, the approximate relaxation time T_R is given by

$$T_R = \tau \frac{1 - r_e^2}{f(r_e)} = - \tau \frac{r_e}{\frac{1}{2}\hbar\Omega_o\beta} = \tau \frac{\tanh(\frac{1}{2}\hbar\Omega_o\beta)}{\frac{1}{2}\hbar\Omega_o\beta} \tag{21}$$

and, for $\frac{1}{2}\hbar\Omega_o\beta$ sufficiently small (sufficiently high temperature of the stable equilibrium state $\underline{r}_e$),

$$T_R \approx \tau \left[1 - \frac{1}{3}(\tfrac{1}{2}\hbar\Omega_o\beta)^2 + \frac{2}{15}(\tfrac{1}{2}\hbar\Omega_o\beta)^4 - \dots\right] \tag{22}$$

It is interesting to note that our intrinsic relaxation or redistribution mechanism shows in this approximation an explicit temperature dependence which in principle should be experimentally verifiable, for example as discussed in the next section.

5. A SINGLE-PARTICLE MAGNETIC RESONANCE EXPERIMENT

As a first attempt to search for an experimental verification of our hypotheses and, in particular, of the implications of Equation 1, we consider a very low intensity (essentially single-particle) beam of spin-1/2 particles entering a suitable magnetic resonance apparatus. During its residence time in the apparatus, each single particle experiences a time-dependent spatially-uniform applied magnetic field.

In the laboratory reference frame, we assume that inside the magnetic resonance apparatus the external magnetic field has components given by

$$\underline{H}_M(t) = (H_{M1}\cos\omega t, H_{M1}\sin\omega t, H_{M3}) \tag{23}$$

while outside the apparatus, $H_{M1} = 0$. With respect to a reference frame rotating about the third laboratory axis $\underline{k}_3$ at the angular frequency ω, the magnetic field has constant components

$$\underline{H}_M(t) = (H_{M1}, 0, H_{M3})' \tag{24}$$

The magnetic moment operator vector of the spin-1/2 particle with gyromagnetic ratio γ is given by

$$\underline{M} = \gamma\hbar\underline{R} \tag{25}$$

and the Hamiltonian operator by

$$H = \underline{H}_M(t)\cdot\underline{M} = \hbar\Omega(R_1\cos\omega t + R_2\sin\omega t) + \hbar\omega_o R_3 \tag{26}$$

By comparison with Equation 3, we find

$$\Omega_o\underline{\Lambda} = (\Omega\cos\omega t, \Omega\sin\omega, \omega_o) = (\Omega, 0, \omega_o)' \tag{27}$$

where $\Omega = \gamma H_{M1}$, $\omega_o = \gamma H_{M3}$ and $\Omega_o^2 = \Omega^2 + \omega_o^2$.

If d'/dt denotes differentiation with respect to the rotating frame, then $d\underline{r}/dt = d'\underline{r}/dt + \omega\, \underline{k}_3 \times \underline{r}$ and Equation 4 becomes

$$\frac{d'\underline{r}}{dt} = (\Omega_o \underline{\Lambda} - \omega \underline{k}_3) \times \underline{r} - \frac{1}{\tau} K(\underline{r})\, [\underline{r} - r_e \underline{\Lambda}] \tag{28}$$

Due to the time dependence of the Hamiltonian, the mean energy, $\mathrm{Tr}H\rho = \hbar\Omega_o r_e/2$, changes at a rate given by

$$\frac{dr_e}{dt} = \frac{d}{dt}\underline{\Lambda}\cdot\underline{r} = \frac{d\underline{\Lambda}}{dt}\cdot\underline{r} = \frac{d'}{dt}\underline{\Lambda}\cdot\underline{r} = \underline{\Lambda}\cdot\frac{d'\underline{r}}{dt} = \frac{\omega\Omega}{\Omega_o} r_2' \tag{29}$$

where r_1', r_2', r_3' will denote the components of $\underline{r}$ with respect to the rotating frame, i.e., $\underline{r} = (r_1', r_2', r_3')'$.

To find an approximate solution of Equation 28 we will make the following assumptions, that are similar to the so-called "slow-passage" or "steady-state" conditions[7] of standard magnetic-resonance configurations:

(1) the relative change in mean energy during the residence time t_{res} in the apparatus is small, i.e., $|t_{res}\dot{r}_e/r_e| << 1$, so that we can consider vector $\underline{r}_e$ as slowly varying in the rotating frame;

(2) the spin-1/2 system enters the apparatus in a non-idempotent stable equilibrium state with respect to the outside external magnetic field and $\Omega << \omega_o$, so that the vector $\underline{r}$ remains close to $\underline{r}_e$ and we can consider $K(\underline{r}) \approx 1/T_R \approx$ const, as done in Equation 20;

(3) the inherent relaxation mechanism maintains an approximately constant magnetization in the rotating frame, so that we can consider $d'\underline{r}/dt \approx 0$.

Under these assumptions, the solution of homogeneous Equation 28 can be approximated by a slowly-varying quasi-steady solution. Setting $d'\underline{r}/dt = 0$ and considering r_e as constant, Equation 28 yields

$$-(\omega_o-\omega)r_2' - r_1'/T_R = -\Omega\, r_e/T_R\Omega_o \tag{30a}$$

$$(\omega_o-\omega)r_1' - \Omega\, r_3' - r_2'/T_R = 0 \tag{30b}$$

$$\Omega\, r_2' - r_3'/T_R = -\omega_o r_e/T_R\Omega_o \tag{30c}$$

$$\begin{vmatrix} r_1' \\ r_2' \\ r_3' \end{vmatrix} = \frac{r_e}{\Omega_o[1 + \Omega^2 T_R^2 + (\omega_o-\omega)^2 T_R^2]} \begin{vmatrix} \Omega[1+\Omega^2 T_R^2+(\omega_o-\omega)\omega_o T_R^2] \\ -\Omega\omega T_R \\ \omega_o[1+(\omega_o-\omega)^2 T_R^2]+(\omega_o-\omega)\Omega^2 T_R^2 \end{vmatrix} \tag{31}$$

Defining the effective relaxation time

$$T_E = \frac{T_R}{(1+\Omega^2 T_R^2)^{1/2}} \tag{32}$$

and the complex susceptibility

$$\chi = \chi'+i\chi'' = \frac{\mathrm{Tr}\,\rho(M_1-iM_2)}{H_{M1}} = \frac{\gamma^2\hbar}{2\Omega}(r_1'-ir_2') \tag{33}$$

we obtain

$$\begin{vmatrix} \chi' \\ \chi'' \end{vmatrix} = \frac{\gamma^2\hbar r_e}{2\Omega_o[1+(\omega_o-\omega)^2 T_E^2]} \begin{vmatrix} 1 + (\omega_o-\omega)\omega_o T_E^2 \\ -\omega T_E^2/T_R \end{vmatrix} \tag{34}$$

and, from Equations 29 and 31,

$$-\frac{1}{r_e}\frac{dr_e}{dt} = \frac{\omega^2\Omega^2 T_E^2/T_R}{\Omega_o[1 + (\omega_o-\omega)^2 T_E^2]} \tag{35}$$

At the frequency $\omega = \omega_o + 1/\omega_o T_E^2$, the right-hand side of Equation 35 achieves a maximum value $\Omega^2(1+\omega_o^2 T_E^2)/\Omega_o^2 T_R$ which must be much smaller than $1/t_{res}$ for consistency with our assumption (1).

Compared to the typical dispersion and absorption curves observed in conventional magnetic-resonance experiments under slow-passage or steady-state conditions,[7] the real and imaginary parts of the complex susceptibility as given by Equation 34 present asymmetries with respect to the resonance condition $\omega = \omega_o$. Their shape is determined by the parameter T_E which is in turn related to the unknown internal time constant τ and the individual inverse temperature β via Relation 21.

As already discussed, the single-particle relaxation effect predicted here is entirely different from the spin-lattice and spin-spin relaxation effects that dominate in standard magnetic resonance experiments where each single spin-1/2 system is coupled to external degrees of freedom. The effect predicted here would be experimentally verifiable if high resolution measurements could be made on a very diluted beam of spin-1/2 particles so that the only external interactions felt by each single particle are those with the applied magnetic fields.

An experiment on these lines would verify the validity of our two hypothesis, namely, (1) the existence of non-mechanical individual states described by non-idempotent state operators and (2) the new equation of motion describing their irreversible time evolution. The experiment would determine the value of the unknown time constant τ for the spin-1/2 particle or, at least, a lower bound to that value.

6. CONCLUSIONS

We have proposed a new approach towards a satisfactory resolution of the so-called irreversibility dilemma or paradox. Instead of statistical, information-theoretic, macroscopic, phenomenological, or anthropomorphic concepts, we submit that entropy and irreversibility are microscopic physical concepts, in the same sense as energy is a microscopic physical concept, and are defined for each individual physical system, even if composed by a single strictly isolated degree of freedom. To show that a logically consistent approach based on this unconventional premise is feasible, we proposed a generalized quantum dynamical theory for the simplest quantum system, namely, a single isolated two-level system.

In conventional quantum mechanics, the entropy of a single individual strictly isolated system is an undefined concept (entropy-like concepts are defined only for the statistical description of ensembles of such systems). In our generalized quantum dynamics, instead, entropy emerges as a physical observable of every single isolated two-level system, and is defined for each of its individual states. We achieve this by adopting the Hatsopoulos- Gyftopoulos postulate that, in addition to all the traditional individual quantum mechanical states (with individual entropy now defined and equal to zero), there exists a broad class of non-mechanical individual quantum states (inconceivable within conventional mechanics and with nonzero entropy).

In conventional (non-statistical) quantum mechanics, individual states of a single isolated system evolve in time only along reversible paths (Schroedinger equation of motion). Irreversibility has no place within mechanics. To explain a physical reality dominated by irreversible processes, mechanics is invariably complemented by additional postulates (such as those of the statistical, information-theoretic, macroscopic or phenomenological approaches reviewed in Reference 1). In our generalized (non-statistical) quantum dynamics, the additional postulates are the Hatsopoulos-Gyftopoulos hypothesis and the new nonlinear equation of motion proposed by the author. Irreversibility emerges as a microscopic physical phenomenon occuring within the single isolated system in most of its non-mechanical individual states.

The proposed two-level quantum dynamics broadens the quantum mechanical treatment without contradicting any of its successful results. But the generalized theory implies new additional results that are inconceivable within conventional mechanics, such as the single-particle, energy- conserving, internal-redistribution relaxation mechanism discussed in detail in the paper.

We believe that our proposal for a resolution of the irreversibility dilemma is logically coherent and consistent with all the successful results of quantum mechanics, it provides a new perspective to the description of nonequilibrium phenomena, and it is definite and explicit enough to imply new detailed predictions that, at least in principle, should be experimentally verifiable.

ACKNOWLEDGEMENTS

The author is indebted to Professor L. Amerio, Politecnico di Milano, Italy, for suggestions concerning the material in Appendix B. The work was supported in part by a grant from the Thermo Electron Corporation.

APPENDIX A - FROM EQUATION 1 TO EQUATION 4

In terms of the representation of state operators given by Relation 2a, the eigenvalues of ρ are $p_+ = (1+r)/2$ and $p_- = (1-r)/2$ where $r = |\underline{r}| = p_+ - p_-$ and $r \leq 1$. If $F(x)$ is a function of the real variable x, then operator $F(\rho)$ may be written as

$$F(\rho) = \frac{1}{r}[p_+F(p_-) - p_-F(p_+)]I + \frac{1}{r}[F(p_+) - F(p_-)]\rho \qquad \text{(A-1a)}$$

$$= \frac{1}{2}[F(p_+) + F(p_-)]I + \frac{1}{r}[F(p_+) - F(p_-)]\underline{r}\cdot\underline{R} \qquad \text{(A-1b)}$$

and, in particular,

$$\rho\ln\rho = \frac{1}{4}[\ln\frac{1-r^2}{4} + r\ln\frac{1+r}{1-r}]I + \frac{1}{2}[\ln\frac{1-r^2}{4} + \frac{1}{r}\ln\frac{1+r}{1-r}]\underline{r}\cdot\underline{R} \qquad \text{(A-2)}$$

$$\mathrm{Tr}\rho\ln\rho = \frac{1}{2}[\ln\frac{1-r^2}{4} + r\ln\frac{1+r}{1-r}] \qquad \text{(A-3)}$$

Using Relation 3a and the commutation rules obeyed by the spin operators, we find

$$\frac{1}{2}\{H,\rho\} = \frac{1}{2}\hbar\Omega_o[\frac{1}{2}(\underline{\Lambda}\cdot\underline{r})I + \underline{\Lambda}\cdot\underline{R}] \qquad \text{(A-4)}$$

$$\mathrm{Tr}\rho H = \frac{1}{2}\hbar\Omega_o\underline{\Lambda}\cdot\underline{r} \qquad \text{(A-5)}$$

$$\mathrm{Tr}\rho H^2 = (\frac{1}{2}\hbar\Omega_o)^2 \qquad \text{(A-6)}$$

$$\mathrm{Tr}\rho H\ln\rho = \frac{1}{4}\hbar\Omega_o[\ln\frac{1-r^2}{4} + \frac{1}{r}\ln\frac{1+r}{1-r}]\underline{\Lambda}\cdot\underline{r} \qquad \text{(A-7)}$$

$$i[H,\rho] = -\hbar\Omega_o(\underline{\Lambda} \times \underline{r})\cdot\underline{R} \qquad \text{(A-8)}$$

The right-hand side of Equation 1a becomes

$$-\frac{1}{\tau}\,\frac{1-r^{2}}{2r}\ln\frac{1+r}{1-r}\,\frac{\underline{r}\cdot\underline{R}-r_{e}\underline{\Lambda}\cdot\underline{R}}{1-r_{e}^{2}} \tag{A-9}$$

Combining Equation 1 with Relations A-8 and A-9 and the fact that

$$\frac{d\rho}{dt}=\frac{d\underline{r}}{dt}\cdot\underline{R} \tag{A-10}$$

Equation 4 follows immediately.

APPENDIX B - EXISTENCE AND UNIQUENESS OF SOLUTIONS

As shown in Appendix A, for ρ in the set of state operators ($\rho^{\dagger} = \rho \geq 0$, $\mathrm{Tr}\rho = 1$), Equation 1 is equivalent to Equation 4 that we rewrite here as

$$\frac{d\underline{r}}{dt} = \underline{F}(\underline{r}) = \begin{cases} \Omega_o \underline{\Lambda} \times \underline{r} - \dfrac{1 - r^2}{2r} \ln\dfrac{1 + r}{1 - r} \dfrac{\underline{r} - r_e \underline{\Lambda}}{1 - r_e^2} & \text{if } r < 1 \\ \Omega_o \underline{\Lambda} \times \underline{r} & \text{if } r = 1 \end{cases} \qquad \text{(B-1)}$$

where $r = |\underline{r}|$, $r_e = \underline{\Lambda} \cdot \underline{r}$ and $\underline{r} \neq \pm\underline{\Lambda}$. We have seen that if $\underline{r}(t)$ is a solution of Equation B-1 then r_e is a constant with $-1 < r_e < 1$ and Equation 9 is satisfied, i.e.,

$$\frac{dr}{dt} = G(r) = \begin{cases} -\dfrac{1}{\tau} \dfrac{r^2 - r_e^2}{1 - r_e^2} \dfrac{1 - r^2}{2r^2} \ln\dfrac{1 + r}{1 - r} & \text{if } |r_e| \leq r < 1 \\ 0 & \text{if } r = 1 \end{cases} \qquad \text{(B-2)}$$

Here we will show that, for each initial condition in the Bloch sphere, Equation B-1 admits of a unique solution defined for $-\infty < t < +\infty$ and lying entirely in the Bloch sphere.

In the open region $D = \{\underline{r} | r < 1,\ \underline{r} \neq c\underline{\Lambda}\}$, the functions $F_j(r_1, r_2, r_3)$ ($\underline{F} = (F_1, F_2, F_3)$, Equation B-1) and the partial derivatives $\partial F_j / \partial r_k$ are defined and continuous. Therefore, for each $\underline{r}_o$ with $r_o < 1$ there exists a unique complete solution $\underline{r}(t)$ of Equation B-1, defined for $a < t < b$, such that $\underline{r}(0) = \underline{r}_o$.

Because $G(r) < 0$ in D, Equation B-2 implies that $r(t) < r_o < 1$ for every $0 \leq t < b$. Thus, the complete solution remains internal to D and bounded for every $0 \leq t < b$, and it must therefore extend to $b = +\infty$.

The solution, i.e, the one-parameter family of points $\underline{r}(t)$, remains on the plane orthogonal to vector $\underline{\Lambda}$ and defined by the constant $r_e = \underline{\Lambda}\cdot\underline{r}$. It spirals towards the equilibrium point $\underline{r}_e = r_e\underline{\Lambda}$ without ever reaching it at any finite time. This can be seen, for example, by integrating Equation B-2 to obtain

$$t_e = \int_0^{t_e} dt = \lim_{r\to r_e} \int_{r_o}^{r} \frac{dr'}{G(r')} = +\infty \tag{B-3}$$

because in r_e the function $1/G(r)$ is infinite of the same order as $1/(r_e - r)$.

The complete solution, defined for $a < t < +\infty$, either extends to $a = -\infty$ or else it approaches the outer boundary $FD = \{\underline{r}|r = 1\}$ of domain D as t tends to some finite $a < 0$. But the latter case is impossible because integration of Equation B-2 yields

$$a = \int_0^{a} dt = \lim_{r\to 1} \int_{r_o}^{r} \frac{dr'}{G(r')} = -\infty \tag{B-4}$$

where $r_o < 1$. Relation B-4 may be verified by observing that in $r = 1$ the function $-1/G(r)$ is infinite of the same order as the function $1/g(r)$ where

$$g(r) = \frac{1 - r^2}{2}\ln\frac{1 + r}{1 - r} \tag{B-5}$$

and

$$\lim_{r\to 1} \int_{r_o}^{r} \frac{dr'}{g(r')} = \lim_{r\to 1} \int_{r_o}^{r} d\ln\ln\frac{1 + r'}{1 - r'} = +\infty \tag{B-6}$$

We conclude that for each $\underline{r}_o$ in D Equation B-1 admits of a unique solution entirely contained in D for every $-\infty < t < +\infty$. As t tends to $+\infty$, the solution approaches a stable equilibrium point, $\underline{r}_e = r_e\underline{\Lambda}$. As t tends to $-\infty$, the solution approaches the boundary FD. On the boundary FD of its domain of definition, Equation B-1 admits of periodic solutions (the conventional quantum mechanical solutions) which precess around vector $\underline{\Lambda}$ at the angular frequency Ω_o and lie entirely on FD. These periodic boundary solutions could fail to be unique only by leaving the boundary FD in finite time. But this is impossible because of Relation B-4. It is also readily seen that, except for the fixed points $\underline{r} = \pm\underline{\Lambda}$, all boundary solutions are unstable.

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Feb. 7, 84

2.452 J and 22.572 J
Quantum Thermodynamics

Elias P. Gyftopoulos	24-109	3-3804
Gian Paolo Beretta	3-339	3-7921

Class hours Tu Th 1:30 – 3:00

Homework	40%
Mid-term	20%
Final take-home	40%.

Brief history

— Classical mechanics as a theory of nature. It has successfully explained many phenomena. For example, the motions of celestial bodies, the behavior of missiles, etc.

It involves such ideas as system, state, property or observable, changes of properties

— Classical thermodynamics as a theory of nature has also explained certain phenomena successfully. For example, the performance of engines, phase diagrams, chemical reactions.

It involves such ideas as system, state, property or observable, changes of state.

— Classical mechanics and classical thermodynamics have many similarities, such as the ideas just cited, the concept of energy and its conservation, etc. But they also have many differences. For example, in classical mechanics energy = adiabatic availability but in classical thermodynamics energy ≠ adiabatic availability = 0. Again, in classical mechanics there is no concept of entropy. but in classical thermodynamics entropy plays a key role.

— Hence the question "are these two theories related?"

The question has preoccupied the greatest scientists during the past 130 years (off and on).

Many objections but always some answer.
Maxwellian demon.

Names

Szilard
Maxwell, Boltzmann, Gibbs, Jaynes, Einstein to mention just a few.

The answer given under different names and different mathematical expressions is only one:

classical thermodynamics is a statistical description of macroscopic classical mechanics.

information theory

Explain what statistical means

Explain advantages and difficulties

Work to acquire information — Maxwellian demon

Meaning of entropy

— Quantum mechanics as a theory of nature. It includes classical mechanics as a special case but covers a broader class of phenomena

— Some reasons for introducing quantum mechanics

One-slit, two slit experiments.
Orbits around atoms
Photoelectric effect
Black-body radiation } Thermo.
Specific heat

— The relation between classical thermodynamics and quantum mechanics has been addressed over the past 50 years. (Landau, von Neumann, Jaynes Prigogine etc)-It was resolved in a manner similar to that proposed for the contrast between classical mechanics and classical thermodynamics, namely a statistical interpretation.

Objections were also raised
Work of identification.

— Are the laws of classical thermodynamics strictly applicable to macroscopic systems in thermodynamic equilibrium? In 2.451 J we generalized them and made them valid for all systems and all states.

— What are some of the distinguishing features of General Thermo?

State, entropy, all systems all states.

— How does this general thermo fit with other theories?

— To answer this question, we developed quantum thermodynamics. It includes both classical thermo and quantum mechanics (and therefore classical mechanics) as special cases.

— Despite these developments, statistical approaches are useful under certain circumstances.

So the panorama of the theories we will review is

Classical mechanics	Classical statistical mechanics
Quantum mechanics	Quantum 〃 〃
Quantum thermo	Quantum statistical thermo.

Question that emerge

What is a theory of nature? Is it reality itself?
Why and how do we change from theory to theory?
What are the key concepts of a theory?
What are the common concepts of a theory?
What are some applications?
What are some unresolved questions?

Our ultimate objective is to define quantum thermodynamics and show that it includes all of thermo and all of mechanics. Moreover that it is a theory that poses novel and challenging questions for all of physics

Central hypothesis to which we want to respond.

State is that of one system
Entropy is a property of one state of one system

Feb 9, 84.

Brief history.

- Classical mechanics
- Classical thermodynamics
- Statistical explanation of classical thermodynamics

- Quantum mechanics
- Statistical explanation of classical thermodynamics in terms of quantum mechanics

- All statistical theories reflect lack of knowledge, or lack of information.

- Generalize thermodynamics, for all systems and all states.
- Assume that it reflects inherent properties. How can it be explained.

- Develop quantum thermodynamics

- So we have to discuss
  classical mechanics
  quantum mechanics
  quantum thermo
  classical statistical mechanics
  quantum statistical mechani
  quantum statistical thermo

Classical mechanics

— **System**: One particle, one apple, the field in cavity

Degrees of freedom N.

Degrees of freedom are the number of independent ways by which we can change the configuration of the parts of the system. For example for a point particle in space we have 3 degrees of freedom, the three cartesian coordinates.

— **State**: Canonical

$$\left.\begin{array}{c} \underline{\text{Generalized coordinates}} \\ q_1, q_2, \dots, q_N \\ \underline{\text{Generalized momenta}} \\ p_1, p_2, \dots, p_N \end{array}\right\} \begin{array}{l} \text{one for each} \\ \text{degree of} \\ \text{freedom} \end{array}$$

For example, for a system of one particle moving in one dimension x, x may be the coordinate $q_1 = x$ and $p_1 = m\dot{x}$. In other cases, we may use polar coordinates etc.

— **Observables**: Each observable or property is a function of the state, the generalized coordinates and the generalized momenta

In particular, we can define the following

Kinematics
~~Statics~~

- Potential energy

$$V = V(q_1, q_2, \dots, q_N, \beta_1, \beta_2, \dots, \beta_s)$$

β_i = i-th constraint

- Forces

$$f_i = -\frac{\partial V}{\partial \beta_i}$$ body force i-th constraint

$$F_i = -\frac{\partial V}{\partial q_i}$$ interparticle force on i-th degree of freedom.

- Lagrangian function

$$L = T - V$$

$$T = \frac{1}{2}\sum_i \frac{p_i^2}{2m_i}$$ = kinetic energy

- Hamiltonian function

(Can be shown)

$$H = \sum_k^N p_k \dot{q}_k - L = H(p_k, q_k) = H(p, q)$$

Dynamics

Dynamics, or equation of motion, or causal evolution

$$\dot{q}_k = +\frac{\partial H}{\partial p_k} \qquad \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

For an one-dimensional motion of a particle in a box

$$q\,,\,p \qquad h = \frac{p^2}{2m} + V(q) \qquad V(q) = \begin{cases} 0 & 0 \leq q \leq a \\ \infty & q<0\,;\; q>a \end{cases}$$

$$\dot{q} = \frac{p}{m} = \frac{\partial h}{\partial p}\,; \quad \dot{p} = -\frac{\partial V}{\partial q} = -\frac{\partial h}{\partial q} = \begin{cases} 0 \\ -\infty \end{cases}$$

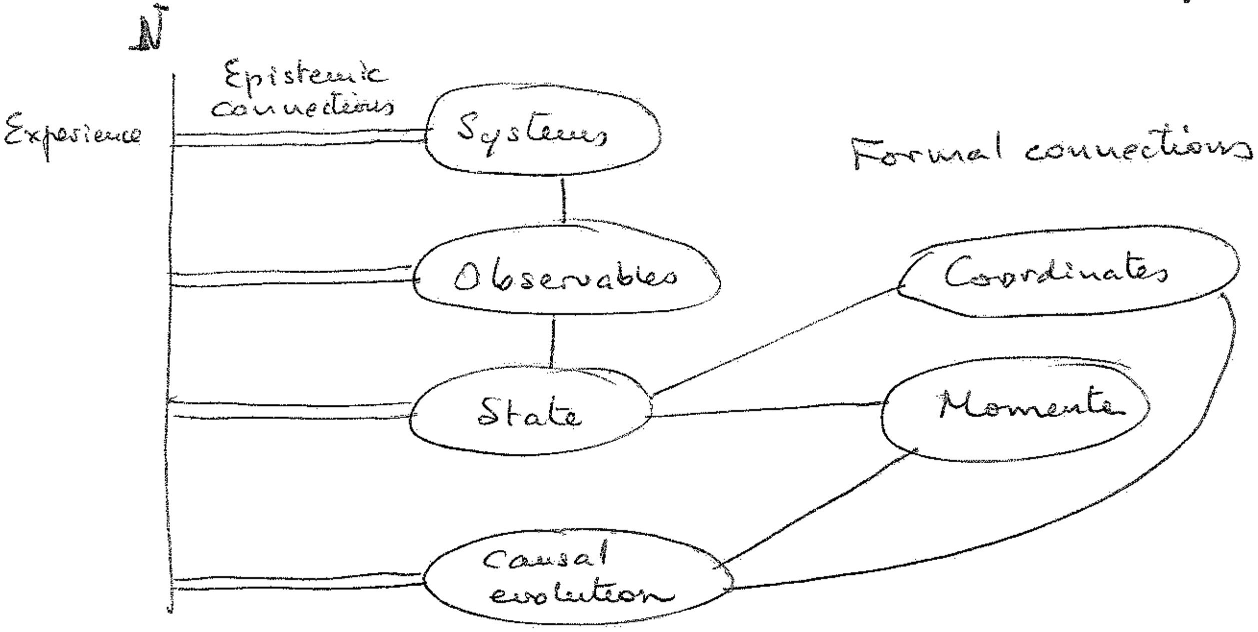
The simple example of classical mechanics gives us an opportunity to bring forth some key elements of the structure of a physical theory or a theory of Nature.

a Experience of world around us, given data

b. Out of this experience, we abstract concepts

c. We develop connections between concepts
These are called formal connections
We also develop connections between concepts and experience
These are called epistemic connections

We can exemplify these statements graphically



The rules of correspondence between experience and concepts and between concepts give structure to a theory of nature

There are many concepts that are common to to all theories, especially the epistemic connections. For example, the concepts of system, observables, state and causal evolution are common. There are others.

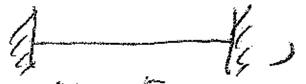
Let us now illustrate some formal connections for classical mechanics.

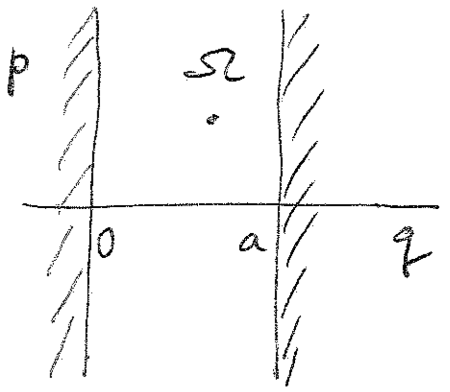
Kinematics

~~States~~

Phase space → space defined by q, p · Ω.

system → region in phase space. The phase space has as coordinates the canonical or generalized coordinates.

For example, for a structureless point particle in a one-dimensional box , the phase space will have coordinates p, q



This is a formal rule of correspondence between system and phase space

state → point in phase space: (q, p) is one state.

observable → function defined on phase space. For example, the energy function

$$h(q,p) = \frac{p^2}{2m} + V(q)$$

value of an observable → value of function associated with observable at a particular point in Ω, at a particular state.

Dynamics

causal evolution → Hamilton's equation of motion

For example

$$\dot{q} = \frac{\partial h}{\partial p} \quad \dot{p} = -\frac{\partial h}{\partial q}$$

Feb. 14, 84

<u>Classical mechanics</u>: Degrees of freedom

Generalized coordinates q

Generalized momenta p

Observables or properties $f(q,p)$

Potential energy V

Kinetic energy T

Lagrangian function $L = T - V$

Hamiltonian function $H = \sum_k p_k \dot{q}_k - L$

$= V + T = H(q,p)$

Equation of motion

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \; ; \; \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

H <u>generator of the motion</u>

<u>Example</u>

q, p $\quad q = x \quad p = m\dot{x}$

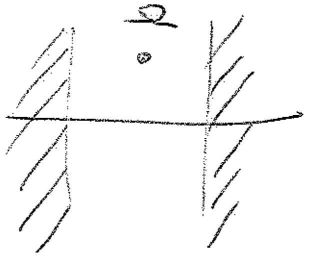
$$h = \frac{p^2}{2m} + V(q) \qquad V(q) = 0 \quad 0 \leq q \leq a$$

$$V(q) = \infty \quad q = 0 \quad q = a$$

$$\dot{q} = \frac{p}{m} = \frac{\partial h}{\partial p} \qquad \dot{p} = -\frac{\partial V}{\partial q} = \begin{cases} 0 & 0 \leq q \leq a \\ \infty & q = 0 \\ -\infty & q = a \end{cases}$$

Formal correspondence

Phase space



System → region in phase space

State → point in phase space

Property / observable → function defined on phase space

value of observable → value of function associated with observable at a particular point in Ω at a particular state

Dynamics → Hamilton's equation of motion

Hamiltonian is the generator of the motion

Paradigm of theory of nature

Example

q, p

$$h = \frac{p^2}{2m} + V(q) \qquad V(q) = \begin{cases} 0 & 0 \leq q \leq a \\ \infty & q = 0 \quad q = a \end{cases}$$

$$\dot{q} = \frac{p}{m} = \frac{\partial h}{\partial p}$$

$$\dot{p} = -\frac{\partial V}{\partial q} = -\frac{\partial h}{\partial q} \begin{cases} 0 & 0 \leq q \leq a \\ \infty & q = 0 \\ -\infty & q = a \end{cases}$$

Measurements

Preparations and Ensembles

~~An~~ ~~idea~~ question that we have not discussed up to now and that plays an important role in all theories of nature is "how do we assign values to observables or properties of systems?"

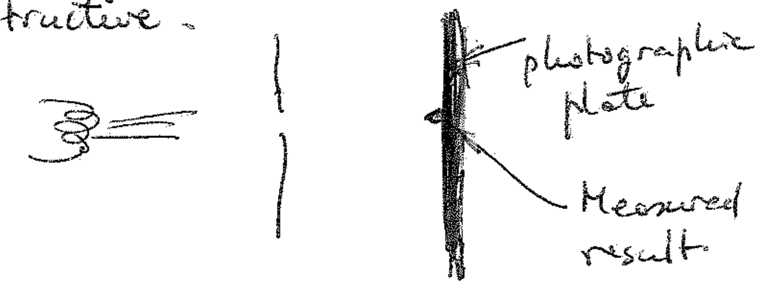
To explore this ~~idea~~ question, we introduce a couple of concepts that are common to all theories

1 Preparation : a reproducible scheme to "accept" a system for study. Such a scheme does not necessarily require an interaction of the preparer with the system

2 Measurement act of an observable : a reproducible scheme of operations on a system for the purpose of obtaining a precise numerical value which by virtue of the chosen experimental arrangement, can be assigned to a definite observable of the system in the condition prior to the measuremen

No errors are assumed here.

This scheme requires necessarily an interaction between the system and the measurement apparatus. It can be even destructive.



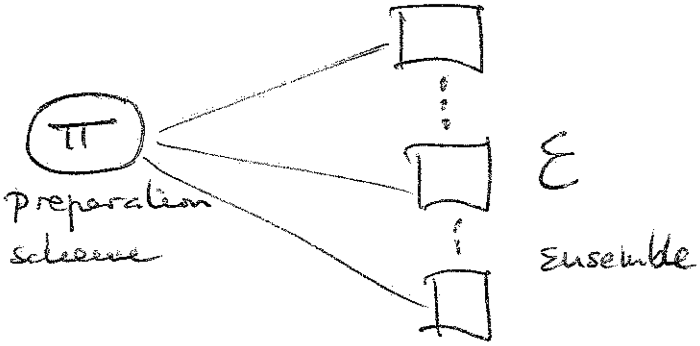
- Question – answer is the feature of measurement
- Errors are not relevant in the foundations of a theory of nature

It is of paramount importance that the observation of an observable be made <u>repeatedly</u> on a systems prepared identically

The <u>repeatability</u> of the measurement results, their <u>pattern</u>, is the data that the theory tries to regularize.

So we have another concept

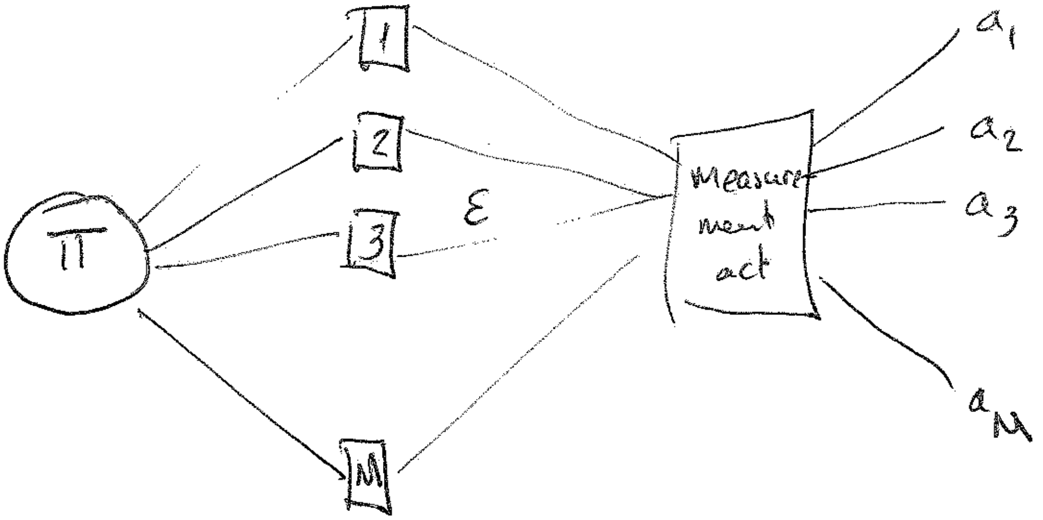
3 <u>Ensemble of identical systems, identically prepared, prepared by the same preparation:</u>



Each member prepared according to scheme Π.

4 Measured value of an observable for a given preparation

Arithmetic mean of measurement results of identica
measurement acts on an ensemble of identical
systems identically prepared.



Ensemble
$M \to \infty$

$$\langle A \rangle = \frac{1}{M} \sum_i^M a_i$$

$M \to \infty$

5 Complete characterization of a preparation:

the set of values $\{\langle A \rangle, \langle B \rangle, \dots\}$ of all conceivable observables

6 Identical preparations, identical ensembles

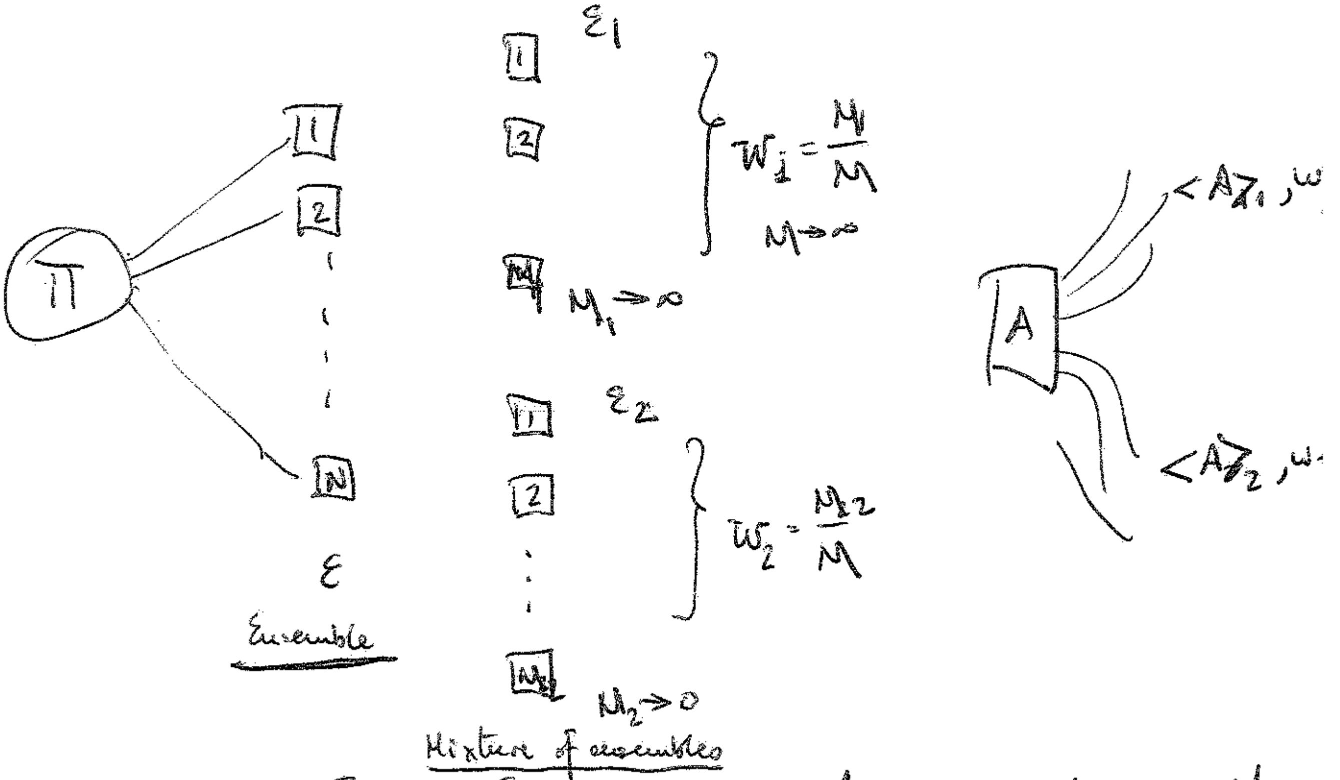
$\Pi_1 = \Pi_2$ if and only if $\langle A \rangle_1 = \langle A \rangle_2$

~~$\mathcal{E}_1 = \mathcal{E}_2$~~ for all conceivable observables.

$$\boxed{\Pi_1 = \Pi_2 \longrightarrow \mathcal{E}_1 \equiv \mathcal{E}_2}$$

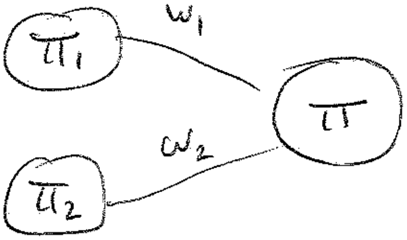
Note: Because in an ensemble $N \to \infty$, any finite subset of members does not affect the value of any observable because its contribution is reduced to zero in the limit $N \to \infty$.

7 Subdivision of ensembles



$$\mathcal{E} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2 \qquad \langle A \rangle = w_1 \langle A \rangle_1 + w_2 \langle A \rangle_2$$

8. We can think of each preparation as a statistical composition (of two or more) preparations (mixtures of ensembles)



$$\Pi = w_1 \times \Pi_1 \oplus w_2 \times \Pi_2$$

$$\mathcal{E} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$$

9. **Homogeneous ensemble $\mathcal{E}^0$ (Homogeneous preparation)**

One that cannot be conceived as a mixture of different subensembles

Any conceivable way of subdividing an $\mathcal{E}^0$ into two subensembles $\mathcal{E}^0 = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$ would yield

$$\mathcal{E}_1 = \mathcal{E}_2 = \mathcal{E}^0$$

$$\langle A \rangle_1 = \langle A \rangle_2 = \langle A \rangle_0$$

$$\langle B \rangle_1 = \langle B \rangle_2 = \langle B \rangle_0$$

$$\vdots \qquad \text{for all observables}$$

10. **Heterogeneous ensemble (heterogeneous preparatio**

A preparation and an ensemble that are not homogeneous.

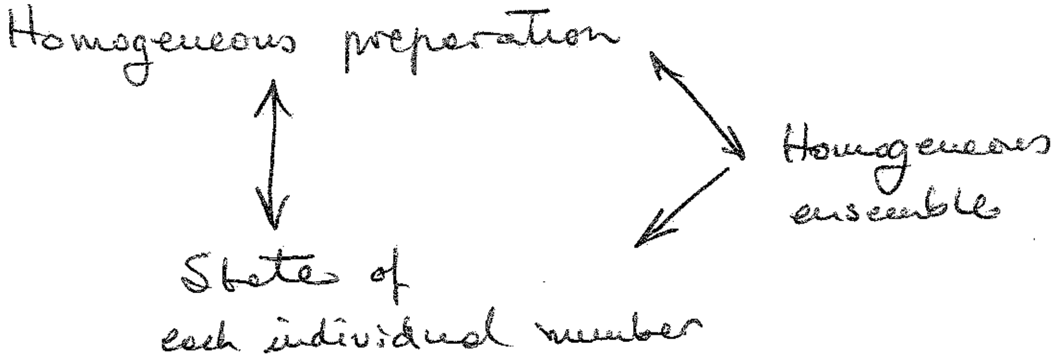
Why is a homogeneous ensemble so important

11. **Every member of a homogeneous ensemble is individually in exactly the same condition as each other member**

If there were members in different ~~states~~ conditions, then a subdivision into different subensembles would be possible

12 Individual state of a system

The condition of an individual system corresponding to a homogeneous preparation. The condition of each individual member of a homogeneous ensemble.



13. The value of an observable is a function of the preparation, "linear" in the statistical weights of its component preparations

$$a(\Pi) = \langle A \rangle_{\Pi}$$

$$\Pi = w_1 * \Pi_1 + w_2 * \Pi_2$$

$$a(\Pi) = \langle A \rangle_{\Pi} = w_1 \langle A \rangle_{\Pi_1} + w_2 \langle A \rangle_{\Pi_2}$$

$$= w_1\, a(\Pi_1) + w_2\, a(\Pi_2)$$

for all observables

(This would not be a good scheme for thermodynamics for nonlinear observables ?)

14. Resolution of a heterogeneous preparation into homogeneous components.

Given any preparation Π, how many ways should there be to resolve it into a statistical composition of homogeneous preparations?

The answer must be one and only one, if the homogeneous preparation is to have a meaning of state

Let us assume there are two different ways. so that

$$\Pi = w_1 * \Pi_1^0 (+) w_2 * \Pi_2^0 = w_3 * \Pi_3^0 (+) w_4 * \Pi_4^0$$

This implies that the ensemble Σ generated by Π has a fraction w_1 of members in state 1

w_2 – – – 2

w_3 – – – 3

w_4 – – – 4

Thus $w_1 w_3$ are in both state 1 and 3

$w_1 w_4$ – – 1 and 4

$w_2 w_3$ 2 and 3

$w_2 w_4$ 2 and 4

$$\sum w_i w_j = 1$$

Can we accept that a single system is simultaneously in more than one state?

So if the state is included as basic characteristic of one individual system, every preparation scheme Π must admit one and only one resolution into homogeneous preparations.

Feb. 16, 84

Preparations and ensembles

- Preparation
- Ensemble
- Measurement of an observable
- Measured value
- Complete characterization of a preparation
- Identical preparations, identical ensembles
- Subdivision of ensembles
- Statistical mixtures of preparations and ensembles.
- Homogeneous ensemble.
- Heterogeneous ensemble
- Individual state of an individual system
- Resolution of a heterogeneous preparation into homogeneous preparations: It is unique.

Feb 23, 84

— Classical mechanics as a preparation, ensemble, and distribution in phase space

$$\rho = \delta(\underline{q}-\underline{q}_0)\,\delta(\underline{p}-\underline{p}_0) = \rho(\underline{q},\underline{p})$$

$$a(\underline{q}_0,\underline{p}_0) = \int_\Omega \rho\, A(\underline{q},\underline{p})\, d\underline{q}\, d\underline{p}$$

— Classical Statistical Mechanics

$$\rho_\Pi(\underline{q},\underline{p})\, d\underline{q}\, d\underline{p}$$

$$\int_\Omega \rho_\Pi(\underline{q},\underline{p})\, d\underline{q}\, d\underline{p} = 1 \; ; \quad \int_\Omega \rho_\Pi(\underline{q},\underline{p})\, A(\underline{q},\underline{p})\, d\underline{q}\, d\underline{p} = a(\Pi)$$

— Statistical composition of preparations $\boxed{\text{Unambiguous theory}}$

$$\rho_\Pi(\underline{q},\underline{p}) = \int_\Omega d\underline{q}_0\, d\underline{p}_0\, \rho_\Pi(\underline{q}_0,\underline{p}_0)\, \delta(\underline{q}_0-\underline{q})\, \delta(\underline{p}_0-\underline{p})$$

- Uniqueness of decomposition in terms of states of classical mechanics

— Equation of motion

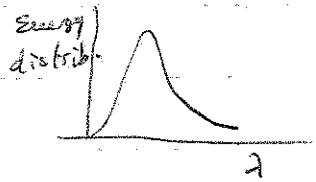
$$\frac{\partial\rho}{\partial t} = [H,\rho] \qquad \frac{d\rho}{dt} = 0$$

Liouville Equation

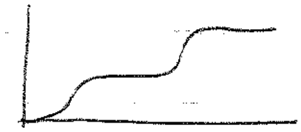
Explain how classical stat mech relates to thermo

Failures of classical mechanics

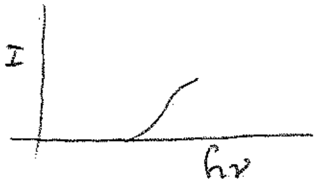
- Black body radiation



- Specific heats



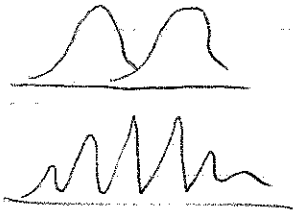
- Photoelectric effect



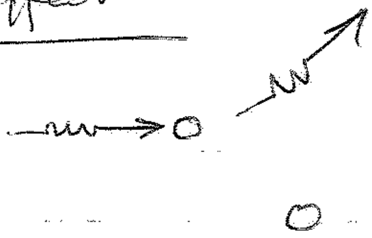
Light waves
Corpuscular nature

- Stability of atoms after discovery of + and − charges and concentration of + in the center

- Two slit experiment

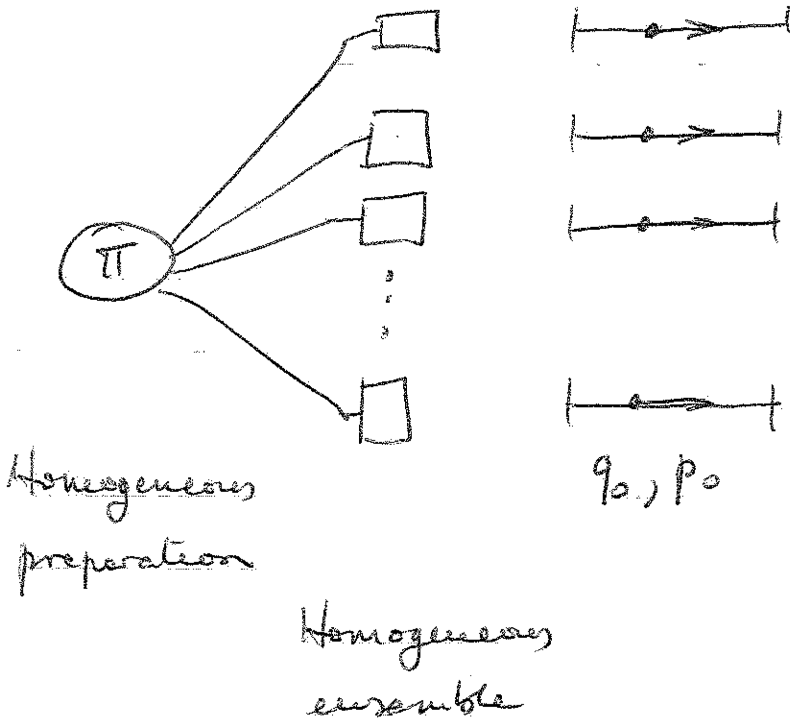


- Compton effect



Let illustrate the ideas of preparations and ensembles in the context of classical mechanics.

Classical mechanics deals with homogeneous preparations in the context of the classical paradigm of physics.



Every single member is in precisely the same condition q_0, p_0

Any subdivision into subensembles would yield a subensemble indistinguishable from any other

Representation of ~~a state~~ preparation as a density in phase space by a distribution ρ.

$$\rho = \delta(q-q_0)\,\delta(p-p_0)\ ;$$ $\rho\, dq\, dp$ = probability of finding system in q to $q+dq$ and p to $p+dp$

$$\iint \rho\, dq\, dp = 1\ ; \qquad \iint \rho\, A(q,p)\, dq\, dp = A(q_0,p_0)$$

For more degrees of freedom

$$\rho = \delta(q_1-q_{10})\,\delta(q_2-q_{20})\cdots\delta(p_1-p_{10})\,\delta(p_2-p_{20})\cdots$$
$$= \delta(\underline{q}-\underline{q}_0)\,\delta(\underline{p}-\underline{p}_0)$$ $\rho\, dq_1 dq_2 \cdots dp_1 dp_2 \cdots = \rho\, d\underline{q}\, d\underline{p}$, etc

Comment on the fact that each system is in a $\overset{\text{classical}}{\wedge}$ state in the context of classical mechanics

Classical statistical mechanics

Classical statistical mechanics is the branch of classical theory that describes heterogeneous preparations.
Heterogeneous preparations may be thought of as arising because of lack of knowledge or because of a systematic variation built in the preparation scheme.
Lack of knowledge: consider range of possibilities
Systematic variation: cut rods in different lengths

We describe a heterogeneous preparation by a distribution (more precisely by a measure) $\rho_\pi(\underline{q}, \underline{p})$ on phase space, such that

$\rho_\pi(\underline{q}, \underline{p})\, d\underline{q}\, d\underline{p}$ = probability that the system is found in a state that lies between $\underline{q}$ and $\underline{q} + d\underline{q}$ and $\underline{p}$ and $\underline{p} + d\underline{p}$

= fraction of systems in the ensembles that are in states between these values

$$\int_{\Gamma} \rho_\pi(\underline{q}, \underline{p})\, d\underline{q}\, d\underline{p} = 1$$

— Value of observable

$$a(\Pi) = \int_\Omega d\underline{q}\, d\underline{p}\ A(\underline{q},\underline{p})\, \rho_\Pi(\underline{q},\underline{p})$$

$$h(\Pi) = \int_\Omega d\underline{q}\, d\underline{p}\ H(\underline{q},\underline{p})\, \rho_\Pi(\underline{q},\underline{p})$$

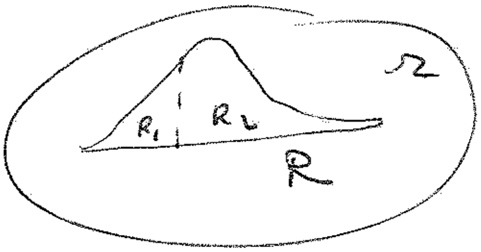
— Statistical composition of two preparations

$$\Pi = w_1 * \Pi_1 (+) w_2 * \Pi_2$$

$$\Big\downarrow$$

$$\rho_\Pi = w_1 \rho_{\Pi_1} + w_2 \rho_{\Pi_2} \qquad \rho_{\Pi_1}, \rho_{\Pi_2} \text{ distributions}$$

Are these two preparations homogeneous? To answer this question, we define the support R of ρ_Π as the region in phase space in which $\rho_\Pi \neq 0$.
Now, we observe that any region R can be subdivided into nonoverlapping subregions in many ways.



For example, $R = R_1 \cup R_2$, define

$$\rho_1 = \begin{cases} 0 & \text{if } \underline{q},\underline{p} \text{ in } R_2 \\ \dfrac{\rho_\Pi}{\int \rho_\Pi\, d\underline{q}\, d\underline{p}} & \text{-- " -- in } R_1 \end{cases} \qquad \Bigg| \qquad \rho_2 = \begin{cases} 0 & \text{if } \underline{q},\underline{p} \text{ in } R_1 \\ \dfrac{\rho_\Pi}{\int_R \rho_\Pi\, d\underline{q}\, d\underline{p}} & \text{.. -- } R_2 \end{cases}$$

$$w_1 = \int_{R_1} \rho_\pi \, d\underline{q} \, d\underline{p} \qquad w_2 = \int_{R_2} \rho_\pi \, d\underline{q} \, d\underline{p}$$

$$w_1 + w_2 = 1$$

Then

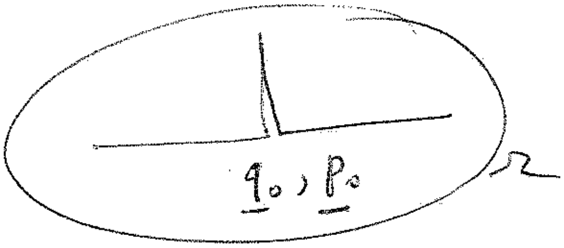
$$\rho_\pi(\underline{q}, \underline{p}) = w_1 \rho_1 + w_2 \rho_2$$

<u>So mathematically, we can always think of a ρ_π as a weighted sum of different ρ's, so these cannot be the unique resolution which corresponds to homogeneous preparations</u>

We can, however, select the support R as a single point in phase space.
Then we can write

$$\rho(\underline{q}, \underline{p}) = \delta(q - q_0)\, \delta(\underline{p} - p_0)$$

[illegible]



$$\rho_\pi(\underline{q}, \underline{p}) = \int_\Omega d\underline{q}_0 \, d\underline{p}_0 \; \rho_\pi(\underline{q}_0, \underline{p}_0)\, \delta(\underline{q}_0 - \underline{q})\, \delta(\underline{p}_0 - \underline{p})$$

These are the only irreducible preparations (homogeneous) which correspond one to one to states. Moreover every ρ_π can be uniquely resolved, the fractions being $\rho(q, p_0$

Consistency check

$$\rho(x) = \int w_1(x')\,\delta(x'-x)\,dx' = w_1(x)$$

$$= \int w_2(x')\,\delta(x'-x)\,dx' = w_2(x)$$

So, the decomposition is unique.

— Equation of motion

We consider a function $A(\underline{q}, \underline{p}, t)$ and wish to find how it changes with time. This change is due to two effects: the implicit changes of $\underline{q}$ and $\underline{p}$ with time, and the explicit change with t. Thus

$$\frac{dA}{dt} = \sum_i^N \left(\frac{\partial A}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial A}{\partial p_i} \frac{dp_i}{dt} \right) + \frac{\partial A}{\partial t}$$

$$= \sum_i^N \left(\frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial A}{\partial t}$$

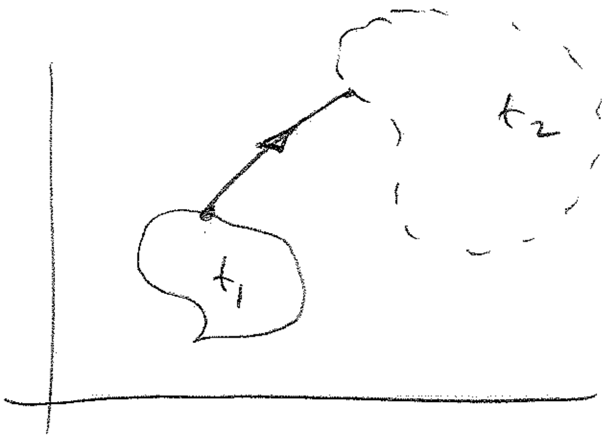
$$= \underbrace{[A, H]}_{\text{Poisson bracket}} + \frac{\partial A}{\partial t}$$

{ Here, we either specify $\frac{dA}{dt}$ or $\frac{\partial A}{\partial t}$.

Now regarding $\rho(\underline{q}, \underline{p}, t)$

$$\frac{d\rho}{dt} = [\rho, H] + \frac{\partial \rho}{\partial t}$$

The question now is "what is the value of $d\rho/dt$?"



Each point is a state.
It evolves according
to the Hamiltonian
laws. Trajectory is
unique. Number
of states inside volume
at t_1 is the same as at time t_2
Volume is one of the <u>Poincaré invariants</u>
Then density ρ (number of points over volume)
is invariant. So

$$\frac{d\rho}{dt} = 0$$

and

$$[\rho, H] + \frac{\partial \rho}{\partial t} = 0$$

or

$$\boxed{\frac{\partial \rho}{\partial t} = [H, \rho]}$$

<u>Liouville equation</u>

<u>Comment about statistical mechanics + thermo
but that it cannot do our job because we
do not have a state more general than classica
assoc. with a system.</u>

A new conceptual abstraction was required. It took decades to develop and had several false starts and misconceptions. It is called quantum mechanics

With the hindsight of 60 years of experience, we can summarize the new ideas that had to be introduced as follows

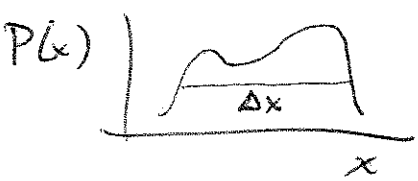
— Upon measurement of an observable, you get a precise answer. For example, you measure energy and you get a precise answer e_1

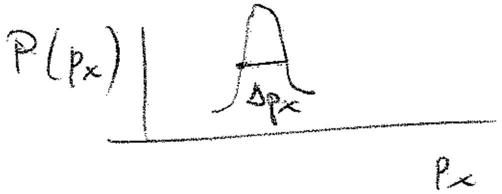
— Upon repeating the same measurement, ~~you get~~ on an identical system, identically prepared (homogeneous preparation), you get again a precise answer but not necessarily the same as the first measurement, etc. For example, you measure energy and you get a precise answer $e_2 \neq e_1$, etc.

— We cannot predict the outcome of a measurement even if we know all there is to know about the system at a given time.

— Results must be described probabilistically. Probabilities are inherent to the nature of things and not the result of lack of knowledge

— In particular, for certain pairs of observables





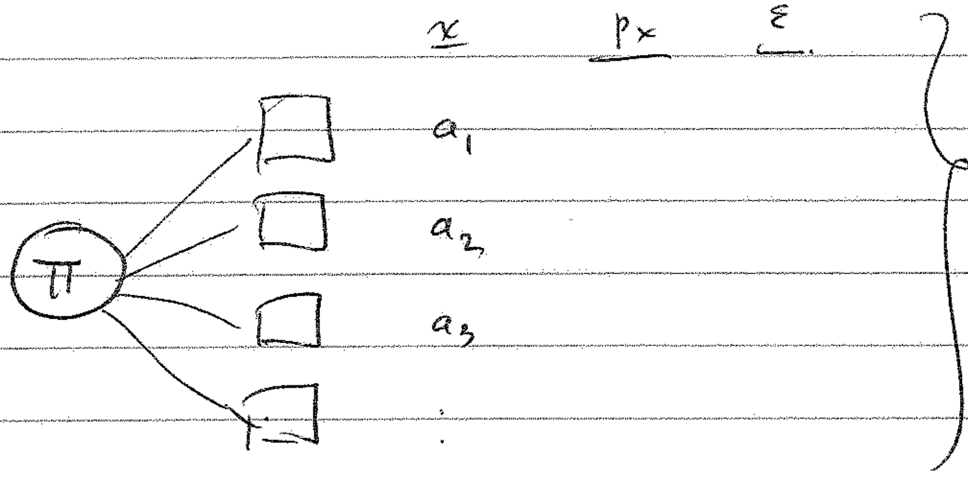
$$\Delta x \, \Delta p_x > h$$

Feb. 28, 84

– Failures of classical mechanics. – Examples

We have to accept that the theory is not valid anymore,

i.e. system → phase space
observable → function
value of observable
state → point in phase space



Quantum Mechanics

$$\overline{\frac{1}{N}\sum a_i}$$
$N \to \infty$

System → Hilbert space

State → Vector in Hilbert space

Observable → Operator on Hilbert space

Value of observable → Functional of of vector

etc.

The new mathematical representation cannot be in terms of phase space and functions on that space.

We must have a structure that can accommodate concepts such

Possible outcomes of measurements	Probability of outcome
e_1	p_{e_1}
e_2	p_{e_2}
$\vdots$	$\vdots$
e_N	p_{e_N}
	$\sum p_i = 1$

On other occasions, questions with yes/no answers might have to be considered

Is the energy e_3 ?

Outcome		Probability of outcome
yes	(1)	p_{e_3}
no	(0)	$1 - p_{e_3}$

It will turn out that we need quantum theory for whi

System → Hilbert space (phase space)
Observable → Operator on Hilbert space (function
State → Vector in Hilbert space (point)
Value of observable → Linear functional of vector. (value of function,
etc.

Mathematical preliminaries

Glossary

$\forall$	for every; for any; for each
$\in$	in; an element of; belonging to
$\exists$	there exists; there is
U	a unique
$\mid$	such that; where.

Scalar field : a set F of objects called "scalars" and denoted by a, b, … (english alphabet) which when subjected to the four arithmetic operation give again elements of the set F. Specifically,

sum $\forall a, b \in F \quad \exists U$ scalar $a+b \in F$

this scalar is called the sum of a and b.

$$\forall a, b, c \begin{cases} a+b = b+a \\ (a+b)+c = a+(b+c) \end{cases}$$

field is commutative

associative

$$\exists 0 \mid \quad 0+a = a$$

there exists a scalar 0
existence of zero

$$\forall a \ \exists (-a) \mid \quad a+(-a) = 0$$

existence of negative

product $\forall$ pair $a, b \in F$ $\exists U$ scalar $ab \in F$ called the product of a and b.

$$\forall\ a, b, c \left\{ \begin{array}{ll} ab = ba & \text{commutative} \\ (ab)c = a(bc) & \text{associative} \end{array} \right.$$

$\exists 1 \mid 1a = a$ existence of unity

$\forall a \neq 0\ \exists a^{-1} \mid aa^{-1} = 1$ existence of reciprocal

$\forall \alpha, b, c$ $a(b+c) = ab + bc$ distributive

Examples: $\mathbb{Q}$ (rational numbers)
$\mathbb{R}$ (real numbers)
$\mathbb{C}$ (complex numbers)

Vector Space V over a scalar field F

Vector space V is a set of objects, called "vectors" and denoted by $\alpha, \beta, \ldots \phi, \psi$ (greek alphabet) which when subjected to addition, and multiplication by a scalar again give elements of the set V. More precisely, they satisfy the following vector space axioms.

addition: $\forall\ \alpha, \beta \in V \quad \exists\, U$ vector $\alpha + \beta \in V$

$\alpha + \beta$ is called the sum of the vectors α, β

$$\forall \alpha, \beta, \gamma \quad \begin{cases} \alpha + \beta = \beta + \alpha & \text{commutative} \\ (\alpha+\beta)+\gamma = \alpha + (\beta + \gamma) & \text{associative} \end{cases}$$

$\exists\, 0_v \in V \ \big|\ \alpha + 0_v = \alpha$ existence of zero vector

$\forall \alpha\ \exists (-\alpha)\ \big|\ \alpha + (-\alpha) = 0_v$ existence of negative vector

multiplication by a scalar

$\forall \alpha \in V$ and $a \in F \quad \exists\, U \quad a\alpha \in V$

$\forall \alpha \qquad 1\alpha = \alpha$

$$\begin{matrix} \forall \alpha, \beta \in V \\ \\ \forall a, b \in F \end{matrix} \begin{cases} a(b\alpha) = ab(\alpha) \\ (a+b)\alpha = a\alpha + b\alpha \\ a(\alpha + \beta) = a\alpha + a\beta \end{cases}$$

Implications

$U \quad 0_v \in V$ uniqueness of zero vector

$U \quad (-\alpha) \in V$ uniqueness of negative vector

$\forall a \quad 0_F\, \alpha = 0_V$

Examples

$\mathbb{R}^3$ the space of three-dimensional analytic geometry (each vector characterized by a length and a direction) Verify all the rules

$\mathbb{R}^N$ generalization to N dimensions

$L^2(a,b)$ square integrable continuous, complex ~~functions~~ $\alpha(t), \beta(t) \dots$ of one variable t on the interval $a \leq t \leq b$

$$\int_a^b |\alpha(t)|^2 dt < \infty$$

$M_N(\mathbb{C})$ $N \times N$ matrices of complex numbers.

Others

Basis of a vector space

a subset $\{\xi_n\}$ of vectors in V such that

1. It spans V, i.e., $\forall \alpha \in V \ \exists \ \{a_n\} \in F \mid$

$$\alpha = \sum_n a_n \xi_n$$

2. The vectors ξ_n are linearly independent, i.e.,

$$\sum_n b_n \xi_n = 0 \quad \underbrace{\text{if and only if}}_{\text{iff}} \quad b_n = 0 \ \forall n$$

Coordinates of a vector α with respect to a basis ξ_n

The scalar coefficients a_n which enter the expansion

$$\alpha = \sum_n a_n \xi_n$$

Dimensionality of vector space V = number of vecto
in a basis. This number is the same for
all bases.

Examples: in $\mathbb{R}^3$ a set of three vectors with different directions. Dimensionality = 3.

in $L^2(a,b)$ the set of functions

$$\xi_n(t) = \exp\left(i n \frac{2\pi}{b-a} t\right) \quad \text{for} \quad n = -\infty, \dots, -1, 0, 1, \dots \infty$$

$$\alpha(t) = \sum_{n=-\infty}^{\infty} a_n \, \xi_n(t).$$ <u>Dimensionality = ∞</u>

Metric Space

A metric space is defined as a vector space in which a "<u>distance</u>", a "metric" d can be defined between any two vectors. In particular, if we denote the distance between α, β as $d(\alpha,\beta)$, then

$$d(\alpha,\beta) \;\Big|\; \forall\, \alpha, \beta, \gamma \in V$$

$$d(\alpha,\beta) \geq 0$$

$$d(\alpha,\beta) = 0 \quad \text{iff} \quad \alpha = \beta$$

$$d(\alpha,\beta) = d(\beta,\alpha)$$

$$d(\alpha,\beta) \leq d(\alpha,\gamma) + d(\gamma,\beta)$$ <u>triangular relation</u>

Examples

$\mathbb{R}^3$ with $d(\alpha,\beta) = (a_1-b_1)^2+(a_2-b_2)^2+(a_3-b_3)^2$

$L^2(a,b)$ with $d(\alpha,\beta) = \sum_{n=-\infty}^{\infty} (a_n-b_n)^2$

The a_i and b_i being the coordinates.

Complete metric space

A metric space V such that every Cauchy sequence is convergent

Cauchy sequence: (α_k) iff $\forall \varepsilon > 0 \ \exists K \mid \forall m,n \geq K$

$$d(\alpha_n, \alpha_m) \leq \varepsilon$$

March 1, 84.

— Scalar field F . $(a, b, ..)$

Sum, zero, negative, product, unity, reciprocal

Examples: Q Rational numbers

R Real numbers

C Complex numbers

— Vector space V over a scalar field F. $(\alpha, \beta, \cdot\cdot\, \psi, \omega)$

addition, multiplication by a scalar, zero, unity, negative ~~unity~~,

Examples: R^3 three dimensional analytic geometry

R^N N-th dimensional " "

$L^2(a,b)$

$$\int_a^b |\alpha(t)|^2 dt < \infty$$

$M_N(C)$ N×N matrices of complex numbers.

— Basis of a vector space $\{\xi_n\}$

$$\alpha = \sum_n a_n \xi_n \qquad \sum b_n \xi_n = 0 \qquad b_n = 0$$

Coordinates of a vector

Dimensionality of vector space

- Metric space : Distance $d(\alpha,\beta)$

$$d(\alpha,\beta) \geq 0$$

$$d(\alpha,\beta) = 0 \text{ iff } \alpha = \beta$$

$$d(\alpha,\beta) = d(\beta,\alpha)$$

$$d(\alpha,\beta) \leq d(\alpha,\gamma) + d(\gamma,\beta)$$

- Complete metric space   Cauchy sequence is convergent

- Cauchy sequence (α_k)
  iff $\forall \varepsilon > 0 \ \exists K \mid \forall m,n \geq K$

$$d(\alpha_n,\alpha_m) < \varepsilon .$$

Normed space

A vector space V equipped with a norm $\|\cdot\|$,

a positive measure, a positive number

$\forall\ \alpha, \beta \in V$, $\forall\ a \in F$, we have the following

$$\|\alpha\| \geq 0$$

$$\|\alpha\| = 0 \quad \text{iff} \quad \alpha = 0_v$$

$$\|\alpha + \beta\| \leq \|\alpha\| + \|\beta\|$$

$$\|a\alpha\| = |a|\,\|\alpha\|$$

Examples $\mathbb{R}^3$ $\quad \|\alpha\| = \sqrt{a_1^2 + a_2^2 + a_3^2}$

$L^2(a,b)$ $\quad \|a\|_1 = \int_a^b |\alpha(t)|\, dt$

$$\|a\|_2 = \sqrt{\int_a^b |\alpha(t)|^2 dt}$$

$$\|\alpha\| = \sqrt{\sum_{n=-\infty}^{\infty} |a_n|^2}$$

Note that a normed space can always be made metric by defining

$$d(\alpha, \beta) = \|\alpha - \beta\|$$

Banach space

A complete normed vector space, a normed space in which every Cauchy sequence is convergent

Scalar (or inner) product space is a

vector space V equipped with an inner product $\langle \cdot , \cdot \rangle$, i.e., a quantity defined such that

~~an inner product is defined such that~~

> **Hilbert Space**
> A complete inner product space

$\forall\ \alpha, \beta, \gamma \in V$ and $a \in F$

$$\langle \alpha, \alpha \rangle \geq 0$$

$$\langle \alpha, \alpha \rangle = 0 \quad \text{iff} \quad \alpha = 0$$

$$\langle \alpha, \beta + \gamma \rangle = \langle \alpha, \beta \rangle + \langle \alpha, \gamma \rangle$$

$$\langle \alpha, \beta \rangle = \langle \beta, \alpha \rangle^{*}$$ complex conjugate

$$\langle \alpha, a\beta \rangle = a \langle \alpha, \beta \rangle$$

Natural norm $\quad \|\alpha\| = \sqrt{\langle \alpha, \alpha \rangle}$

Examples of inner products

$\mathbb{C}^n$ or $\mathbb{R}^n$: The familiar n-dimensional euclidean space

$$x = (\xi_1, \xi_2, \dots, \xi_n) \quad ; \quad y = (\eta_1, \eta_2, \dots \eta_n)$$

Scalar product corresponds to the inner product.

$$\langle x, y \rangle = \sum_k \xi_k^* \eta_k$$

because it satisfies all the rules that we stated about the inner or scalar product.

$L^2(a, b)$, the square integrable complex functions defined on the set $a \le x \le b$ $\int_a^b |f(x)|^2 dx < \infty$

{Lebesgue integrable}

Scalar product

$$\langle f, g \rangle = \int_a^b f^*(x) g(x) \, dx$$

The space of absolute convergent sequences

$$x = (\xi_1, \xi_2, \dots, \xi_k, \dots)$$

$$\sum_{k=1}^{\infty} |\xi_k|^2 < \infty$$

Scalar product

$$\langle x, y \rangle = \sum_k^{\infty} \xi_k^* \eta_k$$

~~Note~~

~~Phase space~~

Hilbert space

A complete, inner product space. $\mathcal{H}$.

It has also a natural norm.

In Hilbert space we have

— Points or vectors or elements $\varphi, \psi, \dots$

The Hilbert space is equipped with a number of properties

— Space is closed under addition, and multiplication by a scalar in $\mathbb{C}$ (complex), i.e.

$$a\varphi + b\psi \in \mathcal{H}$$

given that $a, b \in F$ and $\varphi, \psi \in \mathcal{H}$.

In addition, the Hilbert space is (and has a)

— Complete: every sequence ψ_n converges to ψ in $\mathcal{H}$

— Metric: a distance $d(\psi, \varphi)$ is defined.

— Norm: a norm $\|\psi\|$ is defined

— Inner product: a scalar product $\langle \phi, \phi \rangle$ is defined.

The scalar products satisfies the following relation
For every ψ, φ in $\mathcal{H}$ and a in $\mathbb{C}$:

$$\langle \psi, \psi \rangle \geq 0$$

$$\langle \psi, \psi \rangle = 0 \quad \text{iff} \quad \psi = 0$$

$$\langle \psi, \varphi \rangle^* = \langle \varphi, \psi \rangle$$

$$\langle a\psi_1 + b\psi_2 , \varphi \rangle = a^* \langle \psi_1, \varphi \rangle + b^* \langle \psi_2, \varphi \rangle$$

$$= \langle \varphi , a\psi_1 + b\psi_2 \rangle^* = a^* \langle \varphi, \psi_1 \rangle^* + b^* \langle \varphi, \psi_2 \rangle^*$$

$$= a^* \langle \psi_1, \varphi \rangle + b^* \langle \psi_2, \varphi \rangle$$

In terms of the scalar product, we can define a natural norm and a metric.

$$\| \psi \| = \langle \psi, \psi \rangle^{1/2}$$

$$d(\psi, \varphi) = \| \psi - \varphi \| = \| \psi - \varphi \|$$

$$\boxed{\text{Note that phase space is contained in } \mathcal{H} = \mathbb{R}^{2N}}$$

Hilbert spaces

Examples.

$$\left.\begin{array}{l} \mathbb{C}^n , \ \mathbb{R}^n \\ x = (\xi_1, \dots, \xi_n) \\ \langle x, y \rangle = \sum_k \xi_k^* \eta_k \end{array}\right\} \text{notation}$$

$L^2(a,b)$, the square integrable complex functions defined on the set $a \leq x \leq b$

$$\int_a^b |f(x)|^2 dx < \infty$$

$$\langle f, g \rangle = \int_a^b f^*(x) g(x) \, dx$$

The space of absolute convergent sequences

$$\sum_{k=1}^{\infty} \xi_k^2 < \infty \qquad \langle x, y \rangle = \sum \xi_k^* \eta_k$$

Many more variables

March 6, 84

- Normed space $\| \cdot \|$
- Banach space: A complete normed vector space
- Scalar or inner product $< \cdot , \cdot >$

$$<\alpha, \alpha> \geq 0$$

$$<\alpha, \alpha> = 0 \quad \text{iff} \quad \alpha_v = 0$$

$$<\alpha, \beta + \gamma> = <\alpha, \beta> + <\alpha, \gamma>$$

$$<\alpha, \beta> = <\beta, \alpha>^*$$

$$<\alpha, a\beta> = a<\alpha, \beta>$$

$$\|\alpha\| = \sqrt{<\alpha, \alpha>}$$

- Hilbert space; a complete inner product space.

Examples $\mathbb{C}^n$, $\mathbb{R}^n$

~~$<x, y> = \sum$~~ [illegible]

$L^2(a, \beta)$

$$< f, g > = \int_a^b f^* g \, dx$$

Quantum mechanics.

In quantum mechanics we have again the concepts of $\underbrace{\text{system, observable, value of observable, state}}_{\text{statics}}$

$\underbrace{\text{equation of motion}}_{\text{dynamics}}$

We also have two key characteristics of measurements that are not present in classical mechanics. Specifically, if we consider a homogeneous preparation and the corresponding homogeneous ensembles generated by this preparation, we have to cope with the facts that

- Each measurement of an observable yields in general a different precise answer
- Each answer can be predicted only probabilistical

It turns out that we can accommodate the statics by making a theory of nature that has the following correspondences between concepts and mathematical representations.

System → Hilbert space $\mathcal{H}$.
Observables → Operators on Hilbert space
States ~~State~~ → vector in Hilbert space
Value of observable → functional on Hilbert space

For the dynamics, we have

Dynamics → Schroedinger's equation of motion.

The question now is how we select the operators, the vectors, etc.

There are different ways to approach the answers to these questions, and each textbook or author uses one ~~of~~ more of these

We will use the approach related to that of ~~developed by~~ Dirac. and we will build it up gradually so that we can develop some feeling for its inner workings.

We consider a homogeneous preparation a homogeneous ensemble, and the state of each individual system as being ψ.

We start by considering a <u>special observable</u> Q_a stated in the form of a question, i.e.,

$\underline{Q_a} \equiv$ <u>does measurement of observable A yield answer a</u>?

The possible answers to this question are

<u>Yes</u>
<u>No</u>

and we can arbitrarily associate the <u>value unity</u> with <u>yes</u> and the <u>value zero</u> with <u>no</u>, so that

Yes	1
No	0.

Now if we make measurements of Q_a on a homogeneous ensemble, we can determine the value of Q_a

$$\text{value of } Q_a = \underbrace{\langle Q_a \rangle}_{\text{= fraction of answers } a} = \underbrace{q_a(\psi)}_{\text{= functional on } \mathcal{H}} = \underset{N \to \infty}{\underline{\frac{N_1}{N}(1) + \frac{N_2}{N}(0)}}$$

Clearly $\underline{0 \le q_a(\psi) \le 1}$ <u>unique value</u>.

<u>We see immediately a contrast with C.M. because</u> in C.M. $q_a = \begin{cases} 1 \\ 0 \end{cases}$ whereas here we can also have values in between.

We can consider another observable $Q_{\bar{a}}$ corresponding to the opposite question

$Q_{\bar{a}} \equiv$ does measurement of observable A yield a value different from a?

Again we have two possible answers	Yes	1
	No	0

and then

$$\text{value of } Q_{\bar{a}} = \langle Q_{\bar{a}} \rangle = q_{\bar{a}}(\psi) = \frac{N_1}{N}(0) + \frac{N_2}{N}(1)$$

= fraction of answers $\bar{a}$

$N \to \infty$

= functional on $\mathcal{H}$

and $0 \leq q_{\bar{a}}(\psi) \leq 1$

$$q_a(\psi) + q_{\bar{a}}(\psi) = 1$$

Results of measurements are quantized but value is continuous

We can be a little bit more explicit about our mathematics. We define two subspaces in Hilbert space such that

$$\mathcal{H}_a = \{ \psi \mid q_a(\psi) = 1 \}$$

We call all the ψ's here ψ_a

$$\mathcal{H}_{\bar{a}} = \{ \psi \,/\, q_a(\psi) = 0 \}$$

We call all the ψ's here $\psi_{\bar{a}}$

In other words, for all the ψ_a's the answer would be yes and for all the $\psi_{\bar{a}}$ the answer would be no. ~~to~~ the question "is value of A_{op} equal to a?".

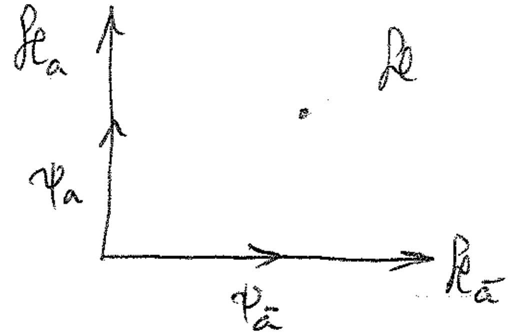
We assume select that ψ_a, $\psi_{\bar{a}}$ are orthogonal,

i.e.

$$< \psi_a , \psi_{\bar{a}} > = 0$$

Because we can always select them orthogonal

Then we say that $\mathcal{H}_a$ and $\mathcal{H}_{\bar{a}}$ are orthogonal subspaces



Clearly the two subspaces are disjoint because the answer to the question cannot be simultaneously yes and no.

Now, what is the functional $q_a(\psi)$? To answer the question, we consider a ψ that is neither in $\mathcal{H}_a$ nor in $\mathcal{H}_{\bar{a}}$ but has components in both $\mathcal{H}_a$ and $\mathcal{H}_{\bar{a}}$. So we write

$$\psi = \psi_a + \psi_{\bar{a}}$$

ψ_a is the projection of ψ onto $\mathcal{H}_a$ $= P_{\mathcal{H}_a}\psi$

$\psi_{\bar{a}}$ is the projection of ψ onto $\mathcal{H}_{\bar{a}}$ $= P_{\mathcal{H}_{\bar{a}}}\psi$

So we define an operator $P_{\mathcal{H}_i}$ which when applied on a vector ψ in $\mathcal{H}$ yields a vector ψ_i in Hilbert subspace $\mathcal{H}_i$ of $\mathcal{H}$. It is called a projection operator or a projector for all i's.

Now

$$\|\psi\|^2 = \|\psi_a + \psi_{\bar{a}}\|^2 = \langle \psi_a + \psi_{\bar{a}}, \psi_a + \psi_{\bar{a}} \rangle$$

$$= \langle \psi_a, \psi_a \rangle + \langle \psi_a, \psi_{\bar{a}} \rangle$$

$$+ \langle \psi_{\bar{a}}, \psi_a \rangle + \langle \psi_{\bar{a}}, \psi_{\bar{a}} \rangle$$

$$= \|\psi_a\|^2 + \|\psi_{\bar{a}}\|^2$$

$$1 = \frac{\|\psi_a\|^2}{\|\psi\|^2} + \frac{\|\psi_{\bar{a}}\|^2}{\|\psi\|^2}$$

So ~~ife~~ ~~we~~ define

$$q_a(\psi) = \frac{\|\psi_a\|^2}{\|\psi\|^2} \qquad q_{\bar{a}}(\psi) = \frac{\|\psi_{\bar{a}}\|^2}{\|\psi\|^2}$$

We satisfy the conditions imposed on the q's. Is it unique?

This simplifies if we select $\|\psi\|^2 = 1$ — ψ is normalized

Note further that

$$\underline{\|\psi_a\|^2 = \underline{\langle \psi_a, \psi_a \rangle} = \underline{\langle \psi, \psi_a \rangle} = \underline{\langle \psi, P_{\mathcal{H}_a} \psi \rangle}}$$

$$\underline{q_a(\psi) = \frac{\langle \psi, P_{\mathcal{H}_a} \psi \rangle}{\langle \psi, \psi \rangle}}$$

$$\underline{q_{\bar{a}}(\psi) = \frac{\langle \psi, P_{\mathcal{H}_{\bar{a}}} \psi \rangle}{\langle \psi, \psi \rangle}}$$

We call $\underline{\mathcal{H} = \mathcal{H}_a \oplus \mathcal{H}_{\bar{a}} \quad \text{direct sum}}$

$$\underline{\psi = P_{\mathcal{H}_a} \psi + P_{\mathcal{H}_{\bar{a}}} \psi .}$$

$$\underline{= \psi_a + \psi_{\bar{a}} .}$$

Note that $\psi = \psi_a \qquad q_a(\psi) = 1 \qquad q_{\bar{a}}(\psi) = 0$

$\psi = \psi_{\bar{a}} \qquad q_a(\psi) = 0 \qquad q_{\bar{a}}(\psi) = 1$

Next, we will consider an observable A with a long list of possible outcomes of measurements of A, i.e.;

$$a_1, a_2, \dots, a_j, \dots$$

We can capitalize on the previous results and formulate the following problem

- What is the operator that represents A?

To answer this question we proceed as follows. For each outcome of a measurement on a homogeneous ensemble we define the question

$$Q_{a_j} \equiv \text{is the result of measurement of observable } A \text{ equal to } a_j\,?$$

If we make an A measurement we answer all these questions.

The arithmetic mean of this question is

$$\langle Q_{a_j} \rangle = q_{a_j}(\psi) = \langle \psi, P_{\mathcal{M}_{a_j}} \psi \rangle$$

where $\langle Q_{a_j} \rangle$ is the fraction of times that we get the value a_j

It follows that the arithmetic mean of A will be

$$\langle A \rangle = a_1 \langle Q_{a_1} \rangle + a_2 \langle Q_{a_2} \rangle + \cdots = \sum a_i \langle Q_{a_i} \rangle$$

We can write this result in functional form so that

$$\underline{a(\psi)} = \sum_i a_i \, q_{a_i}(\psi)$$

$$= \sum_i a_i < \psi, P_{\mathcal{H}_{a_i}} \psi >$$

$$= \sum_i < \psi, a_i P_{\mathcal{H}_{a_i}} \psi >$$

$$= < \psi, \left(\sum_i a_i P_{\mathcal{H}_{a_i}} \right) \psi >$$

Let us define an operator

$$\underline{A \equiv \sum_i a_i P_{\mathcal{H}_{a_i}}}$$

What does it do?

a. $\underline{a(\psi) = < \psi, A \psi >}$

b. $A\psi = \sum_i a_i P_{\mathcal{H}_{a_i}} \psi = \underline{\sum_i a_i \psi_{a_i}}$

Linear operator

$$A \quad \mathcal{H} \to \mathcal{H} \quad , \psi \to A\psi$$

$$A(a\varphi + b\psi) = aA\varphi + bA\psi$$

Identity operator

$$I\psi = \psi \qquad IA = AI = A$$

Projection operator P

$$P^2\psi = P\psi \qquad P^2 = P$$

$$I(\cdot) = \sum \eta_j \langle \eta_j , \cdot \rangle$$

$$= \sum P_{\mathcal{H}_{\eta_j}}(\cdot)$$

Adjoint operator $\langle A^+\psi, \varphi \rangle = \langle \psi, A\varphi \rangle$

Self adjoint $A^+ = A$

Unitary $U^{-1} = U^+$

Recall that we established that if an observable yields values $a_1, a_2,$ upon measurement then it can be represented by an operator

It will be self adjoint because a_i are real

$$A = \sum a_i P_{\mathcal{H}_{a_i}}$$

$$\boxed{A\psi_{a_i} = a_i \psi_i}$$

And if the state is ψ, then the probability or frequency of observing a_i is

$$q_{a_i}(\psi) = \langle \psi, P_{\mathcal{H}_{a_i}} \psi \rangle = \| \psi_{a_i} \|^2$$

$$\psi = \sum \psi_{a_i} = \sum P_{\mathcal{H}_{a_i}} \psi.$$

Now suppose we are given the operator A
How do we proceed?

Eigenvalue problem of a self-adjoint operator

$$A\psi = a\psi$$

Linear Hermitian operator

Solutions are: a_k eigenvalues

α_{kd} eigenfunctions

$$\boxed{A\,\alpha_{kd} = a_k\,\alpha_{kd}}$$

Because the operator is self-adjoint,

$\langle \alpha_m, A a_n\rangle = a_n\langle a_m, a_n\rangle$

$\langle A a_m, a_n\rangle = \langle a_m, A^{\dagger} a_n\rangle = a_m^{*}\langle a_m, a_n\rangle$

$\{\alpha_{kd}\}$ forms an orthogonal (normal) basis for $\mathcal{H}$

a_k are real

Every ψ ~~can be written as~~ of the form

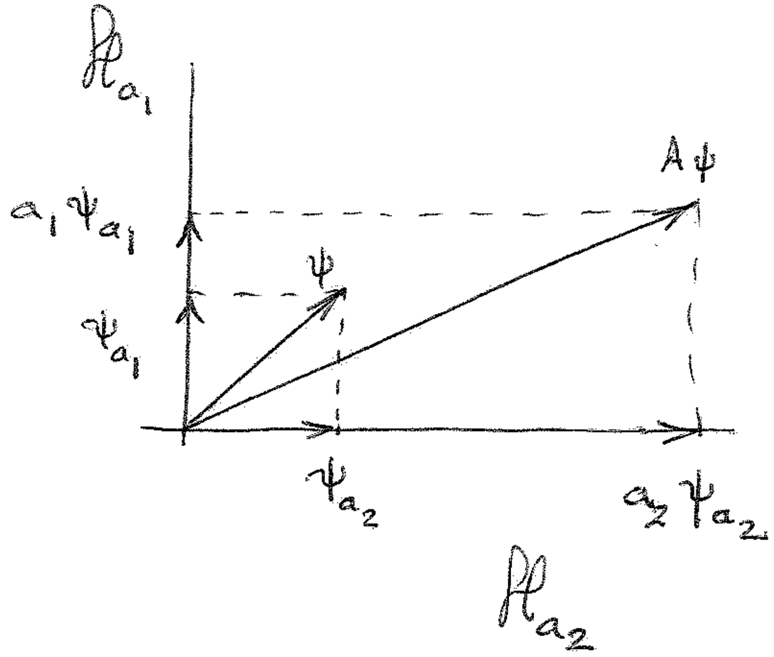
$$\psi = \sum_{d=1}^{D_k} c_d\,\alpha_{kd}$$

is an eigenvector belongi

to a_k

Degeneracy of a_k D_k

$$\mathcal{H}_{a_k} = \left\{ \psi \;\middle|\; \psi = \sum_{d=1}^{D_k} c_d\,\alpha_{kd} \right\}$$


$\mathcal{H}_{a_1}$
$A\psi$
$a_1\psi_{a_1}$
ψ
ψ_{a_1}
ψ_{a_2}
$a_2\psi_{a_2}$
$\mathcal{H}_{a_2}$

March 8, 84

— Correct states into kinematics

— Hilbert space

Vector ψ

Homogeneous preparation

Questions: Q_a measurement of A yields a?

$Q_{\bar{a}}$ – of A does not yield a?

$q_a(\psi)$ fraction of answers a

$q_{\bar{a}}(\psi)$ fraction of answers not a

$$\mathcal{H}_a = \{\psi \mid q_a(\psi) = 1\}$$

$$\mathcal{H}_{\bar{a}} = \{\psi \mid q_a(\psi) = 0\}$$

Direct sum

$$\mathcal{H} = \mathcal{H}_a \oplus \mathcal{H}_{\bar{a}}$$

$$\psi = \psi_a + \psi_{\bar{a}} \qquad \langle \psi, \psi \rangle = 1 = \|\psi\|^2$$

$$q_a(\psi) = \langle \psi, P_{\mathcal{H}_a}\psi \rangle$$ probability

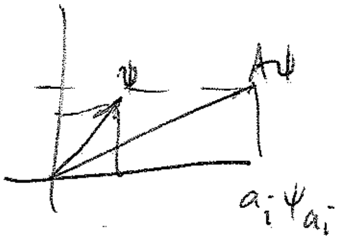
$$q_{\bar{a}}(\psi) = \langle \psi, P_{\mathcal{H}_{\bar{a}}}\psi \rangle$$ – " –

— <u>Observable A</u>

$$\langle A \rangle = a(\psi) = \underline{\sum \langle \psi, \left(\sum_i a_i P_{\mathcal{H}_{a_i}}\right) \psi \rangle}$$

$$= \underline{\langle \psi, A\psi \rangle = \sum_i a_i q_{\mathcal{H}_{a_i}}(\psi) = \sum_i a_i \langle Q_{a_i} \rangle}$$

$$\underline{A = \sum a_i P_{\mathcal{H}_{a_i}}}$$



$$\underline{A\psi = \sum_i a_i P_{\mathcal{H}_{a_i}} \psi = \sum_i a_i \psi_{a_i}}$$

Having established some of the features of vectors, operators, projectors, etc., we will proceed a little more formally in manipulations of · Hilbert space

$\mathcal{H}$

$\psi, \varphi, \ldots$ vectors in Hilbert space $\mathcal{H}$
$a, b, \ldots$ scalars in $\mathbb{C}$
$\langle \psi, \varphi \rangle$ scalar product on $\mathcal{H}$
$\alpha^*, \beta^*, \ldots$ linear functionals on $\mathcal{H}$ } mappings, functions, transformations
$A, B, \ldots$ operators on $\mathcal{H}$

Examples

Operator $A\psi \to \varphi$ — Hilbert to Hilbert $\mathcal{H} \to \mathcal{H}$

Linear functionals on $\mathcal{H}$

functional α^*: takes you from Hilbert $\mathcal{H} \to \mathbb{C}$ Scalar

$$\psi \to \alpha^*(\psi)$$

linear $\alpha^*(a\psi_1 + b\psi_2) = a\,\alpha^*(\psi_1) + b\,\alpha^*(\psi_2)$

Representation Theorem

We are going to define α^* so that

To every α^* on $\mathcal{H}$ there corresponds a unique vector α in $\mathcal{H}$ such that

$$\alpha^*(\cdot) = \langle \alpha, \cdot \rangle$$

Theorem: All bases for a $\mathcal{H}$ have the same number of elements

N = dimensionality of $\mathcal{H}$

Linear operators on $\mathcal{H}$

Operator $A : \mathcal{H} \to \mathcal{H} \quad \psi \to A\psi$

Linear $A(a\psi_1 + b\psi_2) = aA\psi_1 + bA\psi_2$

Identity operator

$$I : \quad I\psi = \psi \quad \text{for every } \psi$$

c-Number operator

$$C : \quad C\psi = c\psi \quad \text{for every } \psi$$

$$CI = c$$

Orthogonal ~~Orthogonal~~ Projection operator or projector

$$P : \quad P^2\psi = P(P(\psi)) = P\psi$$

$$P_1 P_2 = \delta_{12} P_2$$

Coordinates of ψ with respect to an orthonormal basis $\{\eta_j\}$

First we write

$$\psi = \sum_j c_j \eta_j$$

Next we define the mapping η_j^*. We will show that

$$c_j = \eta_j^*(\psi) = < \eta_j , \psi >$$

Indeed

$$\eta_j^*(\psi) = <\eta_j , \sum_i c_i \eta_i > = <\eta_j , \psi >$$

$$= \sum c_i < \eta_j , \eta_i > = \sum_i c_i \delta_{ij} = c_j$$

$$\psi = \sum c_j \eta_j = \sum_j < \eta_j , \psi > \eta_j$$

Remark. The set $\mathcal{H}^*$ of all linear functionals on $\mathcal{H}$ forms a Hilbert space, which is in one-to-one correspondence with $\mathcal{H}$. It is called the dual space of $\mathcal{H}$.

Basis for $\mathcal{H}$.

A set $\{\eta_j\}$ of vectors in $\mathcal{H}$ is called a basis for $\mathcal{H}$ if it is

- complete: i.e. for every ψ in $\mathcal{H}$ there exist c_j such that

$$\psi = \sum_j c_j \eta_j$$

- linearly independent, i.e., $\sum a_j \eta_j = 0$ iff $a_j = 0$ for all j

Orthonormal basis for $\mathcal{H}$

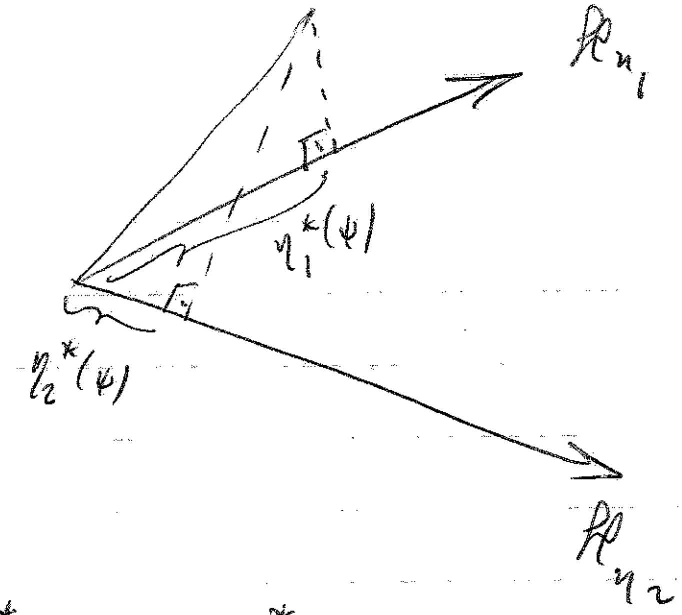
if in addition to being a basis

$$\langle \eta_i, \eta_j \rangle = \delta_{ij} \begin{cases} \langle \eta_j, \eta_j \rangle = 1 & \text{normaliz} \\ \langle \eta_i, \eta_j \rangle = 0 \quad i \neq j & \text{orthogonal} \end{cases}$$

Examples

$$P_{\mathcal{H}_{\eta_1}}\psi = \eta_1\, \eta_1^*(\psi) = \eta_1 < \eta_1, \psi >$$

$$P_{\mathcal{H}_{\eta_2}}\psi = \eta_2\, \eta_2^*(\psi) = \eta_2 < \eta_2, \psi >$$



$$P_{\mathcal{H}_{\eta_1} \oplus \mathcal{H}_{\eta_2}}(\psi) = \eta_1\, \eta_1^*(\psi) + \eta_2\, \eta_2^*(\psi)$$

$$P_{\mathcal{H}_{\eta_1} \oplus \mathcal{H}_{\eta_2}} = \eta_1 < \eta_1, \cdot > + \eta_2 < \eta_2, \cdot >$$

Resolution of identity operator into projectors

$$I(\ ) = \sum_j \eta_j < \eta_j, \cdot > = \sum_j P_{\mathcal{H}_{\eta_j}}(\cdot)$$

Resolution
of identity
into projecto
Completeness

Projection on a d-dimensional subspace $\mathcal{H}_n$

$\{\eta_{i_n}\}$ a basis for $\mathcal{H}_n$ with d vectors
d dimensional

$$P_{\mathcal{H}_n}(\cdot) = \sum_{i_n=1}^{d} P_{\mathcal{H}_{\eta_{i_n}}}(\cdot) = \sum_{i_n=1}^{d} \eta_{i_n} \langle \eta_{i_n}, \cdot \rangle$$

Adjoint operator $A^\dagger$

$\langle A^\dagger \psi, \varphi \rangle = \langle \psi, A\phi \rangle$ for all ψ and ϕ

Self adjoint

$$A^\dagger = A$$

Unitary

$$U^{-1} = U^\dagger \qquad U = \exp(iG) \qquad G^\dagger = G$$

?

Preserves norm: $\|U\psi\| = \|\psi\|$

Preserves scalar product $\langle U\psi, U\varphi\rangle = \langle \psi, \phi \rangle$

$\langle \psi, U^\dagger U \varphi \rangle$

$\langle \psi, U^{-1} U \varphi \rangle$

March 13, 84

$\mathcal{H}$

$\psi, \varphi, \ldots$ vectors

$a, b, \ldots$ scalar

$\langle \psi, \varphi \rangle$ inner product

α^*, β^* linear functionals

A, B operators

$$\alpha^*(\psi) \qquad \overset{\mathcal{H}}{\psi} \to \overset{\mathbb{C}}{\mathbb{C}}$$

Functionals

Linear $\alpha^*(a\varphi + b\psi) = a\alpha^*(\varphi) + b\alpha^*(\psi)$

Representation theorem $\alpha^*(\cdot) = \langle \alpha, \cdot \rangle$

Basis $\{\eta_j\}$ $\quad \psi = \sum c_j \eta_j \quad \sum b_j \eta_j = 0 \quad b_j = 0$

Orthonormal basis for $\mathcal{H}$

$$\langle \eta_i, \eta_j \rangle = \delta_{ij} \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

Continuum

$\langle \eta_{q'}, \eta_{q''} \rangle$

$\delta(q' - q'')$

Coordinates of ψ

$$\psi = \sum c_j \eta_j \qquad c_j = \langle \eta_j, \psi \rangle = \eta_j^*(\psi)$$

Direct sum

$$\mathcal{H} = \mathcal{H}_{a_1} \oplus \mathcal{H}_{a_2} \oplus \dots$$

Orthogonal eigenspaces

$$A = \sum a_k P_{\mathcal{H}_{a_k}}$$

eigenvalues are results of measurement and each define an eigenspace along which we can take the projection of ψ.

Different operators → different set of eigenvectors
~ set of eigenvalues

skip

$$F(A) = \sum_k F(a_k) P_{\mathcal{H}_{a_k}}$$

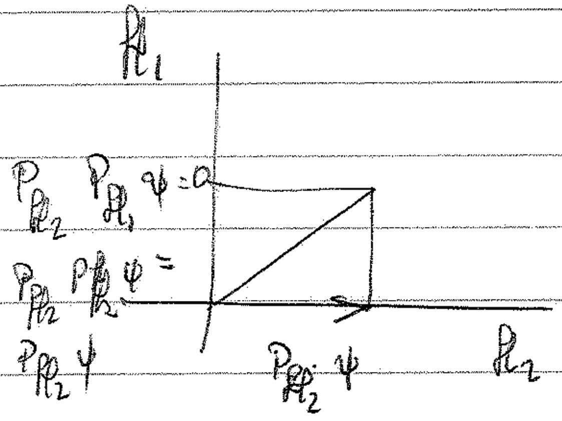
$$F(x) = \sum c_n x^n$$

$$F(A) = \sum c_n A^n$$

but orthogonality implies $P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{a_j}} = \delta_{ij} P_{\mathcal{H}_{a_j}}$

so that

$$A^n = \sum_k a_k^n P_{\mathcal{H}_{a_k}}$$



Recall that

$$P_{\psi} = \psi \langle \psi , \quad \rangle$$

$$P_{\alpha_{kd}} = \alpha_{kd} \langle \alpha_{kd} , \quad \rangle$$

SKIP

$$P_{\mathcal{H}_{a_k}} = \sum_{d}^{D_k} P_{\alpha_{kd}} = \sum \alpha_{kd} \langle \alpha_{kd} , \quad \rangle$$

$$A = \sum_{k} a_k P_{\mathcal{H}_{a_k}} =$$

$$= \sum_{k} \sum_{d}^{D_k} a_k \alpha_{kd} \langle \alpha_{kd} , \quad \rangle$$

$$I = \sum_{k} \sum_{d} \alpha_{kd} \langle \alpha_{kd} , \quad \rangle$$

Commutator of two self-adjoint operators

$$[A, B] = AB - BA$$

$$[A, B](\cdot) = A\big(B(\cdot)\big) - B\big(A(\cdot)\big)$$

When $AB - BA = 0$ A, B commute

Iff A and B share a common eigenbasis, a common set of eigenvectors

Messiah p. 200 for proof

Dirac notation

$$\alpha^*(\ ) = \langle \alpha, \ \rangle$$

Vectors $|\psi\rangle, |\varphi\rangle$ — $|\psi\rangle$ ket vector

Functional $\langle\alpha|$ $\langle\beta|$ — $\langle\alpha|$ bra vector

Scalar product

$$\alpha^*(\psi) = \langle\alpha, \psi\rangle = \langle\alpha|\psi\rangle$$

Operator

$$A(\psi) = |A(\psi)\rangle = A|\psi\rangle$$

$$\langle\varphi, A\psi\rangle = \langle\varphi|A|\psi\rangle = \langle A^\dagger\varphi|\psi\rangle = \langle A^\dagger\varphi, \psi\rangle$$

$$\langle A^\dagger\varphi| = \langle\phi|A$$

Eigenvalue problem notation

$$A|\alpha_{kd}\rangle = a_k|\alpha_{kd}\rangle$$

$$A|kd\rangle = a_k|kd\rangle$$

$$A|\alpha_n\rangle = a_n|\alpha_n\rangle$$

$$A|n\rangle = a_n|n\rangle$$

Matrix representation of operators

Select an orthonormal basis for $\mathcal{H}$ $\{\eta_j\}$

$$P_{\mathcal{H}_{\eta_j}} = \eta_j \langle \eta_j , \ \rangle = |\eta_j\rangle \langle \eta_j|$$

$$I = \sum_j P_{\mathcal{H}_{\eta_j}} = \sum \eta_j \langle \eta_j , \ \rangle = \sum \overset{\text{bra vector}}{|\eta_j\rangle} \overset{\text{ket vector}}{\langle \eta_j|}$$

$\underline{\langle \psi | \varphi \rangle \text{ braket}} = \langle \psi , \varphi \rangle$

$$A = I A I = \sum_j \eta_j \langle \eta_j , \left(A \sum_k \eta_k \langle \eta_k , \ \rangle \right.$$

$$= \sum_{j,k} |\eta_j\rangle \underbrace{\langle \eta_j | A | \eta_k \rangle}_{A^{\eta}_{jk}} \langle \eta_k |$$

$$= \sum |\eta_j\rangle A^{\eta}_{jk} \langle \eta_k | = \sum A^{\eta}_{jk} |\eta_j\rangle \langle \eta_k |$$

$[A^{\eta}_{jk}]$ matrix with respect to $\{\eta_j\}$

The trace of the matrix is independent of representation

$$\underline{\mathrm{Tr}(A)} = \sum_j A^{\eta}_{jj} = \sum_j \langle \eta_j , A\eta_j \rangle = \sum_j \langle \eta_j | A | \eta_j \rangle$$

$$\underline{|\eta_j\rangle = \sum_k |\gamma_k\rangle\langle\gamma_k|\eta_j\rangle = \sum_k \gamma_k \langle \gamma_k , \eta_j \rangle}$$

$$\mathrm{Tr}\,A = \sum_j \langle \eta_j | \underbrace{\sum_k |\gamma_k\rangle\langle\gamma_k|}_{I} A \, | \underbrace{\sum_l |\gamma_l\rangle\langle\gamma_l|}_{I} \eta_j \rangle$$

$$= \sum_{j,l} \langle \gamma_l | \eta_j \rangle \langle \eta_j | \sum_k |\gamma_k\rangle\langle\gamma_k|A|\gamma_l\rangle$$

$$= \sum_{j,l,k} \langle \gamma_l | \eta_j \rangle \langle \eta_j | \gamma_k \rangle \langle \gamma_k | A | \gamma_l \rangle$$

$$= \sum_{l,k} \langle \gamma_l | \underbrace{\Big(\sum_j |\eta_j\rangle\langle\eta_j|\Big)}_{I} | \gamma_k \rangle \langle \gamma_k | A | \gamma_l \rangle$$

$$= \sum_{l,k} \underbrace{\langle \gamma_l | \gamma_k \rangle}_{\delta_{lk}} \langle \gamma_k | A | \gamma_l \rangle = \sum_l A^{\gamma}_{ll}$$

Identity operator

$$\underline{I = \sum_j |\eta_j\rangle\langle\eta_j|}$$

$$\underline{I^{\eta}_{kl} = \sum_j \langle\eta_k|\eta_j\rangle\langle\eta_j|\eta_l\rangle}$$

$$\underline{= \sum_j \delta_{kj}\,\delta_{jl} = \delta_{kl}}$$

$$\underline{\left[I^{\eta}_{kl}\right] = \begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} \qquad \text{any basis}}$$

Adjoint operator

$$\left(A^{\dagger}_{kl}\right)^{\eta} = \langle\eta_k|A^{\dagger}|\eta_l\rangle = \langle\eta_k, A^{\dagger}\eta_l\rangle$$

$$= \langle A^{\dagger}\eta_l|\eta_k\rangle^{*} = \langle\eta_l, A\eta_k\rangle^{*}$$

$$= \langle\eta_l|A|\eta_k\rangle^{*} = A^{*}_{lk}$$

The matrix of the adjoint is the transpose of the complex conjugate of A.

Skip

$$P_\alpha^2\psi = P_\alpha P_\alpha(\psi) = \alpha\langle\alpha, P_\alpha\psi\rangle = \alpha\ \langle\alpha, \alpha\langle\alpha,\psi\rangle\rangle$$

$$= \alpha\langle\alpha,\psi\rangle = P_\alpha(\psi)$$

$$P_\alpha = \alpha\langle\alpha,\ \ \rangle \qquad P_\alpha^\dagger\ ?$$

$$\langle\psi, P_\alpha(\phi)\rangle = \langle P_\alpha^\dagger\psi, \varphi\rangle$$

$$\langle\psi, \alpha\langle\alpha,\varphi\rangle\rangle = \langle\alpha,\varphi\rangle\langle\psi,\alpha\rangle = \langle\psi,\alpha\rangle\langle\alpha,\varphi\rangle$$

$$= \langle\alpha\langle\psi,\alpha\rangle^*, \varphi\rangle$$

$$P_\alpha^\dagger(\psi) = \alpha\langle\psi,\alpha\rangle^* = \alpha\langle\alpha,\psi\rangle = P_\alpha(\psi) \qquad \text{Hermitian}$$

Skip

Representation of an operator

$$A(\cdot) = A|\ \rangle = A = \sum_{jk} |\eta_j\rangle\langle\eta_j|A|\eta_k\rangle\langle\eta_k|$$

$$= \sum_{jk} A^{\eta}_{jk} |\eta_j\rangle\langle\eta_k|$$

$$= \sum_{il} A^{\varepsilon}_{il} |\varepsilon_i\rangle\langle\varepsilon_l|$$

$$A^{\eta}_{jk} = \langle\eta_j|A|\eta_k\rangle$$

$$= \sum_{i,l} \langle\eta_j|\varepsilon_i\rangle\langle\varepsilon_i|A|\varepsilon_l\rangle\langle\varepsilon_l|\eta_k\rangle$$

$$= \sum_{i,l} \langle\eta_j|\varepsilon_i\rangle A^{\varepsilon}_{il} \langle\varepsilon_l|\eta_k\rangle$$

$$[A]_\eta = [U]_{\eta\leftarrow\varepsilon} [A]_\varepsilon [U]_{\varepsilon\leftarrow\eta}$$

Identity

$$I^{\eta}_{jk} = \langle\eta_j|I|\eta_k\rangle = \langle\eta_j|\eta_k\rangle = \delta_{jk}$$

$[I] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ [illegible] basis

Skip

Any unitary operator can be written as

$U = \exp(iG)$ where $G = G^{\dagger}$

$U^{-} = \exp(-iG)$

$$\underline{U^{\dagger} = \exp(-iG^{\dagger}) = \exp(-iG) = U^{-}}$$

$$[\psi]_{\eta} = [U]_{\eta\leftarrow\varepsilon}[\psi]_{\varepsilon}$$

$$\begin{bmatrix} c_1 \\ c_2 \\ \; \end{bmatrix} = \begin{bmatrix} \langle\eta_1|\varepsilon_1\rangle & \langle\eta_1|\varepsilon_2\rangle & \cdots \\ \langle\eta_2|\varepsilon_1\rangle & \langle\eta_2|\varepsilon_2\rangle & \cdots \\ & & \end{bmatrix}\begin{bmatrix} d_1 \\ d_2 \\ \; \end{bmatrix}$$

$$[\psi]_{\varepsilon} = [U]_{\varepsilon\leftarrow\eta}[\psi]_{\eta}$$

Transformation from basis to basis
Unitary transformation

Representation of a vector with respect to a basis

$$|\psi\rangle = \sum_j |\eta_j\rangle\langle\eta_j|\psi\rangle = \sum_j |\eta_j\rangle c_j = \sum \eta_j c_j$$

$$= \sum_i |\varepsilon_i\rangle\langle\varepsilon_i|\psi\rangle = \sum_i |\varepsilon_i\rangle d_i$$

$$c_j = \langle\eta_j|\psi\rangle = \sum_i \langle\eta_j|\varepsilon_i\rangle\langle\varepsilon_i|\psi\rangle = \sum_i \langle\eta_j|\varepsilon_i\rangle d_i$$

$$d_i = \langle\varepsilon_i|\psi\rangle = \sum_j \langle\varepsilon_i|\eta_j\rangle\langle\eta_j|\psi\rangle = \sum_j \langle\varepsilon_i|\eta_j\rangle c_j$$

Define matrix

$$[\mathcal{U}]_{\varepsilon\leftarrow\eta} = \left[\langle\varepsilon_i|\eta_j\rangle\right]$$

$$[\mathcal{U}]_{\eta\leftarrow\varepsilon} = \left[\langle\eta_k|\varepsilon_\ell\rangle\right] = \left[\langle\varepsilon_\ell|\eta_k\rangle^*\right]$$

$$= [\mathcal{U}]^{\dagger}_{\varepsilon\leftarrow\eta} = [\mathcal{U}]^{-1}_{\varepsilon\leftarrow\eta}$$

$$\boxed{\text{So } [\mathcal{U}] \text{ is unitary}}$$

Example We can write the transformation operator $(\eta \leftarrow \varepsilon)$

$$\mathcal{U} = \sum_k |\varepsilon_k\rangle\langle\eta_k|$$

$$U^\dagger = \sum_k |\eta_k\rangle\langle\varepsilon_k|$$

$$UU^\dagger = \sum_{i,j} |\varepsilon_i\rangle\langle\eta_i|\eta_j\rangle\langle\varepsilon_j|$$

$$= \sum_{i,j} |\varepsilon_i\rangle\,\delta_{ij}\,\langle\varepsilon_j| = \sum_i |\varepsilon_i\rangle\langle\varepsilon_i| = I$$

$$U^{\eta}_{jk} = \langle\eta_j|\mathcal{U}|\eta_k\rangle = \langle\eta_j|\varepsilon_k\rangle$$

$$= \sum_\ell \langle\eta_j|\varepsilon_\ell\rangle\underbrace{\langle\eta_\ell|\eta_k\rangle}_{\delta_{\ell k}} = \Big[[U]_{\eta\leftarrow\varepsilon}\Big]_{jk}$$

Eigenvalue problem of self-adjoint operator

$A(\alpha) = a'\alpha$

$A|\alpha\rangle = a|\alpha\rangle \qquad (A - aI)|\alpha\rangle = 0$

~~$|\alpha\rangle$ must be the zero.~~

i.e it must be the zero vector. To be the zero vector, it must have all its components equal to zero with respect to any basis. Take basis $\{\eta_j\}$. Then

$$\langle \eta_j | A - aI | \alpha \rangle = 0$$

or

$$\textcircled{I}$$

$$\sum_k \langle \eta_j | A - aI | \eta_k \rangle \langle \eta_k | \alpha \rangle = 0 \qquad \langle \eta_k | \alpha \rangle = c$$

$$= \sum_k \left(A^{\eta}_{jk} - a\,\delta_{jk} \right) c^{\eta}_k = 0$$

$$\Big[[A]_\eta - a[I] \Big] \Big[\alpha \Big]_\eta = 0$$

$$\begin{bmatrix} A^{\eta}_{11} - a & A^{\eta}_{12} & \\ A^{\eta}_{21} & A^{\eta}_{22} - a & \\ & & \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix} = 0$$

A system of linear homogeneous equations has a solution only if the determinant is zero

$$\det\left([A]_\eta - a[I]\right) = 0$$

How about another basis?

$$[A]_\eta = [U]_{\eta\leftarrow\varepsilon}[A]_\varepsilon[U]_{\varepsilon\leftarrow\eta}$$

$$[U]_{\eta\leftarrow\varepsilon}[U]_{\varepsilon\leftarrow\eta} = I$$

$$\det\left[[U]_{\eta\leftarrow\varepsilon}[A]_\varepsilon[U]_{\varepsilon\leftarrow\eta} - [U]_{\eta\leftarrow\varepsilon}[U]_{\varepsilon\leftarrow\eta}\right] = 0$$

$$= \det[U]_{\eta\leftarrow\varepsilon}\left[[A]_\varepsilon - [I]_\varepsilon\right][U]_{\varepsilon\leftarrow\eta} =$$

$$= \det[U]_{\varepsilon\leftarrow\eta}[U]_{\eta\leftarrow\varepsilon}\left[[A]_\varepsilon - a[I]_\varepsilon\right]$$

$$= \det\left([U]_{\varepsilon\leftarrow\eta}[U]_{\eta\leftarrow\varepsilon}\right]\det\left[[A]_\varepsilon - a[I]_\varepsilon\right]$$

$$= \det\left[[A] - a[I]\right]$$ [illegible] basis

So find a basis in which [A] is diagonal.
Then eigenvalues are diagonal elements.

$$\mathrm{Tr}\,[A] = \sum_j a_j$$

$$\mathrm{Tr}\,[A][B] = \mathrm{Tr}\,AB = \mathrm{Tr}\,BA = \mathrm{Tr}\,[B][A]$$

Quantization; Example of Continuous Spectrum

In classical mechanics a single particle moving only along one dimension is described by q and p

We are going to associate operators Q and P with these observables. These operators are linear Hermitian

$$Q = Q^{\dagger} \qquad P = P^{\dagger}$$

The Hamiltonian function

$$H = \frac{1}{2m} p^2 + V(q)$$

$$H = \frac{1}{2m} P^2 + V(Q) = H^{\dagger}$$

The operators are such that

$$[Q, Q] = 0 \qquad [P, P] = 0$$

$$[Q, P] = i\hbar$$

We will now attempt to solve the eigenvalue problems

$$P|\pi\rangle = p|\pi\rangle$$ Eigenvalues and eigenvectors.

$$Q|k\rangle = q|k\rangle$$

We introduce the operator

$$R(m) = \exp\left(-\frac{imP}{\hbar}\right)$$

m = is real parameter.

$$R^{\dagger}(m) = \exp\left(\frac{imP^{\dagger}}{\hbar}\right) = \exp\left(\frac{imP}{\hbar}\right) = R^{-1}(m$$

So R(m) is a unitary operator if m is real

Now let us evaluate the commutator

$$[Q, R]$$

To do this we must make use of the following relations

$$[QP^2 - P^2Q] = 2i\hbar P$$

$$[QP^l - P^lQ] = l(i\hbar)P^{l-1}$$

$$[Q, F(P)] \equiv i\hbar \frac{\partial F}{\partial P}$$

$$[P, G(Q)] \equiv -i\hbar \frac{\partial G}{\partial Q}$$

$$[Q, F(Q,P)] \equiv i\hbar \frac{\partial F}{\partial P}$$

$$[P, F(P,Q)] \equiv -i\hbar \frac{\partial F}{\partial Q}$$

Then we find

$$[Q, R(m)] = i\hbar \frac{\partial R(m)}{\partial P} = m R(m)$$

$$QR = RQ + mR$$

Now let us apply this operator on vector (ket) $|k\rangle$ Then we find

$$Q\left(R|k\rangle\right) = RQ|k\rangle + mR|k\rangle$$

$$= (q+m)\left(R|k\rangle\right)$$

i.e if $|k\rangle$ is a ket of Q ~~then~~ with eigenvalue q, then $R|k\rangle$ is an eigenket of Q with eigenval $q+m$. Clearly q and m are real since Q

is Hermitian.

R is called a translation operator

Indeed

$$R^{-1}QR = R^{-1}RQ + \xi R^{-1}R$$

$$= Q + \xi$$

Since q is continuous, the orthonormality relation is

$$\langle k'|k''\rangle = \delta(q'-q'')$$

The identity operator is

$$\int_{-\infty}^{\infty} |k'\rangle\, dk' \langle k'| = I$$

Now, we have shown that $R(m)|k\rangle$ is an eigenket of Q with eigenvalue $q+m$

We will now attempt to solve the eigenvalue problems

$$Q\chi_x = x\chi_x$$

The eigenvalues $-\infty < x < \infty$ and continuous. Because Q is self-adjoint, the $\{\chi_x\}$ forms a basis for $\mathcal{H}$.

$$I = \int dx\, \chi_x \langle \chi_x , \ \rangle$$

Orthonormality

$$I(\chi_{x'}) = \int dx\, \chi_x \underbrace{\langle \chi_x, \chi_{x'} \rangle}_{\delta(x-x')} = \chi_{x'}$$

Any vector φ in $\mathcal{H}$ may be represented with respect to the position eigenbasis χ_x by the coordinates $\langle \chi_x, \varphi \rangle$ which are complex functions of the variable x. Let

$$\varphi(x) = \langle \chi_x, \varphi \rangle$$

$$|\varphi\rangle = \int dx\, \chi_x \langle \chi_x, \varphi \rangle = \int dx\, \chi_x \varphi(x)$$

$$|\psi\rangle = \int dx'\, \chi_{x'} \psi(x')$$

$$\langle \varphi, \psi \rangle = \left\langle \int dx\, \chi_x \varphi(x), \int dx'\, \chi_{x'} \psi(x') \right\rangle$$

$$= \iint dx\, dx'\, \varphi^*(x)\, \psi(x') \underbrace{\langle \chi_x, \chi_{x'} \rangle}_{\delta(x-x')}$$

$$\underline{= \iint dx}\, dx'\, \varphi^* \underline{(x)\, \psi(x)}$$

$$Q|\varphi\rangle = Q \int dx\, \chi_x\, \varphi(x)$$

$$= \int dx\, Q \chi_x \varphi(x) = \int dx\, x\, \varphi(x)\, \chi_x$$

$$= \int dx\, \chi_x\, x\, \varphi(x)$$

$$Q|\varphi\rangle(x) = x\, \varphi(x)$$

Similarly, starting with $[Q, P] = i\hbar I$
(~~postulate~~)

$$P|\varphi\rangle(x) = -i\hbar \frac{\partial \varphi(x)}{\partial x}$$

March 15, 84

- Eigenvalue problem of a Hermitian operator

  Linear & self-adjoint

- Eigenvalues, eigenvectors, degeneracy

- Commutator $[A, B] = AB - BA$
- Commuting operators

- Dirac notation

  $\alpha^*(\ ) \Rightarrow \langle\alpha|$ bra Functionals

  $\psi \rightarrow |\psi\rangle$ ket vectors

  $\langle\alpha, \psi\rangle \Rightarrow \langle\alpha|\psi\rangle$ bracket inner product

- Eigenvalue problem

$$A|\alpha_{kd}\rangle = a_k|\alpha_{kd}\rangle$$

$$A|kd\rangle = a_k|kd\rangle$$

$$A|n\rangle = n|n\rangle$$

- Matrix representation

$$\overset{\eta}{A}_{k\ell} = \langle\eta_k|A|\eta_\ell\rangle \ ; \ A = \sum_{ij}|\eta_i\rangle A_{ij}\langle\eta_j|$$

$$\psi\rangle = \sum \eta_j\rangle\, c_j \qquad q_{\eta_j} = \|\psi_{\eta_j}\|^2 = \langle c_j^* \eta_j | c_j \eta_j\rangle$$

— Trace

$$\mathrm{Tr}\, A = \sum_i A^{\eta}_{ii} = \sum A_{\ell\ell} \quad \text{any representation}$$

— Transformation from one basis to another

$$|\psi\rangle = \sum_j |\eta_j\rangle\langle \eta_j|\psi\rangle = \sum |\eta_j\rangle\, c_j \qquad c_j = \langle\eta_j|\psi\rangle$$

$$= \sum_i |\varepsilon_i\rangle\langle\varepsilon_i|\psi\rangle = \sum |\varepsilon_i\rangle\, d_i \qquad d_i = \langle\varepsilon_i|\psi\rangle$$

$$c_j = \sum \langle\eta_j|\varepsilon_i\rangle\, d_i$$

$$\left.\begin{aligned} \left[U\right]_{\varepsilon\leftarrow\eta} &= \left[\langle\varepsilon_i|\eta_j\rangle\right] \\ \left[U\right]_{\eta\leftarrow\varepsilon} &= \left[\langle\eta_k|\varepsilon_\ell\rangle\right] \end{aligned}\right\} \quad \begin{aligned} &\underline{[U] \text{ is unitary}} \\ &[U]_{\eta\leftarrow\varepsilon} = [U]^{\dagger}_{\varepsilon\leftarrow\eta} = [U]^{-1}_{\varepsilon\leftarrow} \end{aligned}$$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ \\ \end{bmatrix} = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}_{\eta\leftarrow\varepsilon} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ \\ \end{bmatrix}$$

$$[\psi]_\eta = [U]_{\eta\leftarrow\varepsilon}\,[\psi]_\varepsilon$$

Matrix in terms of eigenrepresentation

$$A|\alpha_n\rangle = a_n|\alpha_n\rangle \qquad A^{\alpha}_{mn} = \langle\alpha_m|A|\alpha_n\rangle = a_n\delta_{mn}$$

Formulation of a quantum mechanical problem

Quantization

We will illustrate the steps used in quantizing a problem by considering a one-particle system in one dimension.

All the results can be readily generalized to more dimensions and more particles at the expense of more mathematical complexity.

Two observables of our system are position q and momentum p. We are going to represent these observables by Hermitian operators

$$q \to Q \qquad p \to P \qquad Q = Q^{+} \qquad P = P^{+}$$

Q and P not to be confused with question Q and projector P.

These operators must satisfy commutation relations

$$[Q,Q] = 0 \qquad [P,P] = 0$$

$$[Q,P] \equiv QP - PQ = i\hbar I$$

If we had more dimensions noncommutation would be only between conjugate Q and P.

The commutation relations are part of the rules for the formulation of the Hermitian operators

Each of the operators Q and P defines an eigenvalue problem

$$Q|\chi\rangle = x|\chi\rangle \qquad P|\pi\rangle = p|\pi\rangle$$

The eigenvalues x are continuous. The eigenvectors $|\chi\rangle$ are orthonormalized. The eigenvalues p may or may not be continuous. The eigenvectors $|\pi\rangle$ are also orthonormalized. In particular

$$\langle\chi|\chi'\rangle = \delta(x-x') \qquad \text{Dirac delta function}$$

$$\int_{-\infty}^{\infty} |\chi_x\rangle\, dx \langle\chi_x = I$$

The following relations can be readily proven (Louisell 34-43)

~~$$\langle\chi|P|\chi'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle\chi|\chi'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\chi'(\chi)$$~~

~~$$\langle\chi|Q|\chi'\rangle = x\,\delta(x-x')$$~~

$$\langle x | P | x' \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \langle x | x' \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \delta(x - x')$$

$$\langle x | Q | x' \rangle = x' \langle x | x' \rangle = x' \delta(x - x')$$

$$\langle x | F(P) | x' \rangle = F\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \langle x | x' \rangle$$

$$\langle x | V(Q) | x' \rangle = V(x) \langle x | x' \rangle$$

More generally

$$\langle x | F(P) | \psi \rangle = F\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \langle x | \psi \rangle$$

$$= F\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \psi(x)$$

$$\langle x | V(Q) | \psi \rangle = V(x) \langle x | \psi \rangle$$

$$= V(x) \psi(x)$$

Now let us consider the operator corresponding to energy.

We start with the function (Hamiltonian) in C.M.

$$h = \frac{p^2}{2m} + V(q)$$

and form a Hermitian operator

$$H = \frac{P^2}{2m} + V(Q) = H^+$$

We wish to solve the energy eigenvalue problem

$$H|\varepsilon\rangle = e|\varepsilon\rangle$$

We will express this problem in the coordinate representation. The way we do it is as follows

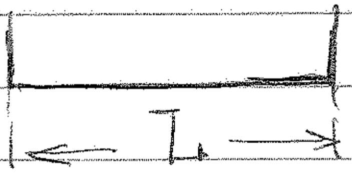
$$\langle x|H|\varepsilon\rangle = e\langle x|\varepsilon\rangle$$

$$\langle x|\frac{P^2}{2m} + V(Q)|\varepsilon\rangle = e\ \varepsilon(x)$$ $\varepsilon(x)$ eigenfunction

e eigenvalue

$$\left[-\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} + V(x)\right]\varepsilon(x) = e\ \varepsilon(x)$$

$V(x) = 0$ Free particle
$ = \infty$



$$e_n = \frac{\hbar^2}{2m}\frac{n^2}{L^2}$$

$$\varepsilon_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\frac{n\pi x}{L}$$

Harmonic Oscillator

Hamiltonian function

$$h = \frac{p^2}{2m} + \tfrac{1}{2} m\omega^2 q^2$$

$$\underline{H = \frac{P^2}{2m} + \tfrac{1}{2} m\omega^2 Q^2 = H^\dagger}$$

Energy eigenvalue problem

$$\underline{H|\varepsilon\rangle = e|\varepsilon\rangle} \qquad \langle x|\varepsilon\rangle = h(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2\right] h(x) = e\, h(x)$$

Method of solution by operator algebra

Define operator $\quad Z = \sqrt{1/2\hbar m\omega}\,(m\omega Q + iP)$

$$Z^\dagger = \sqrt{1/2\hbar m\omega}\,(m\omega Q - iP)$$

Note that $[Z, Z^\dagger] = I$ check

Thus

$$H = \hbar\omega\left[Z^\dagger Z + \tfrac{1}{2} I\right] \; ; \quad N = Z^\dagger Z = N^\dagger$$

Now notice the following

$$N Z = Z Z^\dagger Z = Z \left[Z^\dagger Z \right] = Z \left[\underbrace{Z Z^\dagger - I}_{\text{from commutator}} \right]$$

$$= Z \left(N - I \right)$$

{Meaning of equality}

Check

$$?. \quad N Z^\dagger = Z^\dagger \left(N + I \right)$$

<u>We will consider the eigenvalue problem</u>

$$N | v_n > = n | v_n > = Z^\dagger Z | v_n >$$

Next consider the vector $Z | v_n >$

$$N \left(Z | v_n > \right) = Z \left(N - I \right) | v_n >$$

$$= Z \left(n - 1 \right) | v_n >$$

$$= (n-1) \left(Z | v_n > \right)$$

so $Z | v_n >$ <u>is an eigenvector of N with eigenvalue $(n-1)$</u>

Similarly

$$N Z^{+}|v_n\rangle = Z^{+}(N+I)|v_n\rangle$$

$$= (n+1)\, Z^{+}|v_n\rangle$$

so $Z^{+}|v_n\rangle$ eigenvector of N with eigenvalue $n+1$

If we know eigenvector $|v_n\rangle$ with eigenvalue n we can form the following sequence of eigenvectors with eigenvalues differing by unity.

$$\begin{array}{ccccc} ZZ|v_n\rangle & Z|v_n\rangle & |v_n\rangle & Z^{+}|v_n\rangle & Z^{+}Z^{+}|v_n\rangle \\ n-2 & n-1 & n & n+1 & n+2 \end{array}$$

Now, we wish to show that n is a nonnegative integer.

Indeed

$$\| |v_n\rangle \|^2 = \langle v_n | v_n \rangle \geq 0 \qquad = 0 \text{ iff } v_n = 0_v$$

$$\| Z|v_n\rangle \|^2 = \langle Z v_n | Z v_n \rangle$$

$|Z v_n\rangle$

$$= \langle v_n | Z^{+} Z v_n \rangle = n \langle v_n | v_n \rangle \geq 0$$

Thus $n \geq 0$. —

If $n=0$ $\|Z v_0\|^2 = 0$ $|v_0> = |0>$, $Z|0> = |0>$

because norm $= 0$

If $n \neq 0$ $\|Z^k v_n\|^2 = n(n-1)\cdots(n-k+1) < v_n, v_n >$

k integer

This expression would become negative for $k > n+1$ unless n is integer and then for $k = n+1$ it gives the zero vector, and for $k > n+1$ also the zero vector.

So now we have all the eigenbasis expressed as follows

Eigenvectors: $|0>$ $v_1> = Z^{\dagger}|0>$ - - $|v_n> = \frac{1}{n!} Z^{\dagger n}|0>$
~~orthonormal~~

Eigenvalues 0 1 - - n

$$N|v_n> = n|v_n>$$

$$Z|0> = \cancel{|0>} = 0_v$$

$$Z|v_n> = \sqrt{n}\,|v_{n-1}>$$

$$Z^{\dagger}|v_n> = \sqrt{n+1}\,|v_{n+1}>$$

Energy eigenvalues

$$e_n = \hbar\omega\left[n + \frac{1}{2}\right]$$

Alternatively, we can express the eigenvectors

$$|\nu_n\rangle = \frac{(Z^{\dagger})^n}{\sqrt{n!}}|0\rangle$$

normalized $\langle 0|0\rangle = 1.$

<u>Orthonormality</u> $\langle \nu_{n'}|\nu_{n''}\rangle = \delta_{n'n''}$

<u>Completeness</u> $\sum |\nu_n\rangle\langle \nu_n| = I$

In the N-representation, the matrix elements of Z, Z^+, N are

$$\langle \nu_n|Z|0\rangle = 0$$

N = number operator

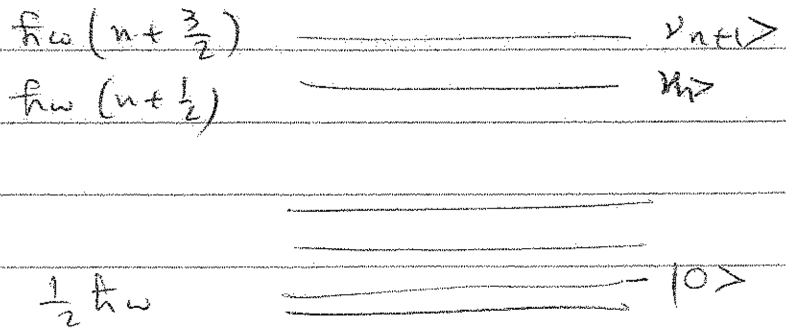
$$\langle \nu_n|Z|\nu_{n'}\rangle = \sqrt{n'}\ \delta_{n,n'-1}$$

Z^+ creation

Z annihilatio

$$\langle \nu_n|Z^+|\nu_{n'}\rangle = \sqrt{n'+1}\ \delta_{n,n'+1}$$

$$\langle \nu_n|N|\nu_{n'}\rangle = n'\ \delta_{n',n''+1}$$



Eigenfunctions

$$h_n(x) = N_n \exp\left(-\frac{\alpha^2 x^2}{2}\right) H_n(\alpha x)$$

$$N_n = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right)^{1/2} \qquad \alpha^4 = \frac{m^2\omega^2}{\hbar^2}$$

$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{d^n(\exp -\xi^2)}{d\xi^n}$$

$$h_0(x) = \frac{\alpha^{1/2}}{\pi^{1/4}} \exp\left(-\frac{\alpha^2 x^2}{2}\right)$$

$$h_1(x) = \frac{\alpha^{1/2}}{2^{1/2}\pi^{1/4}} 2\alpha x \exp\left(-\frac{\alpha^2 x^2}{2}\right)$$

Beretta March 20, 84

Summary of Quantum Mechanics

	Concepts	Mathematical Structure
Kinematics :	System	– Set in Hilbert space $\mathcal{H}$ on $\mathbb{C}$ Dimensionality N.
	Observables	– Operators on $\mathcal{H}$. Self-adjoint.
	Measurement results (spectrum)	– List of N real numbers. They are eigenvalues of operator $A = \sum_i a_i P_{\mathcal{H}_{a_i}}$
	Homogeneous preparations (states)	– Vectors in $\mathcal{H}$
	Frequency of measurement results	– In state ψ, frequency $q_{a_i}(\psi) = \frac{\langle \psi, P_{\mathcal{H}_{a_i}} \psi \rangle}{\langle \psi, \psi \rangle}$
	Value of an observable	– $\langle A \rangle_\psi = \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}$
Dynamics:	Causal evolution	– Schroedinger equation $\dot{\psi} = -\frac{i}{\hbar} H \psi$.

— Given two vectors, do they represent different states?

Theorem: If a vector $\psi_2 = c\psi_1$, where $c \in \mathbb{C}$, then ψ_1 and ψ_2 represent the same state.

Proof: The two vectors represent the same state in the sense that they yield the same frequencies and same values for all conceivable observables. (The word conceivable must be considered in the context of QM).

Indeed

$$\langle A \rangle_{\psi_2} = \frac{\langle \psi_2, A\psi_2 \rangle}{\langle \psi_2, \psi_2 \rangle} = \frac{\langle c\psi_1, Ac\psi_1 \rangle}{\langle c\psi_1, c\psi_1 \rangle} = \frac{cc^* \langle \psi_1, A\psi_1 \rangle}{cc^* \langle \psi_1, \psi_1 \rangle} = \langle A \rangle_{\psi_1}$$

$\forall A$

Even if we normalize ψ, i.e., $\|\psi\| = 1$, still there many ψ's that correspond to the same state since for $c = \exp(ib)$, $cc^* = 1$ and $\|c\psi\| = \|\psi\| = 1$.

To avoid this multiplicity of vectors corresponding to the same state and generalize our mathematical structure we will represent states by projection operators onto one-dimensional subspaces and create a more general Hilbert space as follows

Instead of a vector, let us consider a projector onto a direction as the state. Then we have a unique correspondence between state and projector because

$$P_{\psi_1} = P_{\psi_2} \quad \text{iff} \quad \psi_2 = c\psi_1$$

$$P_\psi(\cdot) = \frac{\psi < \psi, \circ >}{< \psi, \psi >}$$

Let us explore the properties of projectors somewhat more carefully.

We consider a general operator P and the corresponding eigenvalue problem

$$P \pi_{kd} = p_k \pi_{kd}$$ where $\{\pi_{kd}\}$ is a linearly indepen normalized set.

Then

$$P = \sum_k p_k P_{\mathcal{H}_{p_k}}$$ $\mathcal{H}_{p_k}$ subspace of $\mathcal{H}$ defined by all the eigenvectors π_{kd} correspondin to p_k.

A basis for subspace $\mathcal{H}_{p_k}$ is $\pi_{k1}, \pi_{k2}, \ldots \pi_{kD_k}$

where D_k is the dimensionality of $\mathcal{H}_{p_k}$ or, equivalentl the degeneracy of p_k

$$P_{\mathcal{H}_{p_k}}(\cdot) = \sum_{d=1}^{D_k} \pi_{kd} \langle \pi_{kd}, \cdot \rangle$$

For a one-dimensional projector onto π we have

$$P_\pi = \pi \langle \pi, \cdot \rangle \quad \text{and} \quad \operatorname{Tr} P_\pi = \sum_i \left[P_\pi \right]_{ii}^{\eta}$$

if we select $\{\eta\} \mid \{\pi, \eta_2, \eta_3 \cdots \}$ then

$\operatorname{Tr} P_\pi = 1$ because all the η's are $\perp$ to π.

Using this result, we find

$$\begin{aligned} \operatorname{Tr} P_{\mathcal{H}_{pk}}(\cdot) &= \operatorname{Tr} \sum_{d=1}^{D_k} \pi_{kd} \langle \pi_{kd}, \cdot \rangle \\ &= \sum_{d=1}^{D_k} \operatorname{Tr} \underbrace{\left(\pi_{kd} \langle \pi_{kd}, \cdot \rangle \right)}_{1} = D_k \end{aligned}$$

and

$$\begin{aligned} \operatorname{Tr} P &= \operatorname{Tr} \sum_k p_k P_{\mathcal{H}_{pk}} = \sum_k \operatorname{Tr} \left(p_k P_{\mathcal{H}_{pk}} \right) \\ &= \sum_k p_k \operatorname{Tr} \left(P_{\mathcal{H}_{pk}} \right) = \sum_k p_k D_k \end{aligned}$$

What are the eigenvalues of a projection operator P? We know that a projection operator is idempotent, i.e.,

$$P^2 = P$$

Thus

$$P\pi_{kd} = p_k \pi_{kd} = P^2\pi_{kd} = p_k P \pi_{kd} = p_k^2 \pi_{kd}$$

so that

$$(p_k^2 - p_k)\pi_{kd} = 0 \qquad p_k^2 - p_k = 0$$

or

$$p_k = \begin{cases} 0 \\ 1 \end{cases}$$

Accordingly, a projection operator is nonnegative $(P \geq 0)$ and self-adjoint. In general

$$\mathrm{Tr}\,P = D.$$

Now, we can summarize, that <u>one-dimensional</u> projectors have the following features

$$P^\dagger = P, \text{ nonnegative }; (P \geq 0) ; \mathrm{Tr}\,P = 1 ; P^2 = P.$$

We are ready to consider a new structure (mathematical structure) for quantum mechanics.

- Start with a Hilbert space $\mathcal{H}$ on $\mathbb{C}$ $\dim \mathcal{H} = N$.
- $A, B, \ldots$ operators on $\mathcal{H}$.
- Consider all operators that are <u>self-adjoint</u>.

Define: $\mathcal{L}\{\mathcal{H}\} = \{$ set of all self adjoint operators on $\mathcal{H}\}$

To make a Hilbert space out of this set, we must equip it with a scalar product

In fact, we make it a Hilbert space on real numbers by defining $(\cdot, \cdot)$

$$\underline{(A, B) = Tr(AB) = Tr(BA) = (B, A)}$$

Define linear functional on $\mathcal{L}\{\mathcal{H}\}$ as

$$a^*(\cdot) = (A, \cdot) = Tr(A\,\cdot)$$

$$a^*(P_\psi) = Tr(A P_\psi) = \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}$$

Hilbert space	$\mathcal{L}\{\mathcal{H}\}$
States	P_ψ
Observables	Linear functionals a^*
Values	Value of a^*

March 22, 84

Kinematics

	Math. Structure of Q.M.	Math. Structure of C.M.
System:	Hilbert space $\mathcal{H}$ and $\mathcal{L}(\mathcal{H})$ Scalar product in $\mathcal{L}(\mathcal{H})$	Phase space Ω and function on Ω represented as $\mathcal{B}(\Omega)$ Scalar product
	$(A,B) = \mathrm{Tr}(AB)$	$(a,b) = \int_\Omega a b \, d\Omega$
	$\mathcal{L}(\mathcal{H})$ self-adjoint operators on $\mathcal{H}$	a, b functions
Observable:	Linear functional on $\mathcal{L}(\mathcal{H})$	Linear functions on $\mathcal{B}(\Omega)$
	$a^*(\cdot) = (A, \cdot)$ $= T(A \, \cdot)$	$a^*(\cdot) = (a, \cdot)$ $= \int a \cdot d\Omega$
	With each functional, we have a uniquely associated operator A	With each functional, we have a uniquely associated function a.
	Let $L \in \mathcal{L}(\mathcal{H})$ $a^*(L) = \mathrm{Tr}(AL)$ $= (A, L)$	

Frequency of outcome of value a_i of observable A	$q_{a_i}(\cdot) = (P_{\mathcal{H}_{a_i}}, \cdot)$ $= \mathrm{Tr}(P_{\mathcal{H}_{a_i}} \cdot)$ Observable A admits of operator representation (self-adjoint) $A = \sum a_i P_{\mathcal{H}_{a_i}}$	$q_{a_i} = (\delta_{a_i}, \cdot)$ $= \int \delta_{a_i} \cdot d\Omega$ $a = \int a_j \delta_{a_j} d\Omega$
State (Homogeneous preparation)	Vector in $\mathcal{H}$ Projection operator on $\mathcal{L}(\mathcal{H})$. Point in $\mathcal{L}(\mathcal{H})$ such that $P \geqslant 0$; $\mathrm{Tr}\, P = 1$; $P = P^2$	Point in Ω Element in $\mathcal{S}(\Omega)$ "Point" δ in $\mathcal{D}(\Omega)$ with $\delta \geqslant 0$; $\int \delta \, d\Omega = 1$; $\delta^2 =$
Value of observable	Value of the functional at the state a^* at point P of state $a^*(P) = \mathrm{Tr}(AP)$	Value of functional $a^*(\cdot)$ $a^*(\delta) = \int a \delta \, d\Omega$

Dynamics

Causal evolution	$P(t)$ motion of state trajectory in $\mathcal{S}(\mathcal{H})$	$\delta(t)$ motion of state trajectory in $\mathcal{P}(\Omega)$
	$\dot{P} = -\frac{i}{\hbar}\left[H, P\right]$	$\dot{\delta} = -\{h, \delta\}$
	Schroedinger-von Neumann equation	Poisson bracket
		$\{h,\delta\} = \frac{\partial h}{\partial q}\frac{\partial \delta}{\partial p} - \frac{\partial \delta}{\partial q}\frac{\partial h}{\partial p}$
		Hamilton-Liouville equation

Statistics

Heterogeneous preparations

$\Pi = w_1 \times \Pi_1^0 + w_2 \Pi_2^0$	$f = w_1 \delta_1 + w_2 \delta_2$
Point W in $\mathcal{L}(\mathcal{H})$ with $w \geq 0$ $\quad \mathrm{Tr}\, W = 1$ but not idempotent	"point" f in $\mathcal{D}(\Omega)$ $f \geq 0; \quad \int f \, d\Omega = 1$
$a^*(W) = (A, W)$ $= \mathrm{Tr}(A W)$ $= w_1 \mathrm{Tr}(A P_1) + w_2 \mathrm{Tr}(A P_2)$ $= w_1 (A, P_1) + w_2 (A, P_2)$ $= w_1 a_1^*(P_1) + w_2 a^*(P_2)$	$a^*(f) = (a, f) =$ $= \int a f \, d\Omega$ $= w_1 \int a \delta_1 \, d\Omega + w_2 \int a \delta_2 \, d\Omega$

Consistency ~~questions~~ conditions for statistics

1. $\forall A$, and preparation $\Pi = w_1 * \Pi_1 + w_2 * \Pi_2$
we must have that A_Π be the weighted average of the results of the component preparations

$$\langle A \rangle_\Pi = w_1 \langle A \rangle_{\Pi_1} + w_2 \langle A \rangle_{\Pi_2}$$

Π_i need not be homogeneous.

This condition is satisfied by both C.M. and Q.M. statistics.

2. If Π is homogeneous, and yet $\Pi = w_1 \Pi_1 + w_2 \Pi_2$ with $w_1, w_2 > 0$ then $\Pi_1 = \Pi_2 = \Pi$

This condition is satisfied by both C.M. and Q.M.

3. Every heterogeneous preparation admits a unique decomposition into homogeneous components.

Ok for C.M.
But in Q.M. the answer is not Ok.

April 3, 84

Questions

1 How many stable equilibrium states are there?
2 Can all the energy be extracted adiabatically from any state?
3. Are all processes reversible?

Answers in General Thermodynamics

1. One and only one for each value of the energy.
2. No, except for some states. For example, no energy can be extracted adiabatically from a stable equilibrium state.
3. Not necessarily. Irreversible processes are conceivable but not required.

Answers in Quantum Mechanics

1. Equilibrium states $\rho(t) = \rho(t_0)$; $\dot{\rho}(t) = 0$

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] = 0$$

Hence H and ρ share a common eigenbasis, i.e. if the eigenbases are:

$$H \quad \{\varepsilon_1, \varepsilon_2, \dots \}$$

$$P_\psi \quad \{\psi, \dots \}$$

then ψ coincides with one of the eigenvectors of H.

$$H|\varepsilon_{kd}\rangle = e_k|\varepsilon_{kd}\rangle$$

$\dot{P} = 0$ iff P is a projector on one of the eigen-vectors of H. Thus we can write

$$P = |\varepsilon_{kd}\rangle\langle\varepsilon_{kd}|$$

$$\langle E\rangle_{eq} = \langle P|H|P\rangle = e_k = \mathrm{Tr}(HP)$$

$$= \mathrm{Tr}\left(H|\varepsilon_{kd}\rangle\langle\varepsilon_{kd}|\right)$$

$$= \langle\varepsilon_{kd}|H|\varepsilon_{kd}\rangle$$

Conclusions:
- There are no equilibrium states if the energy is different from each of the energy eigenvalues, i.e., $\langle E\rangle \neq e_k$ for all k.
- If $\langle E\rangle = e_k$, then there are infinitel many equilibrium states $(\infty^{D_k - 1})$ for an energy eigenvalue that is D_k degene rate.

Stability of equilibrium

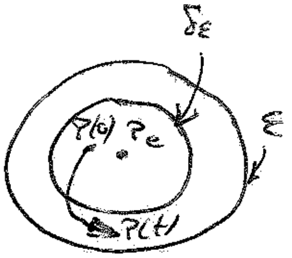
We will examine this question by the method of Liapunoff. (Is this the correct approach?)

Equilibrium state P_e is stable iff $\forall \varepsilon > 0$ there exists a δ_ε such that for every motion $P(t)$ with $P(0)$ whose distance from P_e is

$$\| P(0) - P_e \| < \delta_\varepsilon$$

$P(t)$ is

$$\| P(t) - P_e \| < \varepsilon$$



In Q.M.

$$\| P(t) - P_e \| = \| P(0) - P_e \|$$

because U commut
with P_e

Proof is very easy. ~~Remember that~~

$$\| \cdot \|^2 = (\cdot , \cdot) \qquad \| A \|^2 = \mathrm{Tr}\, A^2$$

$$P(t) = U_t \, P(0) \, U_t^{-1}$$

$$U_t = \exp\left(-\frac{i}{\hbar} t H \right)$$

Conclusion: According to this criterion, all equilibriu
states are stable, and there can be many
stable equ. states for a degenerate energy eigenv

2. In classical mechanics, an adiabatic process is described by a time dependent Hamiltonian $h(p, q, t)$
By analogy, in quantum mechanics an adiabatic process is also described by a time dependent Hamiltonian operator $H(t)$
Then the time evolution of the state is described by the equation of motion

$$\dot{P} = -\frac{i}{\hbar}\left[H(t), P\right]$$

$$P(t) = U_t \, P(0) \, U_t^{-1}$$

$$U_t = \exp\left(-\frac{i}{\hbar}\int_0^t H(t')\,dt'\right)$$

$$\langle \dot{E} \rangle = \frac{d}{dt}\langle H(t), P(t) \rangle$$

$$= \mathrm{Tr}\left(\dot{H} P\right)$$ so ~~energy~~ changes

Let us assume that the minimum energy state of the system is $P_{|\varepsilon_{0d}\rangle}$ e_0 = minimum energy eigenvalue

Starting from state $P(0)$, the question is can we find an adiabatic process to take us to the ground state $P_{|\varepsilon_{0d}\rangle}$?
The answer <u>is yes,</u> we can always find a Ha-

miltonian $H(t)$ which generates a motion from any given $P(0)$ to $P_{|\varepsilon_{od}>}$ at $t = \tau$ and such that $H(0) = H(\tau)$

The proof of this answer is in Von Neumann's book. It proceeds as follows
Given any pair of states (projectors) P_1 and P_2 there exists always a unitary operator U such that

$$P_2 = U P_1 U^{-}$$

For every unitary operator we can write

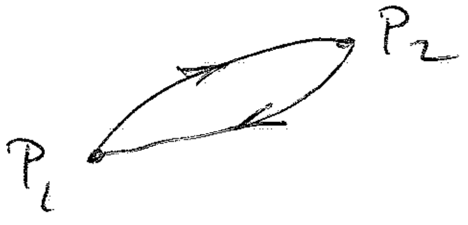
$$U = \sum |\varepsilon_k><\eta_k| = \exp(iG) \qquad G = G^+$$

The projectors P_1 and P_2 are unidimension

$$P_1 = |\eta_1><\eta_1| \qquad P_2 = |\varepsilon_1><\varepsilon_2|$$

$$\{\eta_1, \eta_2 \cdots \qquad \} \qquad \{\varepsilon_1, \varepsilon_2, \cdots \}$$

3. Reversibility. All processes are reversible in Q.M.



April 5, 84

Summary

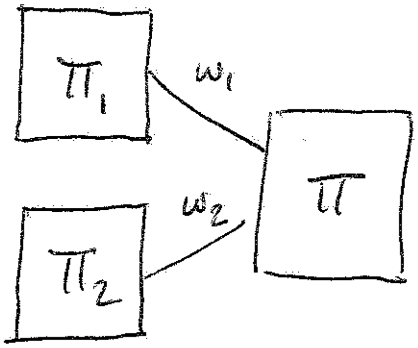
Questions	Answers	
	QM & CM	Gen. Thermo.
How many stable equ. states are there for each value of the energy	None when $\langle E \rangle \neq e_K$ Many for $\langle E \rangle = e_K$, the number being defined by the degeneracy of e_K $(\infty^{D_K - 1})$	One and only one.
Are there states from which we cannot extract all the energy adiabatically?	No	Yes, but not all of them.
Are there processes that are not reversible?	No, all processes are reversible.	Perhaps.

All these statements pertain to homogeneous preparations.

The answers to the questions reveal a conflict. How do we bridge the gap between mechanics & thermodynamics?

One approach is via statistical mechanics. Specificall it is argued that answers in Q.M. are correct for homogeneous preparations whereas answers in thermo are correct for heterogeneous preparations and do not hold for homogeneous preparations.

Statistical preparations



etc. $\Pi = w_1 * \Pi_1 + w_2 * \Pi_2$

List all possible states $P_1, P_2, \ldots$

Assign to each state a probability or statistical weight, so that $w_1, w_2 \ldots$

Energy $\langle E \rangle_{\Pi} = \sum_i w_i * \langle E \rangle_{\Pi_i}$

$$1 = \sum w_i$$

How do we determine w_i?

We decide to assign w_i in the least biased manner compatible with our information. So we must find a logical measure of our uncertainty

We use as criterion the measure of uncertainty proposed by Shannon

$$u(\{w_i\}) = -\sum_i w_i \ln w_i$$

$$u(0, 0, \ldots, 1, \ldots 0) = 0$$

$$u\left(\frac{1}{N}, \frac{1}{N}, \ldots \frac{1}{N}\right) = \ln N$$

We maximize uncertainty subject to our knowledge.

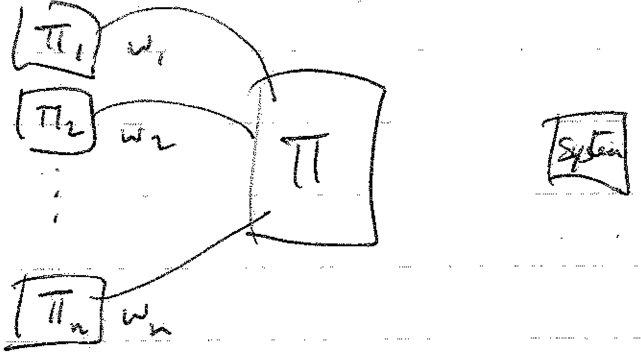
April 10, 84.

Statistical Mech

— All ind. states of a system are correctly described by Q.M.

— Consider many possible states

Construct a heterogeneous preparation



Select w_i in the least biased manner
according to info available

Maximize $u(\{w_i\}) = -\sum_i w_i \ln w_i$

Procedure

1 Select possible states, $\{P_1, P_2 \dots \}$
projection operators.

2 Select info that is
given, known values
of observables $\langle A \rangle$
List values of observables for possible states $\langle A_i \rangle_1, \langle A \rangle_2 \dots$ $\langle B_i \rangle_1, \langle B_i \rangle_2 \dots$

3 Find least biased $w_i\}$ by

maximizing

$$-\sum w_i \ln w_i$$

subject to the info. $\sum_i w_i = 1$

$$\sum_i w_i \langle A \rangle_i = A$$

$$\sum w_i \langle B \rangle_i = B$$

$$w_i = \frac{\exp(-\lambda_A \langle A \rangle_i - \lambda_B \langle B \rangle_i)}{\sum_i \exp(-\lambda_A \langle A \rangle_i - \lambda_B \langle B \rangle_i)}$$

$\left.\begin{matrix}\lambda_A = \\ \lambda_B = \end{matrix}\right\}$ uniquely determined by $\langle A \rangle$ and $\langle B \rangle$

Special example

Observable A is the energy, E

" B is the number of particles N

The set of possible states must be energy eigenbasis

Single particle Maxwell – Boltzmann

$$w_i = \frac{\exp(-\beta \varepsilon_i)}{\sum_i \exp(-\beta \varepsilon_i)}$$

Special example

Observable A is the energy E

Observable B is fixed number N of particles

$$w_i = \frac{\exp(-\beta e_i)}{\sum_i \exp(-\beta e_i)} \qquad e_i \text{ energy 'eigenvalues}$$

If we have a single particle, then w_i is Maxwell-Boltzmann distribution.

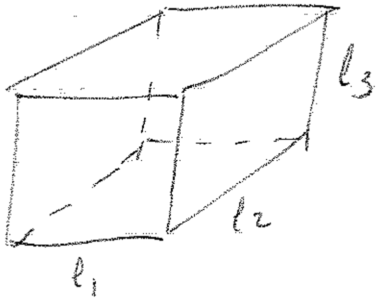
Alternative form

$e_1 \quad e_2 \qquad\qquad e_M$ eigenvalues

$D_1 \quad D_2 \qquad\qquad D_M$ degeneracies

$$w_n = \frac{D_n \exp(-\beta e_n)}{\sum_m D_m \exp(-\beta e_m)}$$

Particle in a box



$$e_{n_1,n_2,n_3} = \pi \frac{\hbar^2}{2m}\left[\left(\frac{n_1}{l_1}\right)^2 + \left(\frac{n_2}{l_2}\right)^2 + \left(\frac{n_3}{l_3}\right)^2\right]$$

How many eigenvalues $e_{n_1 n_2 n_3} \leq E$?

Answer $\frac{1}{6}\pi\left(\frac{2mE}{\pi^2\hbar^2}\right)^{3/2}\underbrace{l_1 l_2 l_3}_{V}$

$D(E)\,dE = \frac{mV}{2\pi^2\hbar^3}\sqrt{2mE}$ $\qquad D(E)$ density

$$w(E)\,dE = \frac{2\beta^{3/2}}{\pi^{1/2}} E^{1/2}\exp\left(-\beta E\right)$$

$$E = \frac{1}{2}mv^2$$

$$w(|v|) = 4\pi\left(\frac{m\beta}{2\pi}\right)^{3/2} v^2 \exp\left(-\frac{m\beta v^2}{2}\right)$$

April 12, 84

Review of Statistical QM or Quantum Statistical Mechanics

(1) Every system is always in some definite though perhaps unknown state.

(2) State is described by a one dimensional projector P on $\mathcal{H}$ $(P^{+} = P ; P \geq 0 , P^2 = P ; \mathrm{Tr}\, P = 1)$

List all possible states $P_1 , P_2 , \ldots$
Assign to each a statistical weight $w_1 , w_2 , \ldots$
according to some rule, i.e., maximize $-\sum_i w_i \ln w_i$
subject to known information.

(3) The extrinsically uncertain situation is described by the statistical operator

$$W = \sum w_i P_i \qquad \text{(von Neumann statistical operator)}$$

$$W^{+} = W \quad ; \quad W \geq 0 \quad ; \quad \mathrm{Tr} W = 1$$

$$\langle A \rangle = \sum w_i \langle A \rangle_i = \sum w_i \mathrm{Tr}\, A P_i = \mathrm{Tr}\, A W$$

The decomposition of $W = \sum w_i P_i$ implies that the state of the system is P_i with probability w_i

Inconsistency

Statements (1) (2) and (3) lead to an unbearable inconsistency.

Theorem by von Neumann.

There no extrinsic uncertainty iff the statistical operator W is itself one-dimensional. i.e., $W^2 = W$.

Corollary: (Schroedinger) 1936: if there is extrinsic uncertainty, i.e., $W \neq W^2$, then W admits many (∞) different decompositions into weighted sums of 1-dimensional projectors

$$W = \sum w_i P_i = \sum w_i' P_i'$$

Meaning according to QSM

The system is concurrently in many states.

This contradicts statement ①

— Park proposed (1968) to accept the math but reject the notion of state.

— Alternatives

give up #3

give up #2

Amer. Jl. of Physics

— ~~Park (1968) proposed (to accept the math) and reject the notion of state. It is fraught with ambiguities. A system can never be thought of being in a state~~

— ~~Alternative give up #3.~~

— ~~" statement #2.~~

Change.

W

A resolution: modify 1, or 2, or 3

1 reject concept of state   system never in a physical state.

2 keep 1 and 2 but modify math in (3)
Risk uncertainty of contradictory exp. evidence

3 keep state but modify step 2. by adapting the math of step (3) to describe the states, not any more the situations with extrinsic uncertainty.

H&G
automatically all successes are guaranteed.
in the region where that math is backed by exp

April 19, 1984

- States in Q.M. are described by intrinsic uncertainties which are represented by projectors P.
- Quantum statistical mechanics deals with situations which require extrinsic uncertainties as to which is the actual state of the system. Each situation is described by a statistical operator

$$W = \sum_i w_i P_i$$

A difficulty with this description is that it mixes irrecoverably the two essentially distinct types of uncertainty, the intrinsic and the extrinsic.

- In addition, we would like to consider the laws of thermodynamics as fundamental.

Hypothesis by H & G

Quantum Thermodynamics

States of QM are only a subset of the conceivable states of a system. QM is valid only for that subset of states

Quantum thermodynamics is valid for all states.

The states are defined as follows

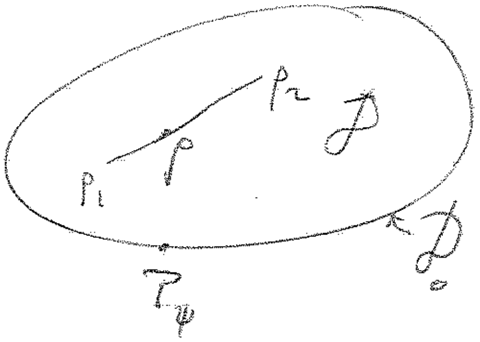
QM: Set of objects $\mathcal{D}_0 = \{ P \mid P = P^\dagger ; P \geq 0 ; \mathrm{Tr} P = 1 ; P^2 = P \}$

QT: ... $\mathcal{D} = \{ \rho \mid \rho = \rho^\dagger ; \rho \geq 0 ; \mathrm{Tr} \rho = 1 \}$

$\mathcal{D}$ is a convex set

$\rho \neq$ is a linear combination of ρ_1, ρ_2

$\mathcal{D}_0$ contains the extreme points of the convex set $\mathcal{D}$.



$$\rho = \alpha \rho_1 + (1-\alpha)\rho_2 \quad \text{if} \quad \rho_1, \rho_2 \in \mathcal{D}$$

$$0 < \alpha < 1$$

if ρ belongs to the set the set is convex.

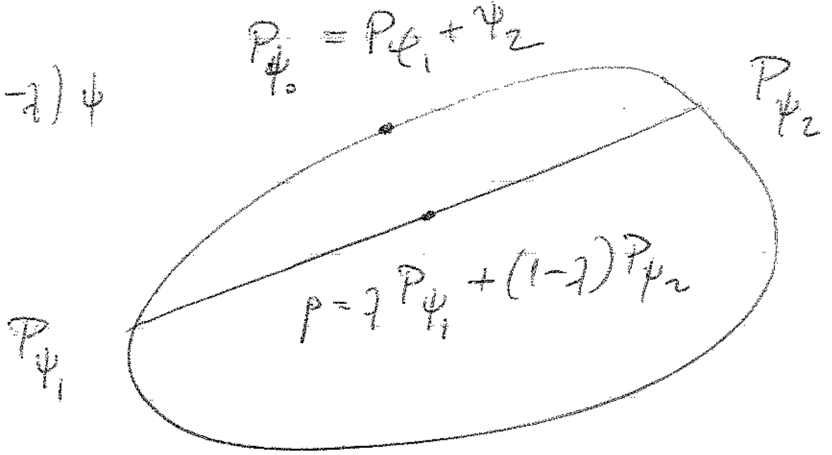
$\psi = P_\psi$, ρ is an extreme point

$$\rho = \lambda \rho_1 + (1-\lambda)\rho_2 \qquad \rho = \rho_1 = \rho_2$$

	Q M	Q T
System:	Hilbert space $\mathcal{H}$ and $\mathcal{L}(\mathcal{H})$ with scalar product $\mathrm{Tr}(AB) = (A, B)$.	
Observable:	Linear functional on $\mathcal{L}(\mathcal{H})$: $a(\cdot) = \mathrm{Tr}(A\cdot)$	
Spectrum of observable	Set of all possible outcomes of measurements of an observable. They are the eigenvalues of the operator A associated with the observable. The operator can be written as $A = \sum_i a_i P_{\mathcal{H}_{a_i}}$	
Binary observable Q_{a_i}	$q_{a_i}(\cdot) = \mathrm{Tr}(P_{\mathcal{H}_{a_i}} \cdot)$	
State	Projector $P_i \in \mathcal{P}_0$	Density operator $\rho \in \mathcal{P} \supset \mathcal{P}_0$
Value of an observable for a state	Value of functional $\mathrm{Tr}(AP)$	$\mathrm{Tr}(\rho A)$
State property	Functional $s(\cdot)$	
Value of state property	Value of functional $s(P)$	$s(\rho)$

Emphasize difference

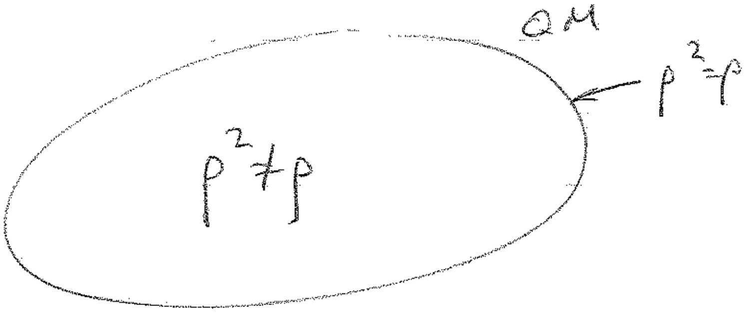
$\psi_0 = \lambda\psi + (1-\lambda)\psi$



Causal evolution

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho]$$

?



First step

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho]$$

For unitary evolution

$$\rho(t) = U_t\rho(0)U_t^{-1}$$

$$U_t = \exp\left(-\frac{i}{\hbar}tH\right)$$

Solutions: unitary, reversible. However not all reversible processes are unitary.

<u>Search</u> of a state property to represent entropy

$$s(\cdot) \qquad \frac{d}{dt} s(\rho) \geq 0 \qquad \forall \rho$$

$$s(\rho) = 0 \qquad \rho^2 = \rho$$

$s_A + s_B = s_{AB}$ for independent states of different systems

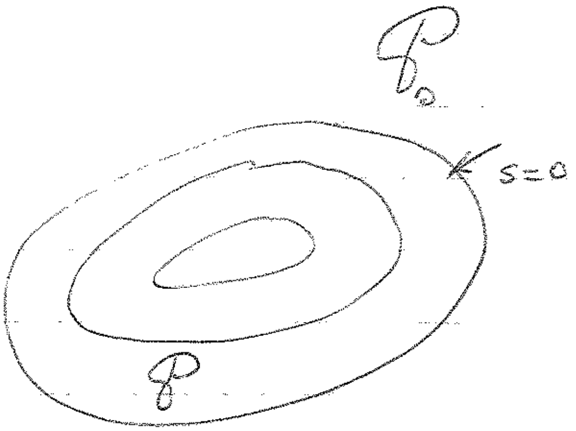
$$\underline{s(\rho) = c \operatorname{Tr} \rho \ln \rho .}$$

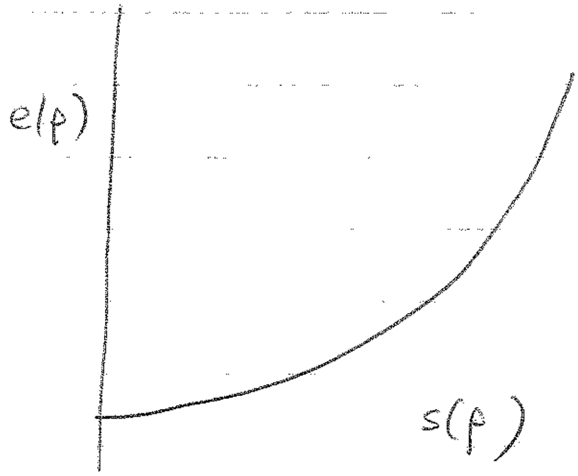
Passed out
- Found. of Phys - Papers
- ACS paper
- Beretta two-level system paper

4/24/84

Comparison of QM and QT

Construct an energy vs. entropy diagram





Take fixed $n(\rho) = Tr\,\mathcal{N}\rho = N$
" $e(\rho) = Tr\,H\rho = E$

On the set

$$\mathcal{P}(E,N) \equiv \left\{ \rho \subset \mathcal{D} \;\middle|\; Tr\,H\rho = E;\; Tr\,\mathcal{N}\rho = N \right\}$$

functional $s(\rho)$ has a maximum, and the maximum is achieved at a unique state

$$\rho_0(E,N) = \frac{\exp\left[-\beta(E,N)H + \nu(E,N)\mathcal{N}\right]}{Tr\,\exp\left[-\beta H + \nu\mathcal{N}\right]}$$

The values of β and ν are defined by the relations

$$\mathrm{Tr}\,\rho_0 H = E \quad \text{and} \quad \mathrm{Tr}\,\rho_0 \eta = N.$$

If N is an eigenvalue of η (integer) or $\eta = NI$ then

$$\rho_0 = \frac{\exp(-\beta(E) H)}{\mathrm{Tr}\exp(-\beta(E) H)}$$

We define the functional

$$\Omega(E) = -\ln \mathrm{Tr}\exp(-\beta H)$$ or equivalently

$$\Omega(\beta) = -\ln \mathrm{Tr}\exp(-\beta H)$$ since E is related to β.

$$s(\rho_0) = -k\,\mathrm{Tr}\,\rho_0 \ln \rho_0$$

$$= -k\,\mathrm{Tr}\,\rho_0 \left[-\beta H - I \ln \mathrm{Tr}\exp(-\beta H)\right]$$

$$= k\beta E - k\,\Omega(\beta)$$

$$\left.\frac{\partial s}{\partial E}\right)_{N,H} = k\beta + kE\frac{d\beta}{dE} - k\frac{d\Omega}{dE}$$

$$\frac{d\Omega}{dE} = - \frac{\mathrm{Tr}\exp(-\beta H)\ (-\beta' H)}{\mathrm{Tr}\exp(-\beta H)}$$

$$= \beta' \,\mathrm{Tr}\,\rho_0 H = \beta' E$$

Thus

$$\frac{\partial s}{\partial E} = k\,\beta(E) = \frac{1}{T(E)}$$

<u>T = temperature</u>

$$dT = -kT^2 d\beta$$

$$c_H = \left.\frac{dE}{dT}\right|_{N,H} = -\frac{1}{kT^2}\frac{dE}{d\beta}$$

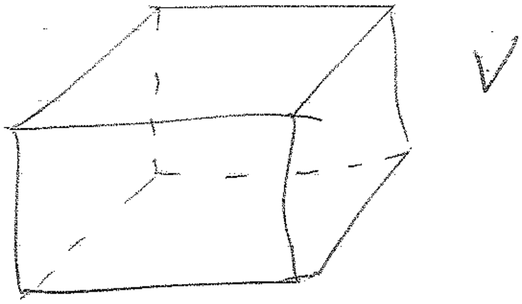
$$\frac{d\Omega}{d\beta} = - \frac{\mathrm{Tr}\left(-\exp(-\beta H)\ H\right)}{\mathrm{Tr}\exp(-\beta H)} = E$$

$$\frac{d^2\Omega}{d\beta^2} = \left\{ \frac{-\left[\mathrm{Tr}\exp(-\beta H)\,H^2\right]\mathrm{Tr}\exp(-\beta H) - \\ - \mathrm{Tr}\left(-\exp(-\beta H)\,H\right)\,\mathrm{Tr}\left(-\exp(-\beta H)\,H\right)}{\left[\mathrm{Tr}\exp(-\beta H)\right]^2} \right.$$

$$= -\mathrm{Tr}\,\rho_0 H^2 + \left(\mathrm{Tr}\,\rho_0 H\right)^2 = -\Delta e^2(\rho_0) = \frac{dE}{d\beta}$$

$$c_H = \frac{1}{kT^2} \, \Delta e^2 \left(\rho_0(E) \right) > 0$$

Pressure



$$H = \frac{p^2}{2m} + V(Q)$$

$$= H(V)$$

$$\mathcal{P}(E, N, V) = \left\{ \rho \in \mathcal{P} \;\middle|\; \mathrm{Tr}\, H(V)\rho = E \; ; \; \mathrm{Tr}\, N\rho = N \right.$$

$$\rho_0(E, V) = \frac{\exp\left(-\beta(E, V)\, H(V) \right)}{\mathrm{Tr} \exp(-\beta H)}$$

$$p = - \left. \frac{\partial E}{\partial V} \right|_{N, S}$$ along stable equilibrium states

$$= \left. \frac{\partial (E - TS)}{\partial V} \right|_T$$

April 26,84

QM states in $\mathcal{P}_0 \equiv \{ P \text{ on } \mathcal{H} \mid P^\dagger = P ; P \geq 0 ; \mathrm{Tr}\, P = 1 ; P^2 = P \}$

QT states in $\mathcal{P} \equiv \{ \rho \text{ on } \mathcal{H} \mid \rho^\dagger = \rho ; \rho \geq 0 ; \mathrm{Tr}\, \rho = 1 \}$

Equation of motion for QM states Schroedinger – von Neumann

$$\frac{dP}{dt} = -\frac{i}{\hbar}[H, P]$$

Solution $P(t) = U(t)\,P(0)\,U^{-1}(t)$; $U(t) = \exp\left(-\frac{i}{\hbar} t H\right)$

Equilibrium states $[H, P_e] = 0$, all stable in $\mathcal{P}_0$

Energy: $\mathrm{Tr}\, H P(t) = E = \text{const.}$

Motions are all <u>reversible</u>

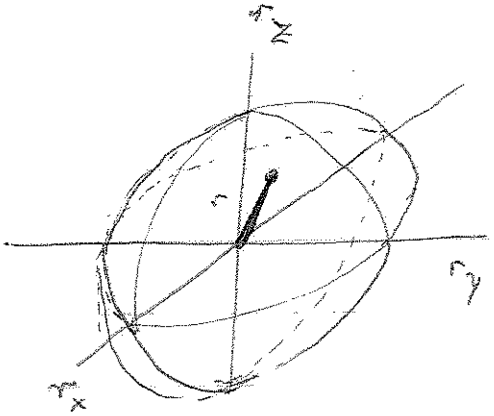
Two-level system ; $\dim \mathcal{H} = 2$

$$[P] = \frac{1}{2}\begin{bmatrix} 1 - r_z & r_x - i r_y \\ r_x + i r_y & 1 + r_z \end{bmatrix} \qquad P = P^\dagger \qquad \mathrm{Tr}\, P = 1$$

Eigenvalues are determined by

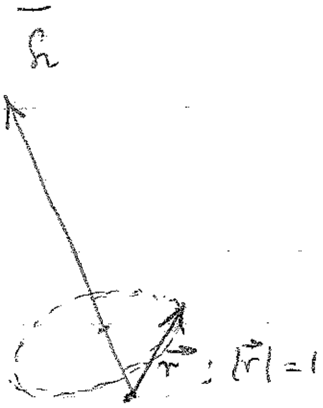
$$r^2 = r_x^2 + r_y^2 + r_z^2 \leq 1 \quad ; \quad P \geq 0$$
$$r^2 = 1 \quad ; \quad P^2 = P$$

Block sphere



$$\vec{r} = \begin{bmatrix} r_x \\ r_y \\ r_z \end{bmatrix} \qquad r^2 = 1$$

$$P \in \mathcal{B}_0$$



Motion is generated by H

$$[H] = \begin{bmatrix} h_0 + h_z & h_x - ih_y \\ h_x + ih_y & h_0 - h_z \end{bmatrix}$$

$$\bar{h} = \begin{bmatrix} h_x \\ h_y \\ h_z \end{bmatrix}$$

Equation of motion can be written as

$$\dot{\vec{r}} = \Omega_0 \frac{\vec{h} \times \vec{r}}{|\vec{h}|} \qquad \Omega_0 = \frac{2}{\hbar} |\vec{h}|$$

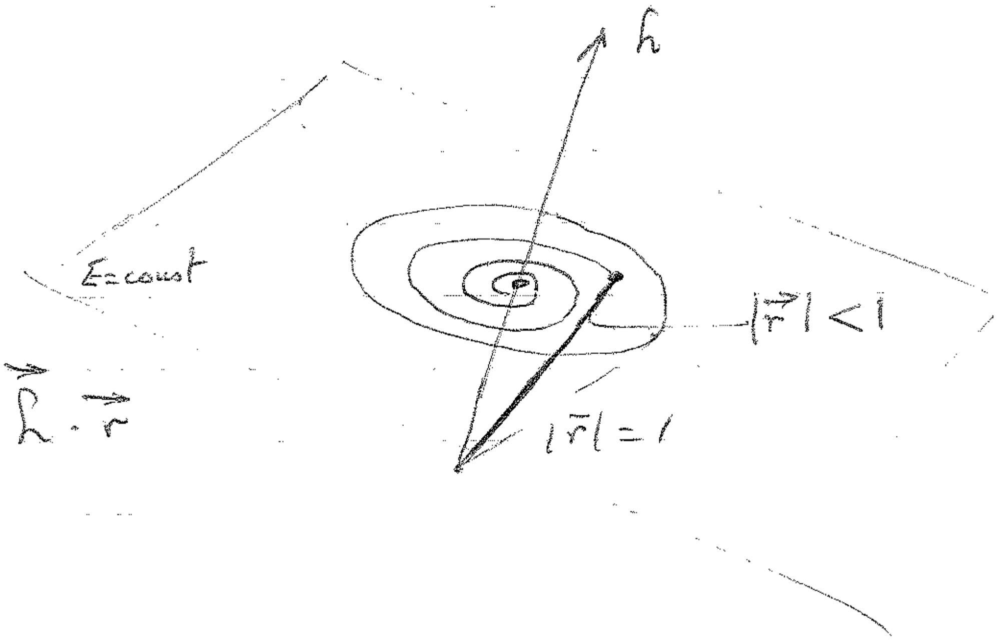
$$h_0 + \vec{h} \cdot \vec{r} = E = \text{energy} = \text{const}$$

In QT

$$[\rho]_\nu = \frac{1}{2}\begin{bmatrix} 1-r_z & r_x+ir_y \\ r_x-ir_y & 1+r_z \end{bmatrix}_{(\nu)}$$

$r^2 = r_x^2 + r_y^2 + r_z \leq 1$ $\rho \geq 0$

QT states $\mathcal{P}_0$ extended to $\mathcal{P}$ $P^2 \neq P$.



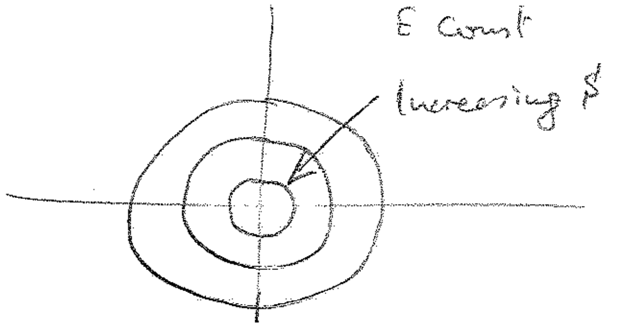
$\mathrm{Tr}\, H\rho = E \rightarrow \vec{h}\cdot\vec{r}$

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho]$$

$$-k\,\mathrm{Tr}\,\rho\log\rho = S = -\frac{1}{2}\left[(1+r)\ln(1+r) + (1-r)\ln(1-r) - \ln 4\right]$$

$[H,\rho_e] = 0$ equilibrium states

$$\vec{r} = r_e\vec{\Lambda} = r_e\frac{\bar{h}}{|\bar{h}|}$$



Conditions on equation of motion for isolated system

- $\dot{\rho} = F(\rho)$ autonomous
- Solutions $\rho(t)$ must remain in $\mathcal{P}$ at all t
  $-\infty < t < \infty$
- $\mathrm{Tr}(H\rho(t)) = \text{const} = E$
- $\forall$ values E: only one stable equilibrium states to each E.
- $-k\,\mathrm{Tr}\rho\ln\rho$ nondecreasing ; $\dot{s} \geq 0$
- For $\rho(0)$ in $\mathcal{P}_0$ $\dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho]$ $\forall\ t$
  (limit of idempotent QM states)

Proposed equation for a single constituent.

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau}\,\frac{\begin{vmatrix} \rho\ln\rho & \rho & \frac{1}{2}(H\rho + \rho H) \\ \mathrm{Tr}\rho\ln\rho & 1 & \mathrm{Tr}H\rho \\ \mathrm{Tr}H\rho\ln\rho & \mathrm{Tr}H\rho & \mathrm{Tr}H^2\rho \end{vmatrix}}{\underbrace{\begin{vmatrix} 1 & \mathrm{Tr}H\rho \\ \mathrm{Tr}H\rho & \mathrm{Tr}H^2\rho \end{vmatrix}}_{\Delta e^2(\rho)}}$$

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau}\Bigg[\rho \ln\rho + \rho\,\frac{\mathrm{Tr}H\rho\,\mathrm{Tr}H\rho\ln\rho - \mathrm{Tr}H^2\rho\,\mathrm{Tr}\rho\ln\rho}{\mathrm{Tr}H^2\rho - (\mathrm{Tr}H\rho)^2}$$

$$+ \frac{1}{2}(H\rho + \rho H)\,\frac{\mathrm{Tr}\rho\ln\rho\,\mathrm{Tr}H\rho - \mathrm{Tr}H\rho\ln\rho}{\mathrm{Tr}H^2\rho - (\mathrm{Tr}H\rho)^2}\Bigg]$$

The nonlinear term.

$$\frac{0}{0} \Rightarrow \mathrm{Tr}(H^2\rho) = (\mathrm{Tr}H\rho)^2 \qquad \rho \text{ is dispersionless ?}$$

$$\rho = \begin{bmatrix} 0 & 0 & - & - & - & 0 \\ 0 & 0 & \ddots & & & \\ & & \begin{bmatrix} p_1 & 0 & \\ 0 & p_2 & \ddots \\ & & p_D \end{bmatrix} & & & \\ & & & 0 & & \\ & & & & 0 & 0 \\ 0 & & & & 0 & 0 \end{bmatrix}$$

$$\rho = \sum_{d_k}^{D} p_{d_k} |\varepsilon_{d_k}\rangle\langle\varepsilon_{d_k}|$$

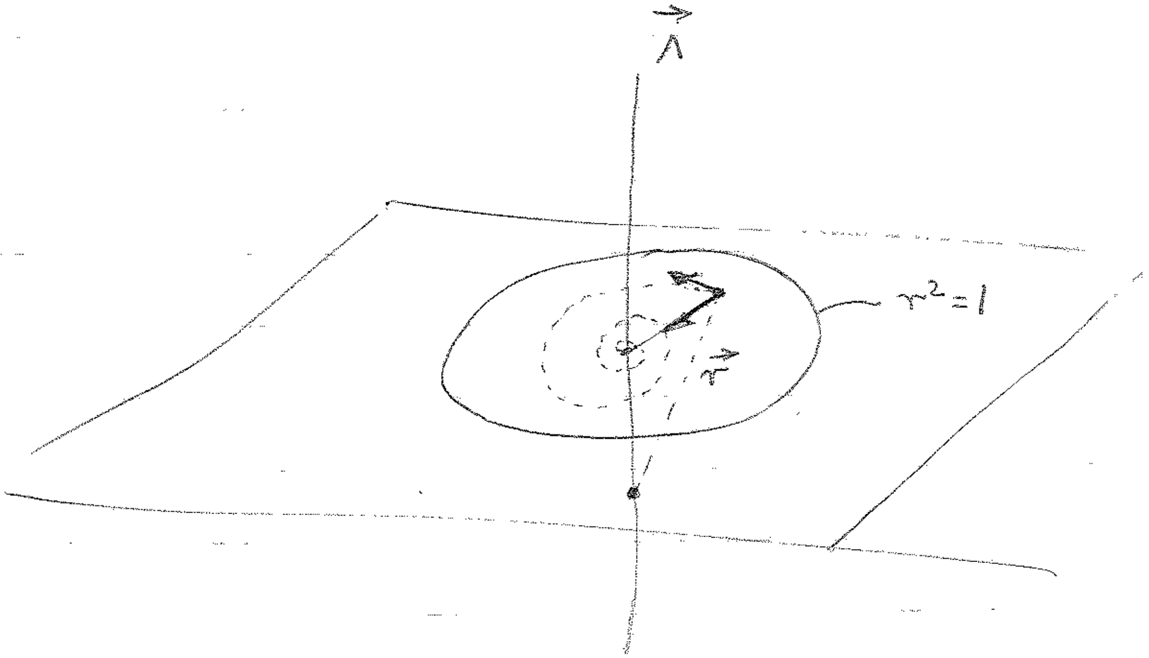
Then

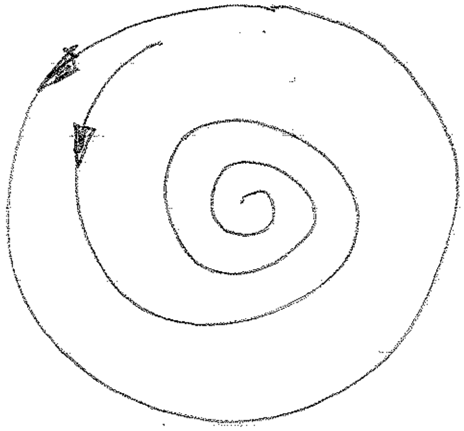
$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau}\begin{vmatrix} \rho\ln\rho & \rho \\ \mathrm{Tr}\rho\ln\rho & 1 \end{vmatrix}$$

If H nondegenerate then ρ Q.M. $\rho^2 = \rho$ (Careful)

For two level system

$$\dot{\vec{r}} = \Omega_0 \vec{\Lambda} \times \vec{r} - \frac{1}{\tau} K(\bar{r}) \left[\vec{\Lambda} \times \vec{r} \times \vec{\Lambda} \right]$$





May 1, 84

QT states in $\mathcal{P} = \{ \rho \mid \rho^{+} = \rho;\ \rho \geq 0;\ \mathrm{Tr}\rho\ 1 \}$

QM states in $\mathcal{P}_0 = \{ P \mid P \in \mathcal{P};\ P^2 = P \}$

Dynamics of a single constituent with $\eta = N I$ $(\Delta e^2(\rho) \neq 0)$

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{\tau\, \Delta e^2(\rho)} \begin{vmatrix} \rho \ln \rho & \rho & \frac{1}{2}(H\rho + \rho H) \\ \mathrm{Tr}\rho\ln\rho & 1 & \mathrm{Tr}H\rho \\ \mathrm{Tr}H\rho\ln\rho & \mathrm{Tr}H\rho & \mathrm{Tr}H^2\rho \end{vmatrix}$$

Two-level system

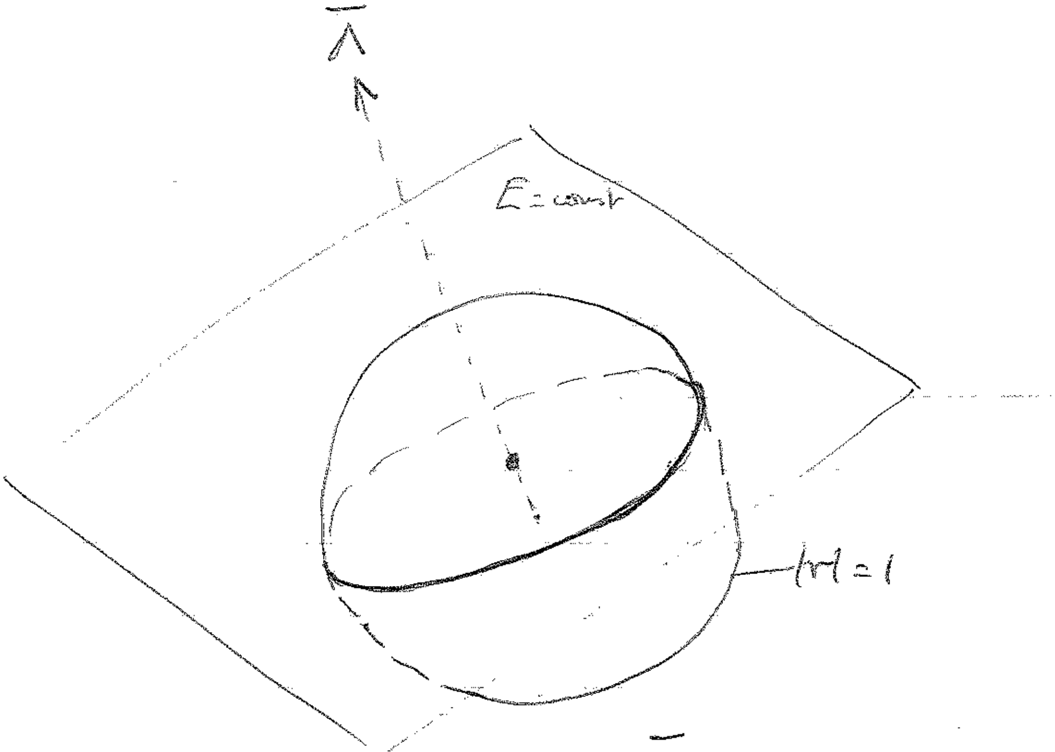
$$[\rho] = \frac{1}{2}\begin{bmatrix} 1 - r_z & r_x - i r_y \\ r_x + i r_y & 1 + r_z \end{bmatrix} \qquad \vec{r} = \begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix} \qquad r^2 \leq 1$$

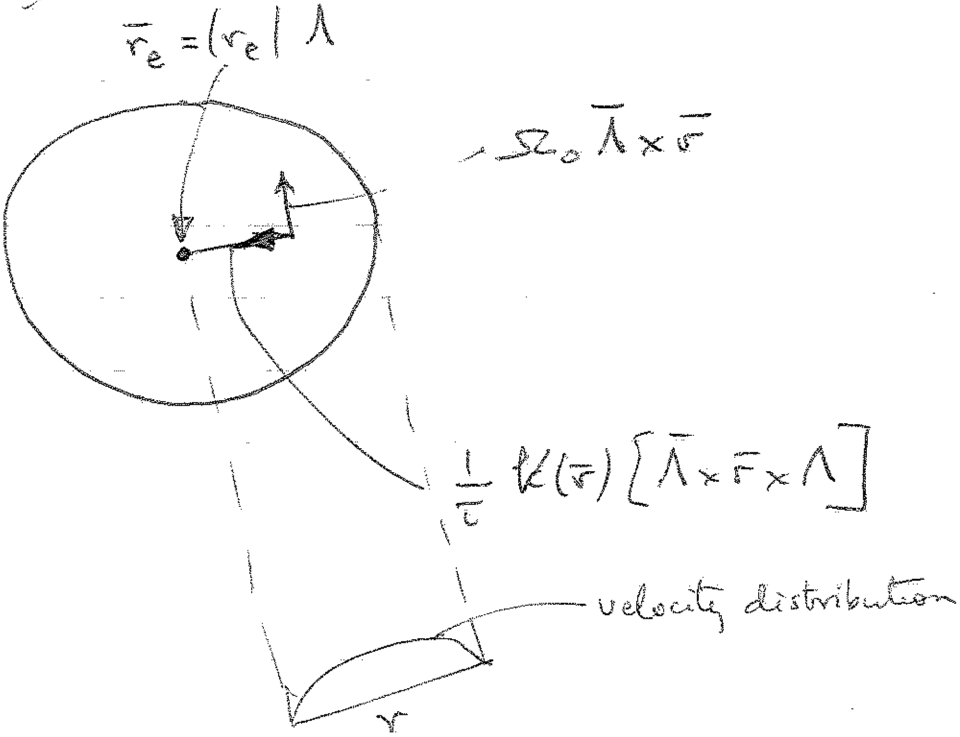
$$[H] = h_0 I + \frac{\hbar \Omega_0}{2}\begin{bmatrix} \lambda_z & \lambda_x - i\lambda_y \\ \lambda_x + i\lambda_y & -\lambda_z \end{bmatrix} \qquad \lambda^2 = 1 \qquad \bar{\lambda} = \begin{pmatrix} \lambda_x \\ \lambda_y \\ \lambda_z \end{pmatrix}$$

$$\dot{\bar{r}} = \Omega_0\, \bar{\lambda} \times \bar{r} - \frac{1}{\tau} K(\bar{r}) \left[\bar{\lambda} \times \bar{r} \times \lambda \right]$$

$$K(\bar{r}) = \frac{1 - r^2}{1 - (\bar{\lambda}\cdot\bar{r})^2} \cdot \frac{1}{2r} \cdot \ln \frac{1+r}{1-r} \quad ; \quad \mathrm{Tr}\, H\rho = \frac{\hbar\Omega_0}{2}\bar{\lambda}\cdot\bar{r} + h_0 = E$$

$= \text{constant}$


$\bar\Lambda$
E = const
$|r| = 1$


$\bar r_e = |r_e|\,\bar\Lambda$
$\Omega_0\,\bar\Lambda\times\bar r$
$\frac{1}{\tau}\,k(\bar r)\left[\bar\Lambda\times\bar r\times\Lambda\right]$
velocity distribution
r

- <u>Cauchy problem</u> – initial value problem

  $\forall \rho_i \in \mathcal{B}$ $\exists$ a unique solution $\rho(t)$, with

  $\rho(0) = \rho_i$; $\rho(t) \in \mathcal{B}$ $\forall t \in (-\infty, +\infty)$

  Assume that this has been proved.

- If initial state is in the set $\rho_i^2 = \rho_i \in \mathcal{B}_0$ then

  $\rho^2(t) = \rho(t) \in \mathcal{B}_0$ and $\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$

  So, solution coincides with <u>Schroedinger equation</u>.

- <u>Conservation of energy</u>

$$\frac{dE}{dt} = \frac{d}{dt}\mathrm{Tr}(H\rho) = \mathrm{Tr}(H\dot{\rho})$$

$$= -\frac{i}{\hbar}\,\cancelto{0}{\mathrm{Tr}\, H(H\rho - \rho H)}$$

$$-\frac{1}{\tau\,\Delta e^2(\rho)} \cancelto{0}{\begin{vmatrix} \mathrm{Tr}\, H\rho \ln\rho & \mathrm{Tr}\, H\rho & \mathrm{Tr}\, H^2\rho \\ \mathrm{Tr}\,\rho\ln\rho & 1 & \mathrm{Tr}\, H\rho \\ \mathrm{Tr}\, H\rho\ln\rho & \mathrm{Tr}\, H\rho & \mathrm{Tr}\, H^2\rho \end{vmatrix}}$$

— <u>Entropy nondecrease</u>

$$\frac{d}{dt} s(\rho|H) = -k \frac{d}{dt} \mathrm{Tr}\,\rho \ln\rho$$

$$= -k\,\mathrm{Tr}\left[\dot\rho \ln\rho + \dot\rho\right] = -k\,\mathrm{Tr}\,\dot\rho \ln\rho$$

$$= \frac{ik}{\hbar}\,\mathrm{Tr}\,[H,\rho]\ln\rho + \frac{k}{\tau\,\Delta e^2(\rho)}\,\mathrm{Tr}\left|\qquad\right|\ln\rho$$

$$= \frac{ik}{\hbar}\overset{=0}{\cancel{\left[\mathrm{Tr}\,H\rho\ln\rho - \mathrm{Tr}\,\rho H\ln\rho\right]}}$$

$$+ \frac{k}{\tau\,\Delta e^2(\rho)} \underbrace{\begin{vmatrix} \mathrm{Tr}\,\rho(\ln\rho)^2 & \mathrm{Tr}\,\rho\ln\rho & \mathrm{Tr}\,H\rho\ln\rho \\ \mathrm{Tr}\,\rho\ln\rho & 1 & \mathrm{Tr}\,H\rho \\ \mathrm{Tr}\,H\rho\ln\rho & \mathrm{Tr}\,H\rho & \mathrm{Tr}\,H^2\rho \end{vmatrix}}_{\text{Gram determinant}} \geq 0$$

— $\dot s = 0$ applies iff $\rho\ln\rho = \rho(\alpha I - \gamma H)$

— An observable represented by operator $C \in \mathcal{L}(\mathcal{H})$ is a <u>constant of the motion</u> iff

$\mathrm{Tr}\,C\rho = \text{const}$ $\qquad \mathrm{Tr}\,C\dot\rho = 0$ for all ρ.

C is a constant of the motion iff $C = \alpha I - \gamma H$.

— A state ρ is called nondissipative iff $\dot{s}(\rho) = 0$

ρ is nondissipative iff $\rho \ln \rho = \rho(\alpha I - \gamma H)$

$$= \rho C = C \rho$$

C = constant of the motion

— A state ρ is equilibrium iff $\dot{\rho} = 0$.

ρ is equilibrium iff nondissipative and commutes with H'

— Equilibrium states

$\rho C = C \rho \qquad C = \alpha I - \gamma H \qquad \rho H = H \rho$

ρ, H share eigenbasis

$H|\varepsilon_j\rangle = e_j|\varepsilon_j\rangle \qquad \rho|\varepsilon_j\rangle = p_j|\varepsilon_j\rangle$

$\rho \ln \rho = \rho C \rightarrow \qquad p_j \ln p_j = p_j(\alpha - \gamma e_j)$

$p_j = b_j \exp(\alpha - \gamma e_j)$

$b_j = \begin{cases} 1 \\ \end{cases}$

$$\sum p_j = 1$$

$$= \exp(\alpha) \sum_j b_j \exp(-\gamma e_j)$$

$$p_j = \frac{b_j \exp(-\gamma e_j)}{\sum_j b_j \exp(-\gamma e_j)}$$

$$\rho_e = \frac{B \exp(-\gamma H)}{\operatorname{Tr} B \exp(-\gamma H)} \qquad B = \begin{bmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 1 & & & \\ & & & 0 & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix}_{\varepsilon_j}$$

$$[\rho_e]_{\varepsilon_j} = \begin{bmatrix} 0 & & & & & \\ & 0 & & & & \\ & & \exp(-\gamma e_3) & & & \\ & & & 0 & & \\ & & & & \exp(-\gamma e_5) & \\ & & & & & \ddots \end{bmatrix} \frac{1}{\operatorname{Tr} B \exp(-\gamma H)}$$

For a fixed energy E

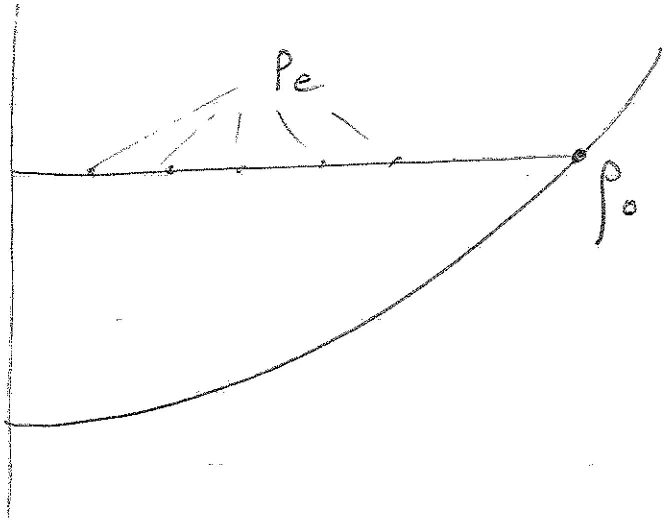
$$E = \operatorname{Tr} \rho_e H = \sum_j e_j p_j$$

$$= \frac{\sum_j b_j e_j \exp(-\gamma e_j)}{\sum_k b_k \exp(-\gamma e_k)}$$

There may be many equilibrium states with energy E. If we specify b_j $(0,1)$ there are 2^N possibilities. Depending on the value of the energy $(\dim \mathcal{H} = N)$ there is at most one equilibrium. ?

For example, if $B = I$ $\{ b_j = 1 \ \forall j \}$ then for $\forall E \in (e_{min}$ to $e_{max})$ there is one equilibrium state

$$\rho_0 = \frac{\exp(-\gamma H)}{\mathrm{Tr}\exp(-\gamma H)}$$



ρ_0 is the only equilibrium state which is strictly positive (all $b_j = 1$)

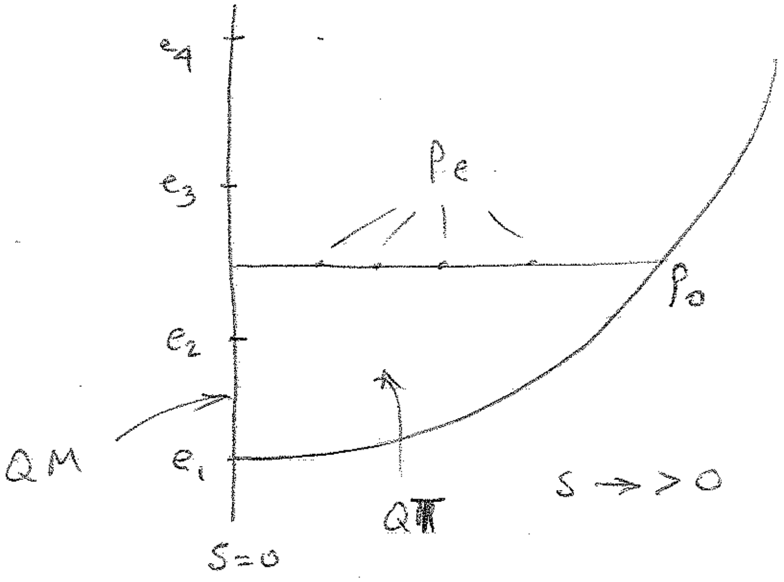
all other ~~zero~~ equilibrium states have zero eigenvalues so any state ρ_n that is nonsingular $(\rho_n > 0)$ is not equilibrium and therefore,

$$\underline{\dot{s}(\rho_n) > 0}$$

May 3, 84

$$\rho_e = \frac{B\exp(-\gamma H)}{\mathrm{Tr}\, B\exp(-\gamma H)}$$

$$[B]_{\varepsilon_i} = \begin{bmatrix} 0 & 0 & 0 & & \\ 0 & 1 & 0 & & \\ 0 & 0 & 0 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$



For each selection of b_j there exists a unique state for a good value of energy (at most one equilibrium state)

We have many equilibrium states for each E, and we have for sure one ρ_0.

The state ρ_0 is the only equilibrium state with energy E and nonsingular (no zero eigenvalues)

$$\rho_0(E) = \frac{1}{\sum_k \exp(-\gamma e_k)} \begin{bmatrix} \exp(-\gamma e_1) & 0 & \\ 0 & \exp(-\gamma e_2) & \\ & & \ddots \end{bmatrix}_e$$

Every equilibrium state is nondissipative.

Every state with no zero eigenvalues (strictly positive) different from $\rho_0(t)$ is dissipative because it is not equilibrium.

Stability of equilibrium.

Liapunov.

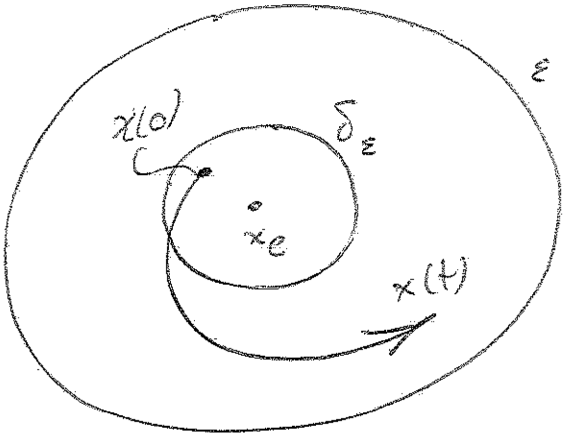
$$\dot{x} = f(x) \qquad x(0) = x_0 \qquad x \in \mathbb{R}^n$$

$\mathcal{R}$

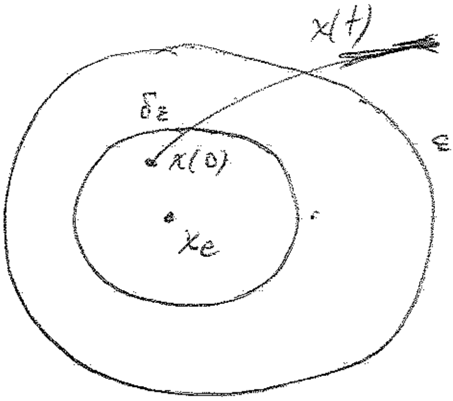
Equilibrium point

$$\dot{x} = 0 \qquad f(x_e) = 0 \qquad x_e(t) = x_e.$$

Stable equilibrium



Stable



Unstable

Differential equations defined on a set having a metric

$d(x,y)$; $d(x,y)=0$ iff $x=y$

$$d(x,y) = d(y,x) \geqslant 0$$

$$d(x,y) + d(y,z) \geqslant d(x,z)$$

$$d(x,y) = \|x-y\|$$

Stable equilibrium state iff

$$\forall \varepsilon > 0, \ \exists \delta_\varepsilon > 0, \ \Big| \ \forall x_0 \ \Big| \ d(x_0, x_e) < \delta_\varepsilon$$

$$d(x(t), x_e) < \varepsilon \quad \forall t$$

Unstable equilibrium state

$$\exists \varepsilon > 0 \quad \forall \delta_\varepsilon > 0 \ \Big| \ \exists x_0 \ \Big| \ d(x_0, x_e) < \delta_\varepsilon$$

$$\exists t \quad d(x(t), x_e) > \varepsilon.$$

Liapunov function –

A Liapunov function $V(x)$ is defined in the neighborhood of an equilibrium state as follows

1. $V(x_e) = 0$
2. $V(\cancel{x})$ continuous at $x = x_e$, i.e., $\forall \xi > 0, \exists \delta_\xi > 0 \,|$

$$\forall x \,,\ d(x, x_e) < \delta_\xi \,,\ \left| V(x) - V(x_e) \right| < \xi$$

3. $V(x) \geq a\big(d(x, x_e)\big)$ where $a(r)$ strictly increasing and positive real function
   $a(0) = 0$; $a(\varepsilon) > 0 \;\forall\, \varepsilon > 0$
   $a(r) < a(s)$ for $r < s$.

4. $V\big(x(t)\big) \leq V\big(x(0)\big) \quad \forall\; t > 0$

Liapunov stability theorem

If $V(x)$ is a Liapunov function in the neighborhood of an equilibrium point x_e, then x_e is a stable equilibrium state

Proof:

1. Consider a solution $x(t)$ with $x(0) = x_0$
If $V(x)$ is a Liapunov function then

$$V(x(t)) \leq V(x_0) \qquad \forall\, t > 0$$

2. $\forall \varepsilon > 0$ select $\xi = a(\varepsilon)$ where $a(r)$ is the function in 3 above (definition of Liapunof function).

3. $\exists\, \delta_\xi = \delta_\varepsilon \qquad \forall x_0 ,\ d(x_0, x_e) < \delta_\varepsilon$

$$|V(x)| < \xi \qquad V(x_0) < \xi = a(\varepsilon)$$

4. $\forall t > 0$

$$a(d(x(t), x_e)) < V(x(t)) \leq V(x_0) < a(\varepsilon)$$

$$d(x(t), x_e) < \varepsilon$$

Let $e(x)$ be an invariant function for the given set of differential equations, i.e.

$$\dot{e}(x) = 0 \qquad \forall\, x$$

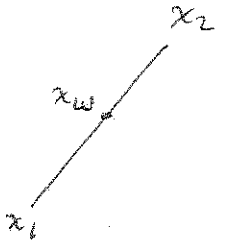
Consider a function $s(x)$

a. $s(x)$ is nonnegative

b. $s(x)$ is concave

$$s(x_\omega) \overset{?}{\leq} \omega\, s(x_1) + (1-\omega)\, s(x_2)$$

$$x_\omega = \omega x_1 + (1-\omega) x_2$$



c. $s(x)$ has a unique maximum at $x_0(E)$ on each set of points $\{x \mid e(x) = E\}$.

d. $s(x(t)) \geq s(x_0) \qquad t > 0$

then

$$V(x) \equiv s(x_0(E)) - s(x)$$

is a liapunov function if x_0 is point of maximum s.

Substitute
E energy
x ρ
s entropy.

May 8, 84

QT states in $\mathcal{P} = \{\rho \text{ on } \mathcal{H} \mid \rho^+ = \rho,\ \rho \geq 0,\ \mathrm{Tr}\rho = 1\}$

Dynamics of single constituent with $\mathcal{N} = NI$ (and $\Delta e^2(\rho) \neq 0$)

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau\,\Delta e^2(\rho)} \begin{vmatrix} \rho \ln \rho & \rho & \frac{1}{2}(H\rho + \rho H) \\ \mathrm{Tr}\rho\ln\rho & 1 & \mathrm{Tr}H\rho \\ \mathrm{Tr}H\rho\ln\rho & \mathrm{Tr}H\rho & \mathrm{Tr}H^2\rho \end{vmatrix}$$

Theorems: on the solutions $\rho(t)$ with $\rho(0)$ in $\mathcal{P}$:

- $\forall t \quad \rho^+(t) = \rho(t) \quad \rho(t) \geq 0 \quad \mathrm{Tr}\rho(t) = 1$
- $\mathrm{Tr}H\dot{\rho} = 0$ energy conservation
- $\dot{s}(\rho) \geq 0$ entropy nondecreasing.
- $\rho_0(E) = \dfrac{\exp(-\beta H)}{\mathrm{Tr}\exp(-\beta H)}$ = equilibrium state
- $V(\rho) = s(\rho_0(E(\rho))) - S(\rho)$ is a Liapunov function near each $\rho_0(E)$, $\forall E$.
- $\rho_0(E)$ is a stable equilibrium state, $\forall E$.
- Any other nondissipative ($\Rightarrow$ equilibrium) state is of the form

$$\rho_0 = \frac{B\exp(-\gamma H)}{}$$

- Every $\rho_e \neq \rho_0(E(\rho_e))$ is unstable.

- For every E there is one and only one stable equilibrium state. Then QT entails a statement of the 2nd law of thermodynamics as a theorem of the dynamics, not as a postulate

Proof of instability

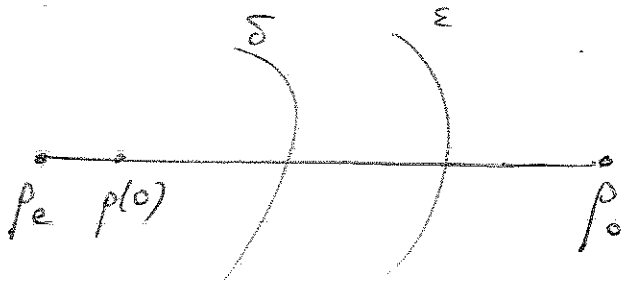
If $\rho_e \neq \rho_0(E)$ the ρ_e has at least one zero eigenvalue

Thus, if $\rho \neq \rho_e(E(\rho))$ and ρ has no zero eigenvalues, then ρ must be dissipative, i.e., $\dot{s}(\rho) > 0$

If $\rho(0)$ has no zero eigenvalues, then $\rho(t)$ has no zero eigenvalues $\forall t$, so $\dot{s}(\rho(t)) > 0 \ \forall t$ and $\rho(t) \to \rho_0(E(\rho(0)))$ as $t \to \infty$

ρ_e is unstable iff $\exists\, \varepsilon > 0, \forall \delta > 0, \exists\, \rho(0) \in \|\rho(0) - \rho_e\| <$

$\exists\, t > 0 \in \|\rho(t) - \rho_e\| \geq \varepsilon$



Take

$\rho(0) = \eta \rho_0(E) + (1-\eta)\rho_e$

$\rho(0)$ has no zero eigenvalues and is arbitrary close to ρ_e

Planck's oscillator $(\dim \mathcal{H} = \infty)$ $N = 1$

Eigenvalues $e_k = \left(k + \frac{1}{2}\right) h\nu$ $k = 0, 1, \ldots \infty$

$$\rho_0 = \frac{\exp(-\beta H)}{Q}$$

$$Q = \operatorname{Tr} \exp(-\beta H) = \sum_k \exp\left(-\beta\left(k + \tfrac{1}{2}\right) h\nu\right)$$

$$= \exp\left(-\frac{x}{2}\right) \sum_k \exp(-kx)$$

$$= \frac{\exp\left(-\frac{x}{2}\right)}{1 - \exp(-x)} = \frac{1}{2 \sinh \frac{\beta h\nu}{2}}$$

$$E = \frac{d}{d\beta}(-\ln Q) = \frac{h\nu}{2} + \frac{h\nu}{\exp(\beta h\nu) - 1} \qquad \beta = \frac{1}{kT}$$

. ——— . ———

<u>Fermi's oscillator</u> $(\dim \mathcal{H} = 2)$ $N = 1$

H eigenvalues $e_k = 0, \varepsilon$ $k = 1, 2$

$$\rho_0 = \frac{\exp(-\beta H)}{Q} = 1 + \exp(-\beta \varepsilon) \quad \times$$

$$E = \frac{\varepsilon}{\exp(\beta\varepsilon) + 1}$$

May 10, 84

Single constituent (or field) with $N \neq N I$.

Field of identical noninteracting coexisting particles, like the electromagnetic field (i.e., radiation, or photons) in a cavity of volume V.

		N
1 particle $\boxed{\Pi} \longrightarrow$	$\mathcal{H}_1$	$1 I_1$
2-particle $\boxed{\Pi} \longrightarrow$	$\mathcal{H}_2 = \mathcal{H}_1 \otimes \mathcal{H}_1$	$2 I_2$
	$\mathcal{H}_n = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$	$n I_n$

Overall Hilbert space – Fock space

$$\mathcal{F} = \mathbb{C} \oplus \mathcal{H}_1 \oplus \mathcal{H}_1 \otimes \mathcal{H}_1 \oplus \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H} \oplus$$

Number of particles operator

$$N = 0 P_{\mathbb{C}} + 1 P_{\mathcal{H}_1} + 2 P_{\mathcal{H}_2} + \cdots + N P_{\mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}$$

How many particles yield eigenvalue e_i for the energy?

$\forall$ eigenvalue e_i of the Hamiltonian H_1, there an operator N_i which represents the occupation number belonging to e_i

$$H = \sum_i e_i n_i \qquad \eta = \sum_i \eta_i$$

Eigenvalue problem for each of the occupation numbers

$$\eta_i \psi_j = n_{ij} \psi_j$$

$\{\psi_j\}$ eigenbasis of all occupation number operators

$$H \psi_j = \sum e_i \eta_i \psi_j$$

$$= \left(\sum_i n_{ij} e_i\right) \psi_j$$

$$E_j = \sum_i e_i n_{ij}$$

$$\eta \psi = \sum \eta_i \psi_j = \sum n_{ij} \psi_j$$

$$N_j = \sum_i n_{ij}$$

* * *

Two classes (important) of such fields

a $n_{ij} = \begin{matrix} 0 \\ 1 \end{matrix}$ Fermi-Dirac fields (Pauli exclusion principle)

b. $n_{ij} = 0, 1, 2 \ldots$ Bose-Einstein ...

Two additional classes

$\langle N \rangle$ is conserved in time

$\langle N \rangle$ is not conserved in time (only example radiation)

Bose-Einstein: Examples	Fermi-Dirac: Examples
Photons	Electron
Neutrons	Protons

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] - \frac{1}{\tau\,\Gamma(\rho)} \begin{vmatrix} \rho \ln \rho & \rho & \frac{1}{2}(H\rho + \rho H) & \frac{1}{2}(\rho N + N\rho) \\ \mathrm{Tr}\,\rho \ln \rho & 1 & \mathrm{Tr}\,H\rho & \mathrm{Tr}\,N\rho \\ \mathrm{Tr}\,H\rho \ln \rho & \mathrm{Tr}\,H\rho & \mathrm{Tr}\,H^2\rho & \mathrm{Tr}\,NH\rho \\ \mathrm{Tr}\,N\rho \ln \rho & \mathrm{Tr}\,N\rho & \mathrm{Tr}\,NH\rho & \mathrm{Tr}\,N^2\rho \end{vmatrix}$$

$\Gamma(\rho)$

If N is conserved; stable equilibrium states

$$\rho_0(E,N) = \frac{\exp(-\beta H + \beta\mu N)}{\mathrm{Tr}\exp(-\beta H + \beta\mu N)}$$

Q partition function

$\langle E \rangle = \mathrm{Tr}\,H\rho$

$\langle N \rangle = \mathrm{Tr}\,N\rho$

$$Q = \mathrm{Tr}\exp(-\beta H + \beta\mu N)$$

$$= \sum \exp(-\beta E_j + \beta\mu N_j)$$

$$= \sum_j \exp\Big(-\beta \sum_i e_i n_{ij} + \beta\mu \sum_i n_{ij}\Big)$$

$$= \sum_j \exp\Big(-\beta \sum_i n_{ij}(e_i - \mu)\Big)$$

Use for Fermions & Bosons

WEAVER 3

May 15, 84

Field of identical indistinguishable noninteracting coexisting particles

Single particle: Hilbert Space $\mathcal{H}_1$, Hamiltonian H_1 with

eigenvalues $e_1\ e_2 \dots e_i$

eigenvectors $\varepsilon_1, \varepsilon_2, \dots \varepsilon_i$

or distinct eigenvalues $e_1\ e_2 \dots e_K$

degeneracy $D_1\ D_2\ \ D_K$

Field: Hilbert (Fock) space $\mathcal{F} = \bigoplus_{j=0}^{\infty} (\mathcal{H}_1)^{\otimes j}$

$H = \sum_i e_i N_i \qquad N = \sum N_i \qquad N_i =$ occupation number associated with eigenvektor ε_i

$H = \sum_K e_K N_K \qquad N = \sum N_K \qquad N_K = \sum_i^{D_K} N_i$ occupation number associated with eigenvalue e_K

Eigenvalue problem for occupation number operators

$N_i |\psi_j\rangle = n_{ij} |\psi_j\rangle$

$n_{ij} = 0, 1$ Fermions

$n_{ij} = 0, 1, 2 \dots$ Bosons

Stable equil. states

N conserved $\quad \rho_0(\mathcal{E}, N) = \dfrac{\exp\left[-\beta(\mathcal{E},N)(H - \mu(\mathcal{E},N)N)\right]}{Q(\mathcal{E},N)}$

$\mathcal{E} = \mathrm{Tr}\, \rho_0(\mathcal{E},N) H$

$N = \mathrm{Tr}\, \rho_0(\mathcal{E},N) N$

η not conserved, photons, $\mu = 0$ $\beta = \beta(E)$ only.

$$\ln Q(E,N) = \sum D_k \ln \left[1 \pm \exp\left(-\beta(E,N)\left(e_k - \mu(E,N)\right)\right)\right]^{\pm 1}$$

+ Fermi-field
− Boson-field

$$N_k = \mathrm{Tr}\, \rho_0(E,N)\, \eta_k = \frac{D_k}{\exp\left[\beta(E,N)\left(e_k - \mu(E,N)\right)\right] \pm 1}$$

Fermi-Dirac
Bose-Einstein
factors

Very dilute $\beta(e_1 - \mu) \gg 1 \rightarrow \exp\left(\beta(e_k - \mu)\right) \gg 1$

$e_k > e_1$

$$N_k \cong D_k \exp(\beta\mu) \exp(-\beta e_k)$$

$$N = \sum_k N_k \cong \exp(\beta\mu) \sum_k D_k \exp(-\beta e_k)$$

$$\frac{N_k}{N} = \frac{D_k \exp(-\beta e_k)}{\sum D_k \exp(-\beta e_k)}$$ Maxwell-Boltzmann

$$H_1 = \frac{p^2}{2m}$$

$e_k = \frac{1}{2} m v_k^2$ $D_k = 1$ velocity distribution M-B.

$$\frac{\mathrm{Tr}\,\rho_0 \mathcal{M}_k}{\mathrm{Tr}\,\rho_0 \mathcal{N}} = \frac{N_k}{N}$$

Radiation in a cavity of volume V (V large)

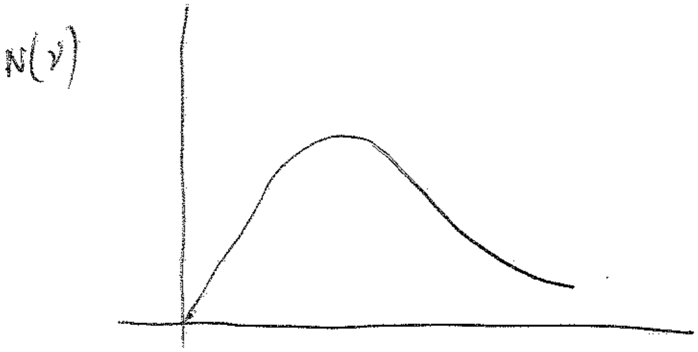
$e_k \rightarrow E = h\nu$

$D_k \rightarrow D(E)$, $D(\nu)$ = number of eigenvalues between ν and $\nu + d\nu$

$$D(\nu) = \frac{4\pi V}{c^3}\nu^2$$

If you account for polarization: multiply by 2

$$N(\nu) = \mathrm{Tr}\,\rho_0 \mathcal{N}_\nu = \frac{8\pi V}{c^3}\,\frac{\nu^2}{\exp(\beta h\nu) - 1}$$

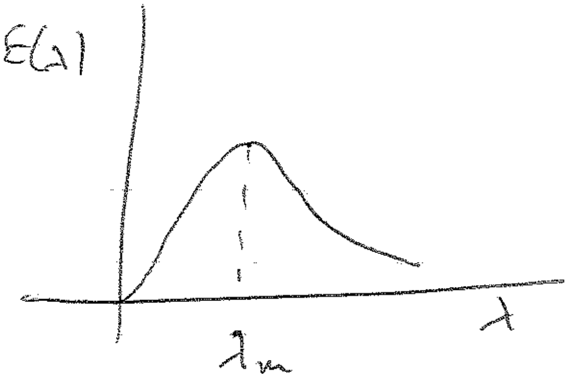


Planck's spectral distribution of blackbody radiation

$$E(\nu) = \frac{h\nu N(\nu)}{V} = \frac{8\pi h}{c^3} \frac{\nu^3}{\exp(\beta h\nu) - 1}$$

$$\nu = \frac{c}{\lambda} \qquad d\nu = -\frac{c}{\lambda^2} d\lambda$$

$$E(\lambda)\, d\lambda = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp(\beta hc/\lambda) - 1} d\lambda$$



$$E'(\lambda_m) = 0 \qquad \beta = \frac{1}{kT}$$

$$\lambda_m T = 0.28978 \text{ cm}\cdot\text{K}$$

Wien displacement law

N = total number of photons

$$= \int_0^\infty d\nu\, N(\nu) = \frac{8\pi V}{c^3} \frac{1}{(h\beta)^3} \int_0^\infty \frac{x^2 dx}{\exp(x) - 1}$$

$$= 2.404 \frac{8\pi V}{c^3} \frac{1}{(h\beta)^3}$$

$$\ln Q = -\int_0^\infty d\nu\, D(\nu) \ln\left(1-\exp(-\beta h\nu)\right)$$

$$= \frac{8\pi V}{3(\beta hc)^3} \underbrace{\int_0^\infty \frac{x^3\,dx}{\exp(x)-1}}_{\pi^4/15}$$

$$\ln Q = \frac{8\pi^5 V}{45(\beta hc)^3}$$

$$E = -\left.\frac{\partial \ln Q}{\partial \beta}\right|_V = \frac{8\pi^5 k^4}{15 h^3 c^3} V T^4$$

$$S = k\beta E + k \ln Q = \frac{32\pi^5 k^4}{45 h^3 c^3} V T^3$$

$$p = \frac{1}{\beta} \left.\frac{\partial \ln Q}{\partial V}\right|_\beta = \frac{8\pi^5 k^4}{45 h^3 c^3} T^4 = \frac{E}{3V}$$

$$N = 2.404 \frac{15}{\pi^4} \beta E$$

$$\frac{pV}{NkT} = 0.9$$

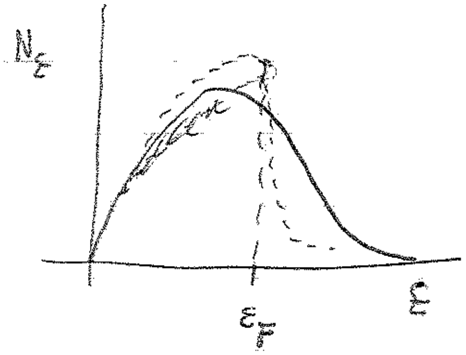
Electrons in a metal

$e_K \rightarrow E$ continuous from the bottom of the conduction band

$$D_K \rightarrow \mathcal{D}(E) = \frac{mV}{2\pi^2 \hbar^3}\sqrt{2mE} \quad \times(2 \text{ for spin})$$

$$N_E = \frac{mV\sqrt{2m}}{\pi^2 \hbar^3} \frac{E^{1/2}}{\exp \beta(E-\varepsilon_F)+1}$$

ε_F = Fermi energy



$$N = \int_0^\infty dE\, N_E$$

$$N_0 = \lim_{\beta\to\infty} N = \int_0^{\varepsilon_F} dE\, N_E = \quad \boxed{\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N_0}{V}\right)^{2/3}}$$

May 17, 84

Statistical interpretation of thermodynamics

— A system is in a state described by a vector or one-dimensional projector

— Because we do not know exactly which vector we consider a number of them and assign a probabilit to each.

— Then we end up with a ρ especially for thermodynamic equilibrium.

Justification

- Infinite system
- Average measurements over infinite time
- Ergodic theories
- Interactions with heat baths

— Many objections have been raised and many attempts have been made to correct things. However, all of them are statistical in nature

Quantum Thermodynamics

- Enlarge the concept of state from P to ρ but homogeneous

- Does this create any problems with the kinematics of Q.M ?
- Does it change any of the numerical results obtain by the other interpretation ?
- Does it require any distinctions between large & small, equilibrium and nonequilibrium?

- Enlarge the dynamics

All the theorems. etc.

- It includes all the dynamics of Q.M.

It includes energy conservation + entropy nondecreas so we do not need thermodynamics in the sense that scattering of solid-state physics are not different sciences than QM

Eliminates all the inconsistencies

2.452J and 22.572J

QUANTUM THERMODYNAMICS

Problem Set #1 Due: February 15, 1983

In a short, schematic and concise paper, review the experimental facts that Classical Mechanics fails to explain.

For each such fact, point out clearly the essential features that Classical Mechanics cannot contemplate and explain why it cannot.

Conclude your paper by condensing in a set of concise statements, each justified by a brief explanation, the ideas that as a result of your analysis emerge as necessary new features of a more complete theory of Nature.

Suggested readings:

Messiah, pp. 3 - 27

Tolman, pp. 180 - 189

Margenau, pp. 307 - 328

Lindsay and Margenau, pp. 387 - 394

(See first handout for complete references).

2.452J and 22.572J

QUANTUM THERMODYNAMICS

Midterm Examination

Due: April 7, 1983

1. Show that, in general, if a vector ψ in Hilbert space evolves according to the Schroedinger equation $\hbar\dot{\psi} = -iH\psi$, where H is the self-adjoint Hamiltonian operator of the system, then the projector P_ψ evolves according to the von Neumann equation $\hbar\dot{P}_\psi = -i[H,P_\psi]$.

2. Show that for any self-adjoint operator A, $\langle\psi|A|\psi\rangle = \mathrm{Tr}AP_\psi$ for every unit-norm vector ψ.

3. Now consider a spin-1/2 system with gyromagnetic ratio γ in a static magnetic field $\vec{H}_m$. The associated Hilbert space is two-dimensional. In a sense, this is the simplest quantum system. Let M_z be the operator corresponding to the observable "magnetic moment in the z-direction". Only two outcomes are possible for an M_z-measurement act, namely, $+\gamma\hbar/2$ and $-\gamma\hbar/2$. Denote the orthonormal eigenbasis of M_z by $|z_+\rangle$ and $|z_-\rangle$. Is there only one? Write the matrix representation of M_z with respect to such basis.

4. Next, consider the set of operators $\{\nu_o,\nu_x,\nu_y,\nu_z\}$ such that their matrix representation with respect to the basis $\{|z_+\rangle,|z_-\rangle\}$ is given by

$$[\nu_o]_z = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad [\nu_x]_z = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$[\nu_y]_z = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad [\nu_z]_z = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Show that these operators form an orthonormal basis for the real space of linear, self-adjoint operators with real scalar product $(A,B) \equiv \mathrm{Tr}AB$. Show that every projector P_ψ can be represented as

$$[P_\psi]_z = \frac{1}{2}\begin{bmatrix} 1+r_z & r_x - ir_y \\ r_x + ir_y & 1-r_z \end{bmatrix}$$

where the real numbers r_x, r_y and r_z are such that $r_x{}^2 + r_y{}^2 + r_z{}^2 = 1$. Thus, every quantum-mechanical state of the two-level system could be represented in an auxiliary three-dimensional space as a point, or vector $\vec{r} \equiv (r_x, r_y, r_z)$, on the surface of a unit-radius sphere known as the Bloch sphere. Draw a sketch of this.

5. Define the "vector" $\vec{\nu} \equiv (\nu_x, \nu_y, \nu_z)$. Note that its "coordinates" are operators! Show that

$$P_\psi = \frac{1}{2}(\nu_o + \vec{r}\cdot\vec{\nu})$$

where $\vec{r}\cdot\vec{\nu} \equiv r_x\nu_x + r_y\nu_y + r_z\nu_z$. With the same notation, the magnetic moment operator "vector" is defined by

$$\vec{M} = \sqrt{2}\,\frac{\gamma\hbar}{2}\,\vec{\nu}$$

By analogy with the classical theory of magnetic dipoles, the Hamiltonian operator is defined by $H = \vec{M}\cdot\vec{H}_m$. It is useful to write H in the form $H = \sqrt{2}\,\vec{h}\cdot\vec{\nu}$ where $\vec{h} \equiv (h_x, h_y, h_z)$. What is the matrix representation of H?

6. Show that if ψ obeys the Schroedinger equation, then the vector $\vec{r}$ obeys the equation

$$d\vec{r}/dt = \vec{\omega} \times \vec{r}$$

where $\vec{\omega} \equiv \gamma\vec{H}_m$. What kind of motion is this in the auxiliary space defined in part 4? Show a typical trajectory on your sketch. Show that the equation for the mean magnetic moment vector $\vec{m}(\psi) \equiv \langle\psi|\vec{M}|\psi\rangle$ is the same as the classical equation for the magnetic dipole moment vector.

7. Now interpret your results as carefully and deeply as you can.

Specifically, address the following questions:

Is the spin system totally equivalent to the classical magnetic dipole?

What are the physical consequences of the fact (show it) that operators M_x, M_y and M_z do not commute?

By measuring magnetic moments in different directions, how many independent sets of measurements should one perform in order to fully determine the state ψ resulting from a given homogeneous preparation?

How would you measure the value of the constant γ?

2.452J and 22.572J

QUANTUM THERMODYNAMICS

Problem Set #4 Due: March 17, 1983

For a given observable A with a spectrum of distinct real values a_1, a_2, ..., a_j, ..., recall the following definitions:

Q_{a_j} = "question-observable" : is A equal to a_j?

$\langle Q_{a_j}\rangle_\psi$ = arithmetic mean of Q_{a_j} – measurements on a homogeneous ensemble of systems all in the same state ψ; also

= frequency of "answer" a_j in A-measurement results

$\langle A\rangle_\psi = \sum_j a_j \langle Q_{a_j}\rangle_\psi$ = arithmetic mean of A-measurement results

$\langle \Delta A^2\rangle_\psi = \sum_j (a_j - \langle A\rangle_\psi)^2 \langle Q_{a_j}\rangle_\psi$ = mean-square deviation of A-measurement results

$\Delta a = (\langle \Delta A^2\rangle_\psi)^{1/2}$ = "uncertainty" in A-measurement results

$q_{a_j}(\psi)$ = functional representing observable Q_{a_j}

$a(\psi)$ = functional representing observable A

$\Delta a^2(\psi)$ = functional representing observable $(A - \langle A\rangle)^2$

$\mathcal{H}_{a_j}$ = (orthogonal) subspace of $\mathcal{H}$ belonging to value a_j

$P_{\mathcal{H}_{a_j}}$ = (orthogonal) projector onto $\mathcal{H}_{a_j}$ (orthogonality: $P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{a_j}} = \delta_{ij} P_{\mathcal{H}_{a_j}}$)

$A = \sum_j a_j P_{\mathcal{H}_{a_j}}$ = self-adjoint operator associated with observable A

1. Show that if $q_{a_j}(\psi) = \langle\psi, P_{\mathcal{H}_{a_j}}\psi\rangle$ and, therefore, $a(\psi) = \langle\psi, A\psi\rangle$ then

$$\Delta a^2(\psi) = \langle\psi, A^2\psi\rangle - \langle\psi, A\psi\rangle^2$$

2. Now consider two observables A and B with associated operators A and B, and define operator $[A,B] = AB - BA$. Show that for every ψ

$$\Delta a^2(\psi)\ \Delta b^2(\psi) \geq \frac{1}{4}\ |\langle\psi,[A,B]\psi\rangle|^2$$

This is the Heisenberg uncertainty principle.

Hints: Recall the Schwarz inequality $\langle\alpha,\alpha\rangle\langle\beta,\beta\rangle \geq |\langle\alpha,\beta\rangle|^2$ valid for any two vectors α and β. Define vectors $\alpha = (A - a(\psi))\psi$ and $\beta = (B - b(\psi))\psi$. Show that $\Delta a^2(\psi) = \langle\alpha,\alpha\rangle$ and $\Delta b^2(\psi) = \langle\beta,\beta\rangle$. Recall that if c is a complex number, then $|c| \geq |\text{Re}(c)| = |(c + c^*)/2|$.

3. As an instructive example, consider a particle in one dimension with $L^2(a,b)$ as the associated Hilbert space. Thus, the state vectors are the square-integrable functions $f(x)$ on $a \leq x \leq b$. Let $Q = x$ be the position operator (i.e., multiplication by x) and $P = -i\hbar\ \partial/\partial x$ (i.e., differentiation by x). Show that $[Q,P] = i\hbar I$ and, therefore, $\Delta q\ \Delta p \geq \hbar/2$. Interpret carefully the physical implications of this position-momentum uncertainty relation.

4. Now return to the general case and let the state vector ψ evolve in time according to the Schroedinger equation of motion $\hbar\dot{\psi} = -\ iH\psi$ where H is the self-adjoint (Hamiltonian) operator associated with the observable energy. Show that $\hbar\dot{a}(\psi) = i\langle\psi,[H,A]\psi\rangle$ (with A = H, this result shows that the energy is a constant of the motion). Define the characteristic time functional $\tau_A(\psi) \equiv (\Delta a^2(\psi))^{1/2}/|\dot{a}(\psi)|$ and show that for any observable A and every state ψ

$$\tau_A(\psi)\ \Delta e(\psi) \geq \hbar/2$$

This is known as the time-energy uncertainty relation. Attempt a careful interpretation of the physical implications of this result.

2.452J and 22.572J

QUANTUM THERMODYNAMICS

Problem Set #5 Due: April 21, 1983

Consider a spin-1/2 system with gyromagnetic ratio γ in a static magnetic field $\vec{H}_m$. We will keep the same notation as in the midterm examination. However, we treat the system according to quantum thermodynamics, not quantum mechanics.

1. Show that the (self-adjoint, unit-trace, nonnegative-definite) state operator ρ can be represented with respect to the $\{|z_+\rangle, |z_-\rangle\}$ basis as

$$[\rho]_z = \frac{1}{2}\begin{bmatrix} 1 + r_z & r_x - ir_y \\ r_x + ir_y & 1 - r_z \end{bmatrix}$$

where the real numbers r_x, r_y and r_z are such that $r_x^2 + r_y^2 + r_z^2 \leq 1$. Thus, every quantum-thermodynamic state of a two-level system can be represented in an auxiliary three-dimensional space as a point, or vector $\vec{r} \equiv (r_x, r_y, r_z)$ with norm $r \equiv |\vec{r}| = (r_x^2 + r_y^2 + r_z^2)^{1/2} = (\vec{r}\cdot\vec{r})^{1/2}$, inside or on the surface of the unit-radius Bloch sphere.

2. Show that

$$\rho = \frac{1}{\sqrt{2}}(\nu_o + \vec{r}\cdot\vec{\nu})$$

$$\vec{m}(\rho) = \frac{\gamma\hbar}{2}\vec{r}$$

and

$$e(\rho) = \vec{h}\cdot\vec{r}$$

where $\vec{m}(\rho)$ is the mean magnetic moment vector and $e(\rho)$ the mean energy for a spin system in state ρ.

3. In the auxiliary Bloch sphere, where do all the states with a given mean energy E lie, i.e., how is the family of states ρ with $e(\rho) = E$ represented in that auxiliary space?

4. The observable represented by the functional $s(\rho) \equiv -k\mathrm{Tr}(\rho\ln\rho)$ plays an important role in quantum thermodynamics. It will be identified with the physical observable entropy. Find the expression of that functional in terms of the scalars r_x, r_y, r_z and show that it depends only on r (careful, this is not a trivial problem, recall the definition of function of an operator).

5. In the auxiliary Bloch sphere, where do all the states with a given mean entropy S lie, i.e., how is the family of states ρ with $s(\rho) = S$ represented in that auxiliary space?

6. For each given value of E, where is in the Bloch sphere the state ρ_o with $e(\rho_o) = E$ and $s(\rho_o)$ greater than any other state with $e(\rho) = E$?

7. On an E versus S diagram, draw with some accuracy the region corresponding to the states of quantum thermodynamics. Where are the states of quantum mechanics? List as many observations as you can on the relations between the Bloch sphere representation of states and the E vs S diagram representation.

Student:

ENZO ZANCHINI

2.452J and 22.572J

QUANTUM THERMODYNAMICS

Problem Set #2

Due: March 13, 1984

Let Ω be the classical phase space of a system with only one degree of freedom and Hamiltonian function h defined on Ω. We can coordinatize Ω using a pair of real variables q and p with dimensions of position and momentum, respectively. But we can also introduce the complex dimensionless variable

$$z \equiv \sqrt{1/2am\omega}\,(m\omega q + ip)$$

where a is a universal constant (with dimensions of angular momentum) and m and ω are characteristic constants of the degree of freedom (with dimensions of mass and frequency, respectively).

1. Show that when the Hamiltonian is regarded as a real function of the variable z and its complex conjugate z^* (i.e., $h(z,z^*) = h^*(z^*,z)$), then the Hamilton equations of motion take the compact form

$$\dot{z} = -\frac{i}{a}\frac{\partial h}{\partial z^*}$$

2. For a one-dimensional harmonic oscillator of mass m and frequency ω, write the Hamiltonian function first in terms of coordinates q and p, then in terms of z and z^*. Write the equation of motion for z(t) and solve it for the initial condition z(0).

PART 1. (HAMILTON EQUATIONS)

$$\boxed{z = \sqrt{1/(2am\omega)}\ (m\omega q + ip)}$$

$$z = \sqrt{\frac{m^2\omega^{\cancel{2}}}{2a\cancel{m}\cancel{\omega}}}\ q + i\sqrt{\frac{1}{2am\omega}}\ p$$

$$\begin{cases} z = \sqrt{\frac{m\omega}{2a}}\ q + i\sqrt{\frac{1}{2am\omega}}\ p \\ z^* = \sqrt{\frac{m\omega}{2a}}\ q - i\sqrt{\frac{1}{2am\omega}}\ p \end{cases} \qquad (1)$$

$$\begin{cases} z + z^* = \sqrt{\frac{2m\omega}{a}}\ q \\ z - z^* = i\sqrt{\frac{2}{am\omega}}\ p \end{cases} \quad (1') \qquad \begin{cases} q = \sqrt{\frac{a}{2m\omega}}\ (z + z^*) \\ p = -i\sqrt{\frac{am\omega}{2}}\ (z - z^*) \end{cases} \quad (1'')$$

$$\left.\begin{array}{l} H = H(q, p, t) \\ q = q(z, z^*) \qquad p = p(z, z^*) \\ H = H(z, z^*, t) \end{array}\right\} \qquad (2)$$

Hamilton equations.

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q} \qquad (2')$$

From $(1'')$:

$$\begin{cases} \dot{q} = \sqrt{\frac{a}{2m\omega}}\ (\dot{z} + \dot{z}^*) \\ \dot{p} = -i\sqrt{\frac{am\omega}{2}}\ (\dot{z} - \dot{z}^*) \end{cases} \qquad (3)$$

By substituting (1) in $H(q, p, t)$, one obtains:

$$H\ (z(q,p),\ z^*(q,p),\ t) \qquad (4)$$

Thus:
$$\begin{cases} \dfrac{\partial H}{\partial q} = \dfrac{\partial H}{\partial z}\dfrac{\partial z}{\partial q} + \dfrac{\partial H}{\partial z^*}\dfrac{\partial z^*}{\partial q} \\ \dfrac{\partial H}{\partial p} = \dfrac{\partial H}{\partial z}\dfrac{\partial z}{\partial p} + \dfrac{\partial H}{\partial z^*}\dfrac{\partial z^*}{\partial p} \end{cases} \qquad (5)$$

From (1):
$$\begin{cases} \dfrac{\partial z}{\partial q} = \sqrt{\dfrac{m\omega}{2\hbar}} \;;\quad \dfrac{\partial z^*}{\partial q} = \sqrt{\dfrac{m\omega}{2\hbar}} \\ \dfrac{\partial z}{\partial p} = i\sqrt{\dfrac{1}{2\hbar m\omega}} \;;\quad \dfrac{\partial z^*}{\partial p} = -i\sqrt{\dfrac{1}{2\hbar m\omega}} \end{cases} \qquad (6)$$

By substituting (6) in (5):
$$\begin{cases} \dfrac{\partial H}{\partial q} = \dfrac{\partial H}{\partial z}\sqrt{\dfrac{m\omega}{2\hbar}} + \dfrac{\partial H}{\partial z^*}\sqrt{\dfrac{m\omega}{2\hbar}} = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\dfrac{\partial H}{\partial z} + \dfrac{\partial H}{\partial z^*}\right) \\ \dfrac{\partial H}{\partial p} = \dfrac{\partial H}{\partial z}\, i\sqrt{\dfrac{1}{2\hbar m\omega}} - \dfrac{\partial H}{\partial z^*}\, i\sqrt{\dfrac{1}{2\hbar m\omega}} = i\sqrt{\dfrac{1}{2\hbar m\omega}}\left(\dfrac{\partial H}{\partial z} - \dfrac{\partial H}{\partial z^*}\right) \end{cases} \qquad (7)$$

By substituting (3) and (7) in (2'):
$$\begin{cases} \sqrt{\dfrac{\hbar}{2m\omega}}\left(\dot{z} + \dot{z}^*\right) = i\sqrt{\dfrac{1}{2\hbar m\omega}}\left(\dfrac{\partial H}{\partial z} - \dfrac{\partial H}{\partial z^*}\right) \\ i\sqrt{\dfrac{\hbar m\omega}{2}}\left(\dot{z} - \dot{z}^*\right) = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\dfrac{\partial H}{\partial z} + \dfrac{\partial H}{\partial z^*}\right) \end{cases} \qquad \text{i.e.:}$$

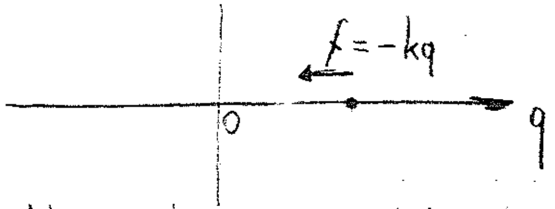
$$\begin{cases} \dot{z} + \dot{z}^* = \dfrac{i}{\hbar}\left(\dfrac{\partial H}{\partial z} - \dfrac{\partial H}{\partial z^*}\right) \\ \dot{z} - \dot{z}^* = -\dfrac{i}{\hbar}\left(\dfrac{\partial H}{\partial z} + \dfrac{\partial H}{\partial z^*}\right) \end{cases} \qquad (8)$$

By summing (8) one obtains: $2\dot{z} = -2\dfrac{i}{\hbar}\dfrac{\partial H}{\partial z^*}$, i.e.:

$$\boxed{\dot{z} = -\frac{i}{\hbar}\frac{\partial H}{\partial z^*}} \qquad (9)$$

PART 2. (HARMONIC OSCILLATOR)

Let us consider a one-dimensional harmonic oscillator of mass m, i.e. a particle of mass m with one degree of freedom, q, subjected to a force $f = -kq$ (i.e. to a potential $V(q)$ such that $-\frac{dV}{dq} = -kq$).



Hamiltonian $H(q,p)$:

$$H = T + V \ ; \quad T = \frac{1}{2} m \dot{q}^2 = \frac{p^2}{2m} \ ; \quad V = k\frac{q^2}{2}$$

$$H(q,p) = \frac{p^2}{2m} + k\frac{q^2}{2} \qquad (10)$$

By setting: $k = m\omega^2$, we have also:

$$H(q,p) = \frac{m\omega^2 q^2}{2} + \frac{p^2}{2m} \qquad (10')$$

where $\omega = \sqrt{\frac{k}{m}}$ has the dimensions of frequency

$$[\omega] = \left[\frac{F}{LM}\right]^{\frac{1}{2}} = \left[\frac{MLT^{-2}}{ML}\right]^{\frac{1}{2}} = [T^{-1}]$$

and turns out to be the frequency of the oscillator (see final solution).

By substituting (1'') into (10'), we obtain:

$$H = \frac{\cancel{m}\omega^2}{2}\frac{a}{2\cancel{m}\omega}(z+z^*)^2 - \frac{1}{2\cancel{m}}\frac{a\cancel{m}\omega}{2}(z-z^*)^2 =$$

$$= \frac{a\omega}{4}\left(z^2 + z^{*2} + 2zz^* - z^2 - z^{*2} + 2zz^*\right) =$$

$$= \frac{a\omega}{4} 4zz^* = a\omega zz^* \qquad (11)$$

Equation of motion:

$$\dot{z} = -\frac{i}{a}\frac{\partial H}{\partial z^*}$$, i.e., from (11):

$$\dot{z} = -i\omega z \qquad (12)$$

Equation (12) can be immediately integrated:

$$\frac{d}{dt}(\ln z) = -i\omega \longrightarrow \ln z = -i\omega t + c' \rightarrow$$

$$\rightarrow \quad \underline{z = c\, e^{-i\omega t}} \qquad (13)$$

Initial condition: $z(0) = c$, and therefore:

$$\boxed{z = z(0)\, e^{-i\omega t}} \, . \qquad (14)$$

The equation of motion (14) shows that $\omega = \sqrt{\frac{k}{m}}$ is the frequency of the harmonic oscillator of mass m in a potential $V(q) = \frac{kq^2}{2}$. In fact, the state vector z is a rotating vector with angular frequency ω.

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Theory of Nature

What is its objective?
It tries to regularize experience. We conceive of humans as spectators of the universe, immersed in the universe.

But what type of experience?
The given. The given is internal, not external to experience. The immediately given. The way nature presents itself to us. But avoid methaphysical aspects. Is God behind it. Has the observer any role in influencing the experience. No. Experience is what is received as a datum. Observe a tree outside. I receive the image of it. That is my datum. Unfortunately much confusion arises on this quite phylosophical point. Is there someone to give us the datum. The same word *data* implies it. What we really should say is instead *habita*, the "had" rather than the given.

Nature vs nature.
Nature : immediate experience from which transition always is made to orderly, conceptual knowledge
nature : immediate experience, including that from which transition cannot be made in a way acceptable to all. (feeling of sorrow, esthetics)

Reification : the act of postulating a thing

seen tree ⟶ physical object, tree

it involves synthesis of experience

integration of the habitum with memory of similar experiences and remembered perceptions

supplementation with the property of permanence

(which could never be abstracted from the data, finite points → line)

Thing vs external object

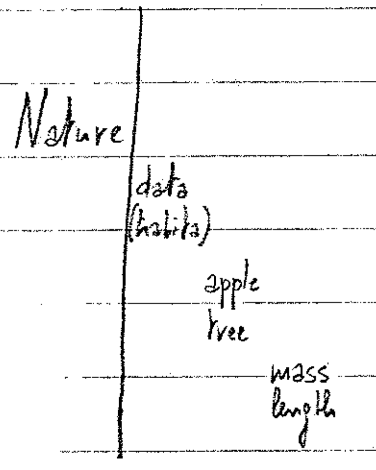
Like a mirage (an inverted palm tree seen at the horizon) vs an apple (Newton)

Thing is closer to Nature than the external object

The objectivity emerges as an additional success in the act of transition from the given to the constructed concept of object

Several times this distinction is not reflected in the language

Take the concept of mass, Newton's apple has mass. Mass is an idea, property of the object, which is adopted using intuitive and somewh abstract means. Yet, if someone throws at you an apple, you say you can "feel" its mass. That feeling is more a thing than an object. It is more close to the plane of Nature than is the concept of mass.



Departure from the immediate: constructs.

Rules of correspondence

immediate ⟶ constructs ⟶ other constr
(the empirical world) (the conceptual realm)

They are not unique. They evolve. "Brown" → wavelength has not always been a rule

There are several types of rules of correspondence. Reification is the simplest. The transition from the unanalyzed visual image of a "tree" to the external object, tree. The less direct transitions, color → wavelength.

The rules of correspondence are not eternally grounded in the nature of things, nor are they immediately suggested by immediate experience They are important parts of every theory of nature and receive their validity from the consistency, the internal neatness and success of the entire explanatory scheme.

Constructs are not wholly determined by perception. In this process there are some methaphysical ~~d~~ aspects such as those of intuition, logic, logical fertility as a requirement of a construct.

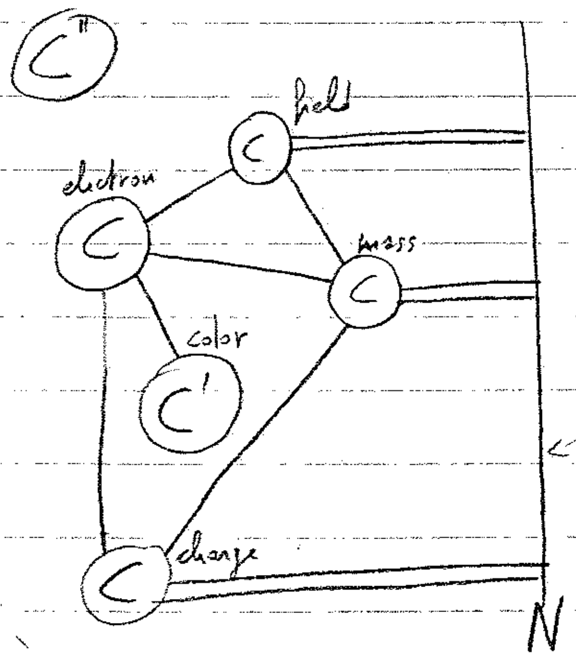
~~Logical~~ Connections between constructs.

Formal connections : a pure logical relation among constructs
(geometrical relations following from the axioms, every connection
between entities that is derivable from postulates

postulate: Newton's law , connection: mass, force, acceleration
Maxwell's equation point charge and its electromag. fiel
Einstein's law of G.R. curvature of space and quantity of matt

These are stable only so long as the postulates are maintained.
They are in a sense hyp-thetical judgements.

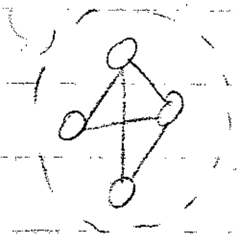
Epistemic connections: those that establish the links between Nature (the immediate given) and the most close constructs.



C' — "color of the electron"
no harm but no way to
connect it to N

C'' — no connections.
irrelevant to a theory
God, has no place in
sci

Nature, the plane of the immediate given



island "universe", born as abstract and then one searches for connections that
[illegible] make them relevant.

The very meaning of "reality" changes as the theory of N. changes, because we change the "lens" through which we interpret the empirical world.

The rules of correspondence give structure to a theory.

There are a number of concepts that ~~we~~ are commonly conceived as having epistemic connections with the immediate and are therefore used as "primitive" objects of the theory of nature. These, rather than individual concepts (apple, tree, ..) are cathegories of such concepts and are common to all the theories that we call physical.

N

- system
- physical observable
- preparation
- homogeneous preparation
- state
- value of an observable
- act of measurement of an observable

The theories differ then by the formal connections between these constructs. Those will be in terms of the mathematical language. Another ~~type~~ class of rules of correspondence will be introduced to form what Kuhn calls the paradigm of a ~~the~~ physical theory

Postulate : concept → mathematical representative

Paradigm : (The set of postulates)

Scientific Revolution : an historical change from an accepted paradigm to a different

System — apple, electron, table, ..., ..., the field in a cavity, a particle a box

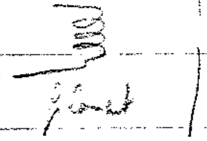
Physical Observable — position, momentum, mass, velocity, ...

the concepts, not the values!

Preparation : a ~~rule~~ reproducible scheme to "accept" systems for study

Telescope aimed at one direction is a rule to accept light for study

The word conveys the idea that a preparation ~~is~~ must be an action on the system. Not so. It does not even require an interaction ~~with~~ with the system. It is just a scheme ~~to select~~ (reproducible) to select systems, possibly for further measure

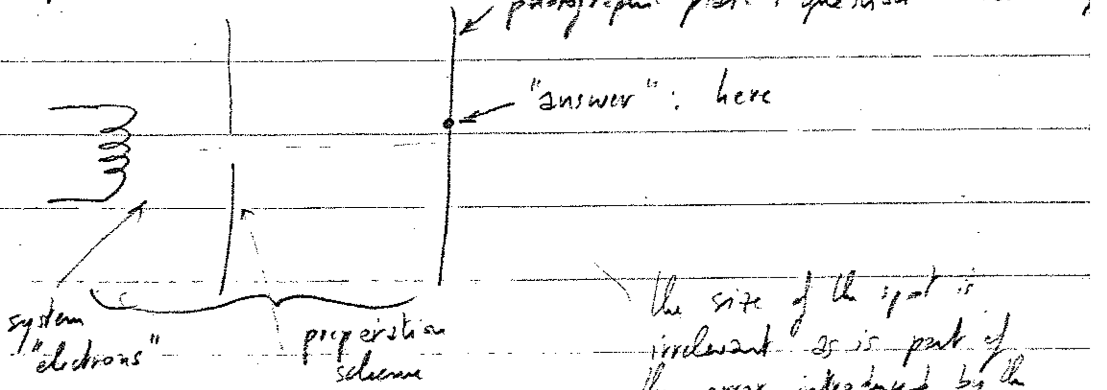


Act of Measurement of an Observable : a reproducible scheme ~~to~~ of operations performed on a system for the purpose of obtaining a numerical value which can, by virtue of the chosen experimental arrangement be assigned to some definite observable.

A "question" posed to the system. to which it "answers" in a definite way.

The "answer" is the numerical value and it is an "exact" value. ~~to other~~ The errors or imprecisions that are due ~~to~~ to the experimental apparatus are not part of the theory. This is another example of those ~~vague~~ epistemic connections, in which the it that "belong" to the system.

So I measure position



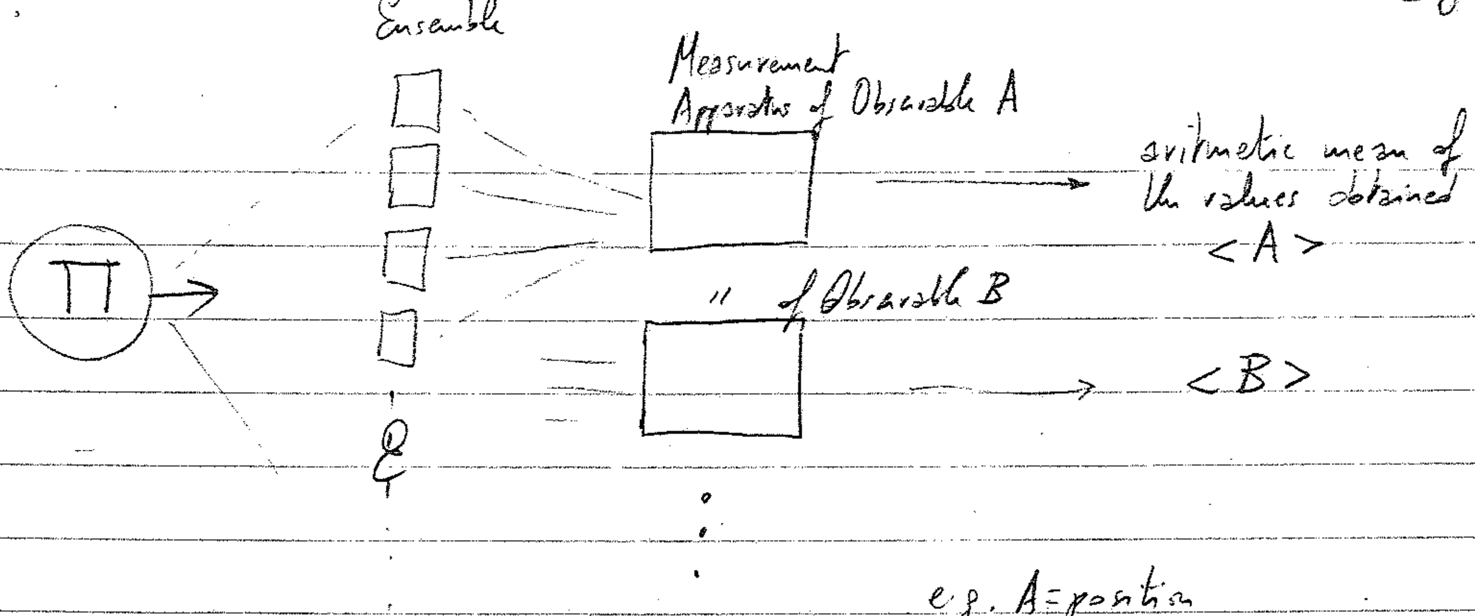
The size of the spot is irrelevant as is part of the error introduced by the photographic plate. With a better plate that would be reduced.

The theory of nature is not concerned with that kind of problems.
~~Heisenberg~~

It is only, Upon repeating a same ~~same~~ measurement ~~an experiment~~ on systems identically prepared that we reach conclusions and decide to regularize the results by building a theory.
Thus, important is the next ~~concept~~ rule of correspondence

$$\text{preparation } \Pi \longrightarrow \underline{\text{ensemble}}^{\mathcal{E}} \text{ of identical systems all prepared by } \Pi$$

How do you characterize a preparation?
By performing measurements of <u>all ~~the~~ conceivable observables</u> of the system



e.g. A = position

B = dispersion in position

C = third moment of the position distribution

D = momentum

⋮

The set of values

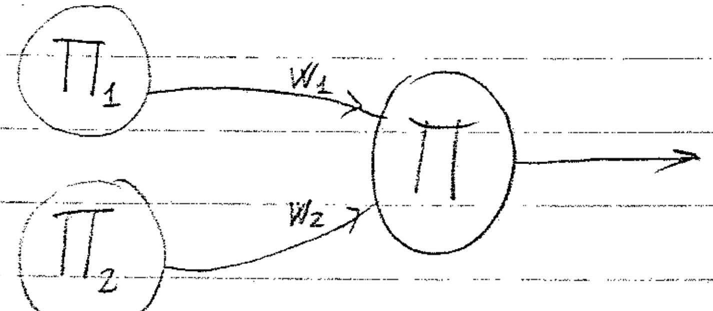
$$\{\langle A\rangle, \langle B\rangle, \ldots\}$$

for all ~~conceivable~~ observables of the system is the complete characterisation of its preparation Π.

Equality $\Pi_1 = \Pi_2$, $\mathcal{E}_1 = \mathcal{E}_2$

Statistical composition of preparations of a system

~~This has to do with the nature of the scheme Π.~~



$0 < w_1, w_2 < 1$

$$\Pi = w_1 \Pi_1 + w_2 \Pi_2$$

we denote this in symbols (bgc only)

Correspondingly, statistical mixing of ensembles

$$\mathcal{E} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$$

Homogeneous Preparation

One that cannot be conceived of as a statistical composition of two different preparations.

If Π^0 is homogeneous and we found two preparations Π_1 and Π_2 such that

$$\Pi^0 = w_1 \Pi_1 + w_2 \Pi_2 \qquad w_1, w_2 \neq 0$$

then $\Pi_1 = \Pi_2 = \Pi^0$.

Conversely, if we have to different preparations $\Pi_1 \neq \Pi_2$ and a given preparation Π is such that

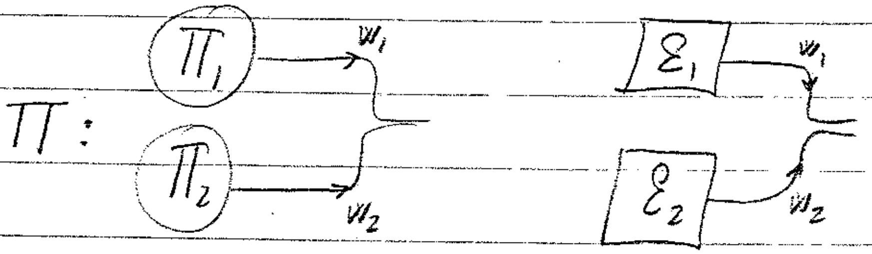
$$\Pi = w_1 \Pi_1 + w_2 \Pi_2 \qquad w_1, w_2 \neq 0$$

then Π is not homogeneous, but heterogeneous.

Statistical composition of ensembles

Follows from the rule $\Pi \rightarrow \mathcal{E}$

$$\Pi_1 \rightarrow \mathcal{E}_1$$
$$\Pi_2 \rightarrow \mathcal{E}_2$$



$$\langle A \rangle = w_1 \langle A \rangle_1 + w_2 \langle A \rangle_2$$

Because the arithmetic mean becomes a weighted sum of means.

Homogeneous ensemble

Follows from above

One that cannot be conceived as a statistical mixture of different ensembles.

It cannot be subdivided into different subensembles. [illegible]

Again an epistemic rule of correspondence

homogeneous ensemble ⟶ (almost) every member is in the same individual state

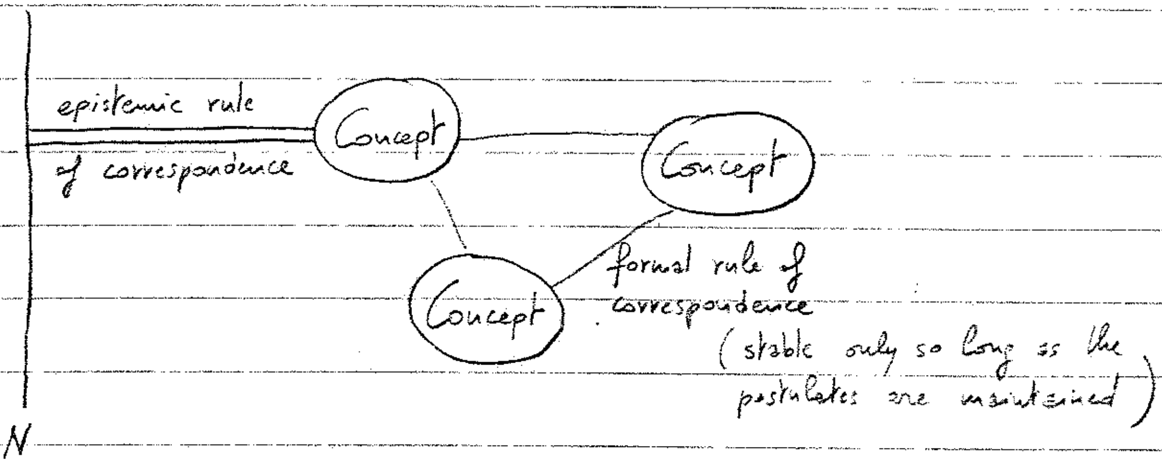
If there were (more than a finite number of) members in different states this would violate definition, we could group them into different subensembles.

Thus, we have

$$\begin{tikzcd}
\text{homogeneous preparation} \arrow[dr] \arrow[dd, dashed] & \\
& \text{homogeneous ensemble} \arrow[dl] \\
\text{individual state} &
\end{tikzcd}$$

$$\begin{tikzcd}
\text{heterogeneous preparation} \arrow[dr] \arrow[dd, dashed] & \\
& \begin{matrix}\text{heterogeneous ensemble} \\ \text{each member is in a state}\end{matrix} \arrow[dl] \\
\text{statistical mixture of different individual states} &
\end{tikzcd}$$

Theory of Nature



Kuhn: "paradigm" of the theory: the set of postulates giving structure to it

scientific "revolution": historical change from one paradigm to a different one

Theories of Nature that we will study:

Classical Mechanics	Classical Statistical Mechanics
Quantum Mechanics	(Quantum Statistical Mechanics)
Quantum Thermodynamics	(Quantum Statistical Thermodynamics)

↑

these are all "non-statistical" theories

To set a common ground on which to compare and grasp the differences between these theories,

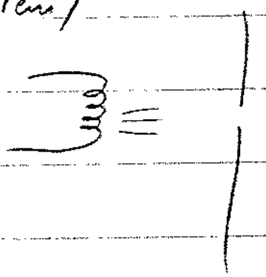
we first identify a set of "primitive" concepts that are common to the theories (common as concepts, but linked among themselves differently)

1. System : apple, table, building, electron, electromagnetic field, particle in a box, field in a cavity, crystal, ...

2. Physical Observable : position, momentum, angular momentum, mass, velocity, acceleration

the concepts, not the values

3. Preparation : a reproducible scheme to "accept" a system for study (does not necessarily require an interaction of the "preparer" with the system)

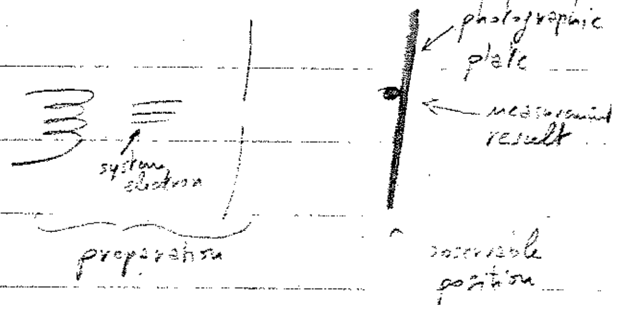


4. Measurement Act of an Observable:

reproducible scheme of operations on a system for the purpose of obtaining a precise numerical value which, by virtue of the chosen experimental arrangement, can be assigned to a definite observable of the system in the conditions prior to measurement.

(requires necessarily an interaction between system and measurement apparatus) (note how demanding restrictive these conditions are

it can even be destructive



"question" - "answer"

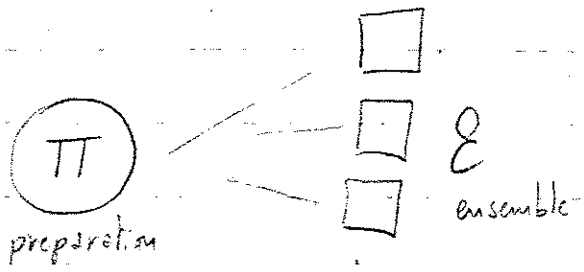
errors in the reading are irrelevant

Note the importance of repeated measurement acts of the same observable on systems prepared identically.

The repeatability of the measurement results, their pattern, are the data that the theory has to regularize.

Thus, a useful concept is that of:

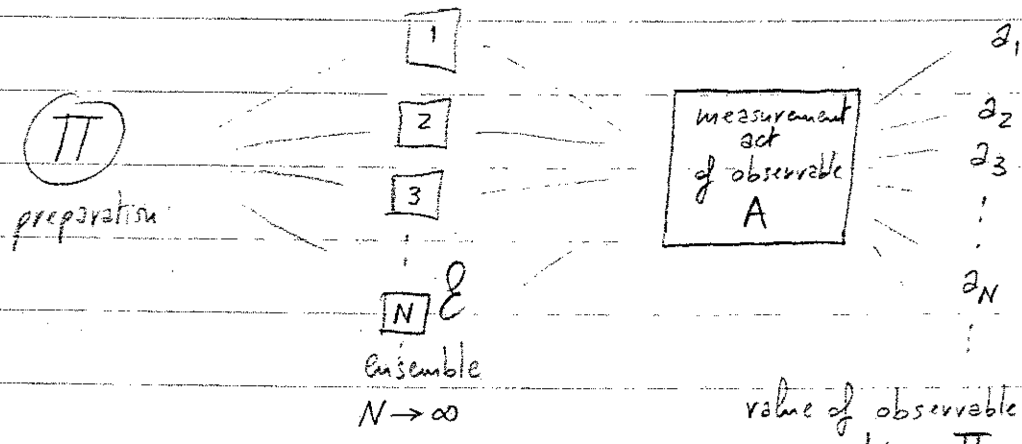
5. Ensemble of identical systems identically prepared:



each member prepared according to scheme Π

6. (Measured) Value of an Observable for a given Preparation:

arithmetic mean of measurement results of identical measurement acts on an ensemble of identical systems identically prepared



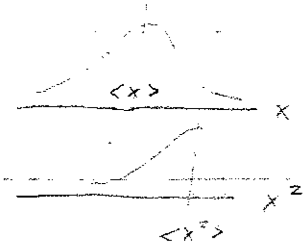
value of observable A for preparation Π is

$$\langle A \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} a_i$$

Examples: position

square of position

velocity



7. Complete Characterization of a Preparation:

the set of <u>values</u> $\{\langle A \rangle, \langle B \rangle, \ldots\}$ of <u>all conceivable</u> observables

8. Identical Preparations (Identical Ensembles):

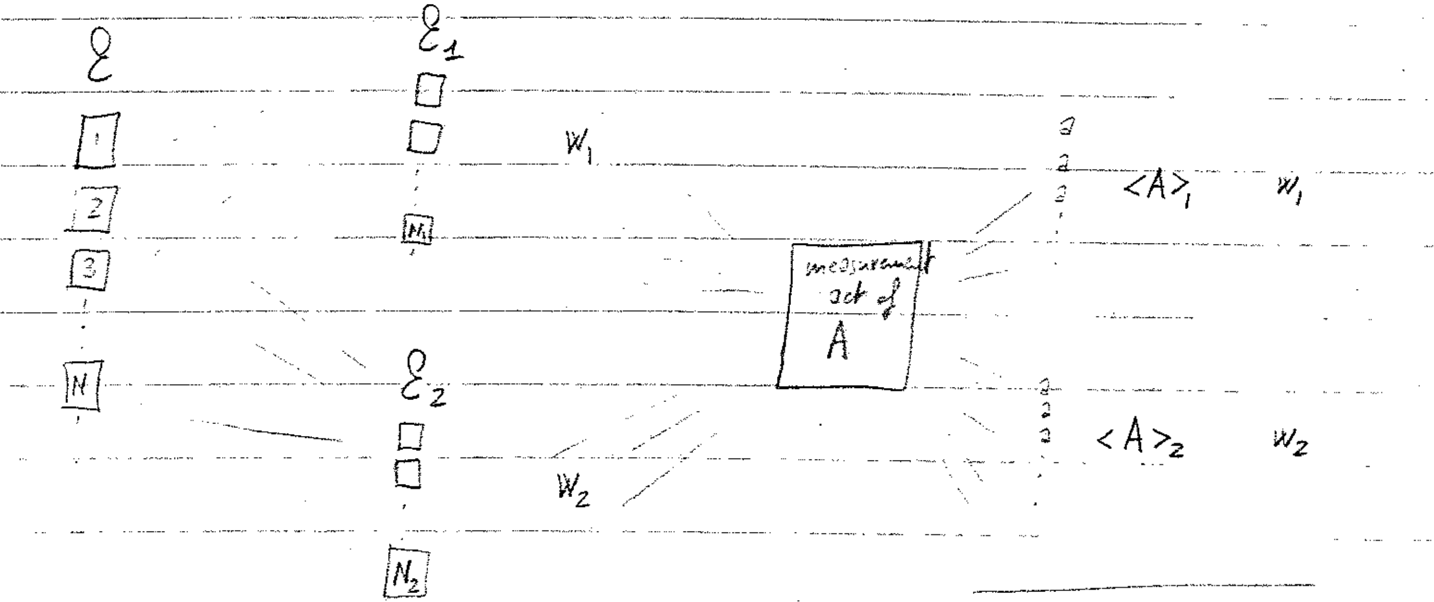
$\Pi_1 = \Pi_2$ if and only if $\langle A \rangle_1 = \langle A \rangle_2$, $\langle B \rangle_1 = \langle B \rangle$

... for all conceivable observables

$\Pi = \Pi \quad - \quad \varrho = \varrho$

Note: because in an ensemble $N \to \infty$, any finite subset of members does not affect the value of any observable because its contribution is washed away by the limit

We will next be concerned about possible subdivisions of an ensemble into subensembles.

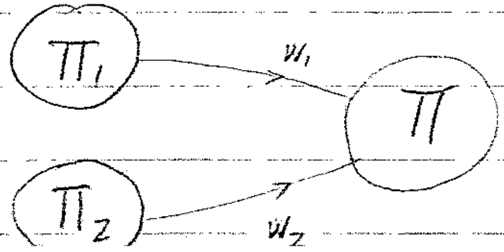


$$<A> = w_1 <A>_1 + w_2 <A>_2$$

$$\mathcal{E} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$$ a "mixture" of ensembles

Therefore, preparation $\Pi (\to \mathcal{E})$ can be conceived as a

9. Statistical Composition of Preparations (Mixture of Ensembles)



$$\Pi = w_1 \Pi_1 + w_2 \Pi_2$$

$$\mathcal{E} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$$

10. Homogeneous Ensemble (Homogeneous Preparation):

One that cannot be conceived as a mixture of *different* *subensembles*.

Any conceivable way of subdividing an $\mathcal{E}^{\circ}$ into two subensembles

$$\mathcal{E}^{\circ} = w_1 \mathcal{E}_1 + w_2 \mathcal{E}_2$$

implies that

$$\mathcal{E}_1 = \mathcal{E}_2 = \mathcal{E}^{\circ}$$

i.e.,

$$\langle A \rangle_1 = \langle A \rangle_2 = \langle A \rangle_0$$
$$\langle B \rangle_1 = \langle B \rangle_2 = \langle B \rangle_0$$
$$\vdots \qquad \text{for all observables}$$

Otherwise heterogeneous

Why is the Homogeneous Ensemble (Homogeneous Preparation) so important?

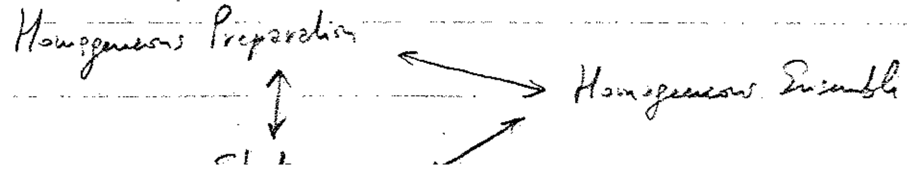
Every member of a homogeneous ensemble is individually in exactly the same condition as all the other members.

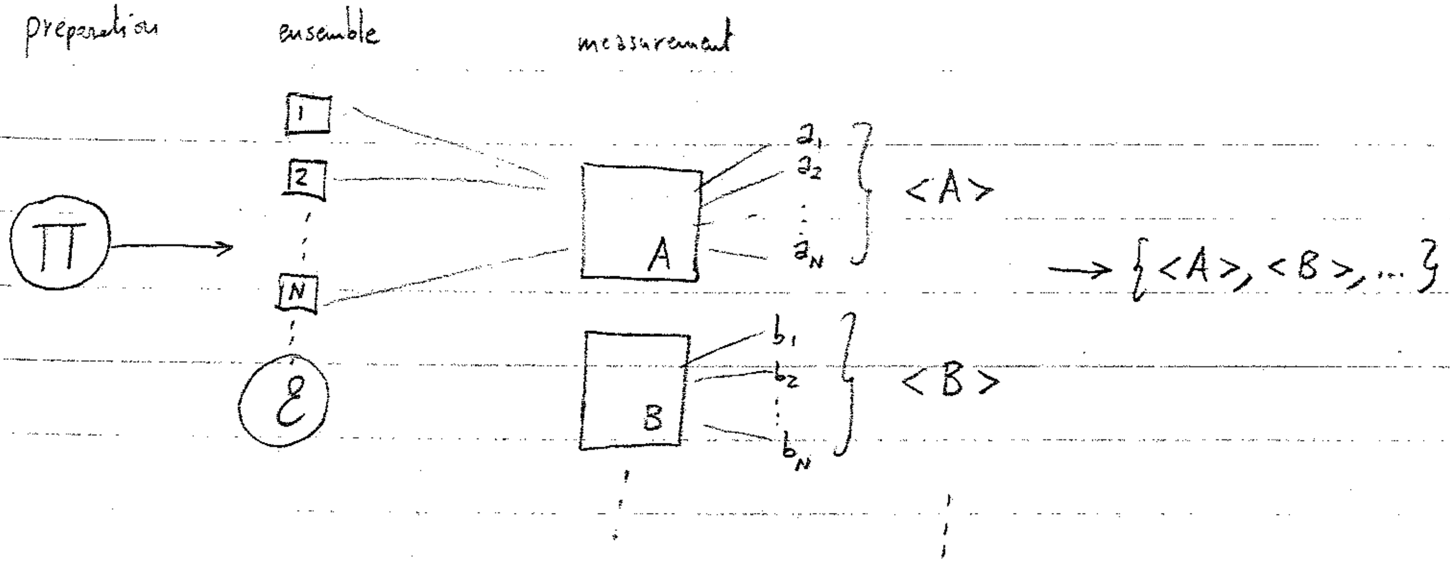
If there were members in different states, then a subdivision into different subensembles would be possible, thus contradicting the definition.

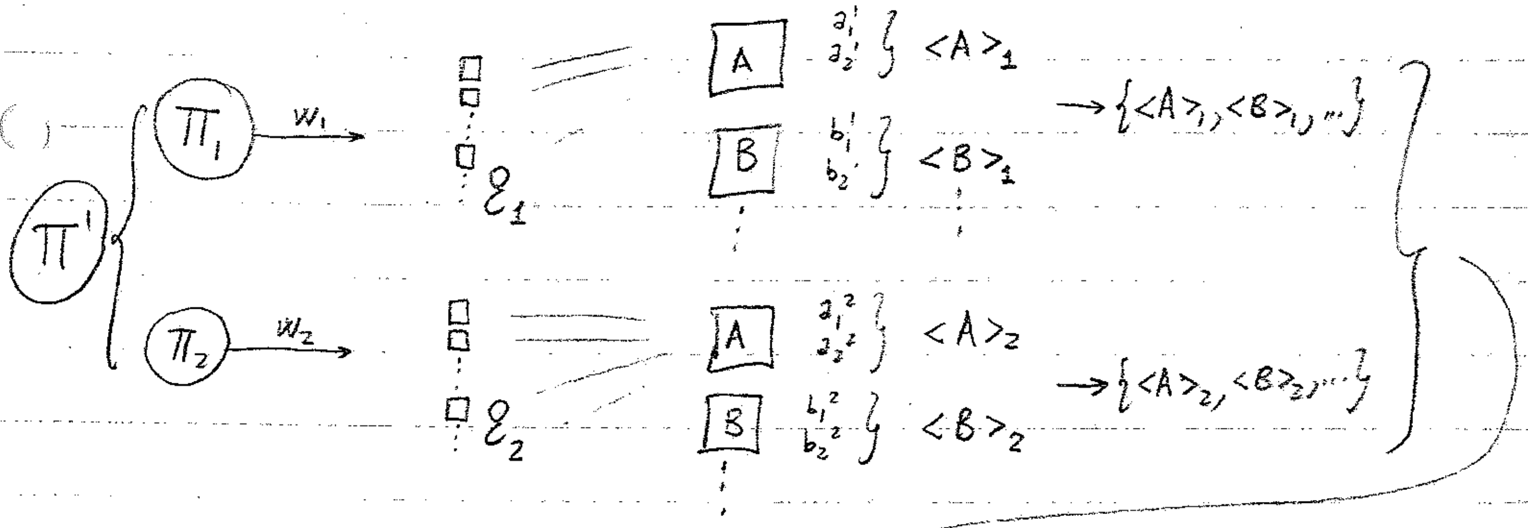
11. (Individual) State of a System

The condition under which it is after a homogeneous preparation.

The condition of each individual member of a homogeneous ensemble







$$\begin{cases} \langle A\rangle' = w_1\langle A\rangle_1 + w_2\langle A\rangle_2 \\ \langle B\rangle' = w_1\langle B\rangle_1 + w_2\langle B\rangle_2 \\ \vdots \end{cases}$$

$$\rightarrow \{\langle A\rangle', \langle B\rangle', \dots\}$$

$$\Pi' = \Pi \quad \text{iff} \quad \langle A\rangle' = \langle A\rangle,\ \langle B\rangle' = \langle B\rangle,\ \dots$$

The value of an observable is a function of the preparation, "linear" in the statistical weights of its component preparation.

$$a(\Pi) = \langle A \rangle_{\Pi}$$

value of observable "A" for preparation Π

arithmetic mean of A-measurement results on an ensemble generated by Π

If $\quad \Pi = w_1 * \Pi_1 \,(+)\, w_2 * \Pi_2$

$$a(\Pi) = \langle A \rangle_{\Pi} = w_1 \langle A \rangle_{\Pi_1} + w_2 \langle A \rangle_{\Pi_2} = w_1\, a(\Pi_1) + w_2\, a(\Pi_2)$$

thus

$$\boxed{a\left(w_1 * \Pi_1 \,(+)\, w_2 * \Pi_2\right) = w_1 \cdot a(\Pi_1) + w_2 \cdot a(\Pi_2) \quad \text{for all observables}}$$

Homogeneous Preparations

A preparation Π° is homogeneous if and only if whenever Π° can be conceived as a statistical composition of two preparations Π_1 and Π_2,

$$\Pi^{\circ} = w_1 * \Pi_1 \ (+) \ w_2 * \Pi_2 \qquad 0 < w_1, w_2 < 1$$

it follows that $\Pi_1 = \Pi_2 = \Pi^{\circ}$, i.e., $a(\Pi_1) = a(\Pi_2) = a(\Pi^{\circ})$ for all observables.

Homogeneous Ensemble : one generated by a homogeneous preparation.

Heterogeneous Preparations

A preparation Π' is heterogeneous if and only if it is possible to conceive it (at least in one way) as a statistical composition of two different preparations Π_1 and Π_2, i.e., there exist $\Pi_1 \neq \Pi_2$ such that

$$\Pi' = w_1 * \Pi_1 \ (+) \ w_2 * \Pi_2 \qquad 0 < w_1, w_2 < 1$$

and, therefore, $a(\Pi') = w_1\, a(\Pi_1) + w_2\, a(\Pi_2)$ for all observables.

Every possible subdivision of a homogeneous ensemble yields subensembles that are identical, i.e., that share the values of all properties.

Individual State of a System

The common individual condition shared by all the members of the homogeneous ensemble to which the system belongs.

Park: "The usefulness of the state concept lies in its reference to individual systems and its participation to the general scheme of causality (initial state of a system implies a final state via physical laws)".

Every member of a homogeneous ensemble is in exactly the same individual state as all the others.

A homogeneous preparation generates systems all in the same individual state.

Resolution of a Heterogeneous Preparation into its Homogeneous Components

Given any Π, how many ways should there be to resolve it into a statistical composition of <u>homogeneous</u> preps.?

Let us assume there are <u>two different ways</u>:

$$\Pi = \underset{\substack{\downarrow \\ \text{state 1}}}{w_1 * \Pi_1^\circ} \; (+) \; \underset{\substack{\downarrow \\ \text{state 2}}}{w_2 * \Pi_2^\circ} = \underset{\substack{\downarrow \\ \text{state 3}}}{w_3 * \Pi_3^\circ} \; (+) \; \underset{\substack{\downarrow \\ \text{state 4}}}{w_4 * \Pi_4^\circ}$$

This implies that the ensemble $\mathcal{E}$ generated by Π has

w_1 members in state 1
w_2 members in state 2
$w_1 + w_2 = 1$

but also

w_3 members in state 3
w_4 members in state 4
$w_3 + w_4 = 1$

Thus

$w_1 w_3$ members are <u>both</u> in state 1 and 3
$w_1 w_4$ — " — 1 - 4
$w_2 w_3$ — " — 2 3
$w_2 w_4$ — " — 2 - 4

$w_1 w_3 + w_1 w_4 + w_2 w_3 + w_2 w_4 = 1$

Can we accept that a single system be simultaneously in two different states?

We conclude that, for the concept of state of an individual system to be correctly included in the theory of nature, every preparation scheme Π must admit one and only one resolution into homogeneous preparations.

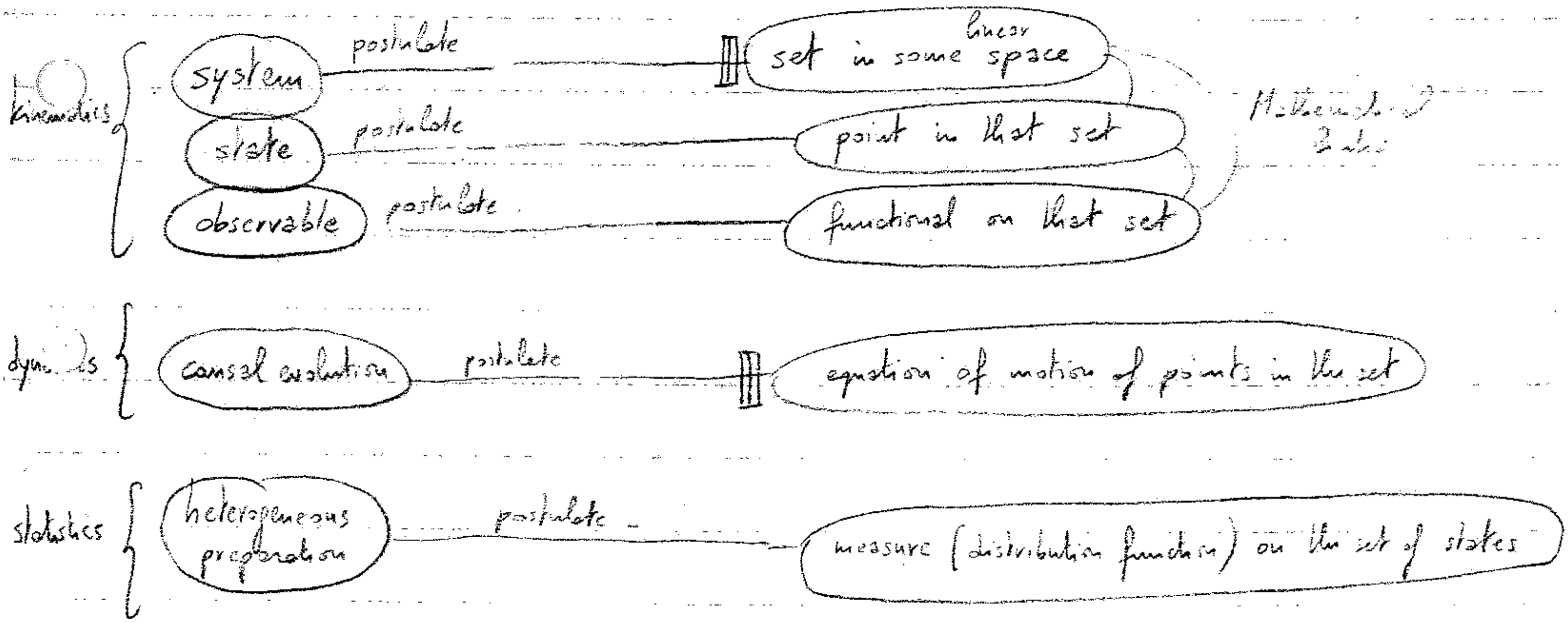
Aspects of a theory of nature.

Kinematics : description of states (homogeneous preparations)

Dynamics : description of the time (causal) evolution of states

Statistics : description of heterogeneous preparations

Mathematical description



Glossary:

$\forall$	for every; for any; for each
$\in$	in; an element of; belonging to
$\exists$	there exists; there is
$\mathcal{U}$	a unique
$\vert$	such that; where

Scalar Field

a set F of objects, called "scalars" and denoted by a, b, ..., which when subjected to the four arithmetic operations again give elements of the set F. More exactly, they satisfy the following (field) axioms:

sum $\forall\, a, b \in F \ \ \exists \mathcal{U}$ scalar $a+b \in F$ called the sum of a and b

$$\forall a,b,c \begin{cases} a+b = b+a & \text{commutative} \\ (a+b)+c = a+(b+c) & \text{associative} \end{cases}$$

$$\exists 0 \,|\quad 0+a = a \qquad \text{existence of zero}$$

$$\forall a \ \exists (-a) \quad a+(-a) = 0 \qquad \text{existence of negative}$$

product $\forall$ pair $a, b \in F \ \ \exists \mathcal{U}$ scalar $ab \in F$ called the product of a and b,

$$\forall a,b,c \begin{cases} ab = ba & \text{commutative} \\ (ab)c = a(bc) & \text{associative} \end{cases}$$

$$\exists 1 \,|\quad 1a = a \qquad \text{existence of unity}$$

$$\forall a \neq 0 \ \exists a^{-1} \quad aa^{-1} = 1 \qquad \text{existence of reciprocal}$$

$$\forall a,b,c \quad a(b+c) = ab + ac \qquad \text{distributive}$$

Examples: $\mathbb{Q}$ (rational numbers), $\mathbb{R}$ (real numbers), $\mathbb{C}$ (complex numbers)

Vector Space V over a field F

a set V of objects, called "vectors" and denoted by $\alpha, \beta, \dots$, which when subjected to addition and multiplication by a scalar again give elements of the set V. More exactly, they satisfy the following (space) axioms:

addition $\forall \alpha, \beta \in V \ \exists \mathcal{U}$ vector $\alpha + \beta \in V$ called the sum of α and β /

$$\forall \alpha, \beta, \gamma \begin{cases} \alpha + \beta = \beta + \alpha & \text{commutative} \\ (\alpha + \beta) + \gamma = \alpha + (\beta + \gamma) & \text{associative} \end{cases}$$

$\exists 0 \in V / \quad \alpha + 0 = \alpha$ existence of zero vector

$\forall \alpha \ \exists (-\alpha) / \quad \alpha + (-\alpha) = 0$ existence of negative vector

multiplication by a scalar $\forall \alpha \in V$ and $a \in F \ \exists \mathcal{U}$ vector $a\alpha \in V$ /

$$\forall \alpha \quad 1\alpha = \alpha$$

$$\begin{matrix} \forall \alpha, \beta \in V \\ \forall a, b \in F \end{matrix} \begin{cases} a(b\alpha) = (ab)\alpha \\ (a+b)\alpha = a\alpha + b\alpha \\ a(\alpha + \beta) = a\alpha + a\beta \end{cases}$$

implications:

$\mathcal{U} \ 0 \in V$ uniqueness of zero vector

$\mathcal{U} \ (-\alpha) \in V, \ (-\alpha) = (-1)\alpha$ uniqueness of negative vector

$\forall \alpha \quad 0_F \alpha = 0_V$

Examples :

$\mathbb{R}^3$ the space of three-dimensional analytic geometry (each vector characterized by a length and a direction, usual parallelogram rule for addition, multiplication by a scalar length $= |a|$ length, direction $= \frac{a}{|a|}$ direction)
Verify that the rules are satisfied.

$\mathbb{R}^N$ generalization to N dimensions

$L^2(a,b)$ square integrable continuous complex functions of one variable t $\alpha(t), \beta(t), \dots$ on an interval $a \leq t \leq b$. $\int_a^b |\alpha(t)|^2 dt < +\infty$

$M_N(\mathbb{C})$ $N \times N$ matrices of complex numbers

Basis for a Vector space

a subset $\{\xi_n\}$ of vectors in V which:

1) span V, i.e., $\forall \alpha \in V \ \exists \{a_n\} \in F \mid \alpha = \sum_n a_n \xi_n$

2) are linearly independent, i.e., $\sum_n b_n \xi_n = 0$ iff $b_n = 0 \ \forall n$

Coordinates of a vector α with respect to a basis $\{\xi_n\}$: $\alpha = \sum_n a_n \xi_n$

Dimensionality of V = number of vectors in a basis (equal for all bases)

Examples:

in $\mathbb{R}^3$ a set of three vectors with different directions

in $L^2(a,b)$ the set of functions $\xi_n(t) = e^{in\frac{2\pi}{b-a}t}$ for $n = -\infty, .., -1, 0, 1$

in fact

$$\alpha(t) = \sum_{n=-\infty}^{\infty} a_n \xi_n(t)$$

Metric Space

A space V equipped with a metric d (or distance), i.e. a real function $d(\alpha,\beta)$ | $\forall \alpha,\beta,\gamma \in V$

$$d(\alpha,\beta) \geq 0$$
$$d(\alpha,\beta) = 0 \quad \text{iff} \quad \alpha=\beta$$
$$d(\alpha,\beta) = d(\beta,\alpha)$$
$$d(\alpha,\beta) \leq d(\alpha,\gamma) + d(\gamma,\beta) \qquad \text{triangular relation}$$

examples:

$\mathbb{R}^3$ with $d(\alpha,\beta) = (a_1-b_1)^2 + (a_2-b_2)^2 + (a_3-b_3)^2$

$L^2(a,b)$ with $d(\alpha,\beta) = \sum_{n=-\infty}^{\infty} (a_n - b_n)^2$

Complete Metric Space

A metric space V such that every Cauchy sequence is convergent.

Cauchy sequence : (α_k) iff $\forall \varepsilon > 0 \ \exists K \mid \forall n, m \geq K, \ d(\alpha_n, \alpha_m) <$

Normed Space

A space V equipped with a norm $\|\cdot\|$, $\forall \alpha, \beta \in V$, $\forall a \in F$

$$\|\alpha\| \geq 0$$
$$\|\alpha\| = 0 \text{ iff } \alpha = 0$$
$$\|\alpha + \beta\| \leq \|\alpha\| + \|\beta\|$$
$$\|a\alpha\| = |a| \|\alpha\|$$

Examples:

$\mathbb{R}^3$ with $\|\alpha\| = \sqrt{|a_1|^2 + |a_2|^2 + |a_3|^2}$

$L^2(a,b)$ with $\|\alpha\|_1 = \int_a^b |\alpha(t)| dt$

or $\|\alpha\|_2 = \sqrt{\int_a^b |\alpha(t)|^2 dt}$

or $\|\alpha\| = \sqrt{\sum_{n=-\infty}^{\infty} |a_n|^2}$

Note that a normed space can always be made metric by defining

$$d(\alpha, \beta) = \|\alpha - \beta\|$$

Banach Space

A complete normed vector space

Scalar (or Inner) Product Space

A vector space V equipped with an inner product $< \cdot , \cdot >$,
$\forall\ \alpha, \beta, \gamma \in V$ and $a \in F$

$$<\alpha,\alpha> \geqslant 0$$
$$<\alpha,\alpha> = 0 \quad \text{iff} \quad \alpha = 0$$
$$<\alpha,\beta+\gamma> = <\alpha,\beta> + <\alpha,\gamma>$$
$$<\alpha,\beta> = <\beta,\alpha>^*$$
$$<\alpha, a\beta> = a<\alpha,\beta>$$

Natural norm: $\|\alpha\| = \sqrt{<\alpha,\alpha>}$

Hilbert Space

A complete inner product space.

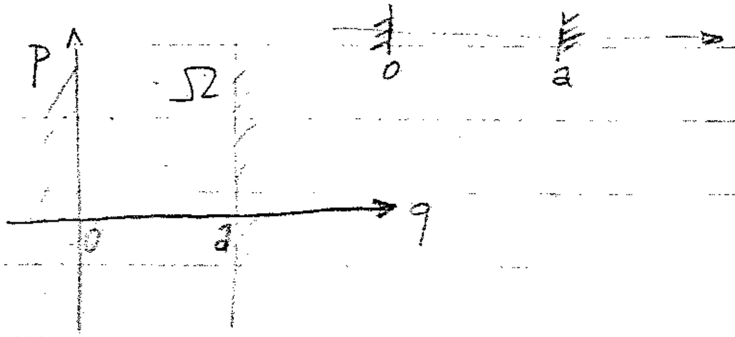
Classical Mechanics

kinematics

system — region in phase-space (usually with canonical coordinates q and p, position and momentum of each degree of freedom)

e.g. particle in a one-dimensional box

phase space



state — point in phase-space (q,p) is a state

observable — function defined on phase-space, for example, the energy: hamiltonian function $h(q,p)$, position q, momentum p

e.g. $$h(q,p) = \frac{p^2}{2m} + V(q)$$

where $$V(q) = \begin{cases} 0 & 0 \leq q \leq a \\ \infty & q \leq 0,\ q \geq a \end{cases}$$

value of an observable — value of function at that point.

dynamics

causal evolution ——— Hamilton's equations of motion

$$\dot{q} = \frac{\partial h}{\partial p} \qquad \dot{p} = -\frac{\partial h}{\partial q}$$

In the example:

$$\dot{q} = \frac{\partial h}{\partial p} = p/m$$

$$\dot{p} = -\frac{\partial h}{\partial q} = -\frac{\partial V(q)}{\partial q} = \begin{cases} 0 & 0<q<a \\ -\infty & q=0,\ q=a \end{cases}$$

$$\dot{h} = \frac{\partial h}{\partial q}\dot{q} + \frac{\partial h}{\partial p}\dot{p} = \frac{\partial h}{\partial q}\frac{\partial h}{\partial p} - \frac{\partial h}{\partial p}\frac{\partial h}{\partial q} = 0$$

If $q=q(t)$ and $p=p(t)$ are the solution of H. eq., then

$$h(t) = h(q(t), p(t)) = \text{const}$$

hence $\frac{p^2(t)}{2m} = \text{const}$

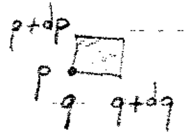
$$p(t) = \pm\sqrt{p^2(t)}$$

Harmonic oscillator: $h(q,p) = \frac{p^2}{2m} + \frac{1}{2}kq^2$

Classical Statistical Mechanics

heterogeneous preparation Π —— a distribution (more precisely, a measure) $f_\Pi(q,p)$ on phase-space, such that

$$f_\Pi(q,p)\,dq\,dp = \text{probability that the system results prepared in a state which lies in the region } \begin{matrix} q - q+dq \\ p - p+dp \end{matrix}$$



such that

$$\int_\Omega dq\,dp\, f_\pi(q,p) = 1$$

value of an observable, e.g., energy, weighted sum of contributions

$$h(\Pi) = \int_\Omega dq\,dp\; f_\Pi(q,p)\, h(q,p)$$

statistical composition of two preparations Π_1 and Π_2 with weights w_1 and w

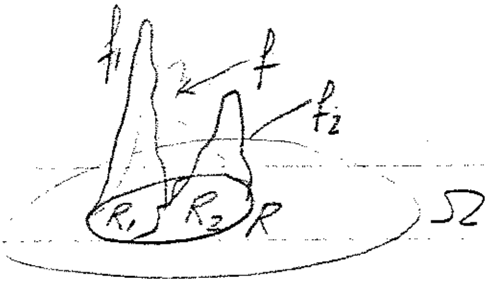
$$\Pi = w_1 * \Pi_1 \;(+)\; w_2 * \Pi_2$$

$$f_\Pi(q,p) = w_1\, f_{\Pi_1}(q,p) + w_2\, f_{\Pi_2}(q,p)$$

homogeneous preparations ?

define the support R of f as region where $f \neq 0$

any region, other than a point, can be subdivided into two $\overset{\text{disjoint}}{\vee}$ subregions $R = R_1 \cup R_2$



Thus, given an $f(q,p)$
and any subdivision $R = R_1 \cup R_2$
define

$$f_1(q,p) = \begin{cases} 0 & \text{if } q,p \text{ in } R_2 \\ \dfrac{f}{\int_{R_1} dq\,dp} & \text{if } q,p \text{ in } R_1 \end{cases}$$

$$f_2(q,p) = \begin{cases} \dfrac{f}{\int_{R_2} dq\,dp} & \text{if } q,p \text{ in } R_2 \\ 0 & \text{if } q,p \text{ in } R_1 \end{cases}$$

and

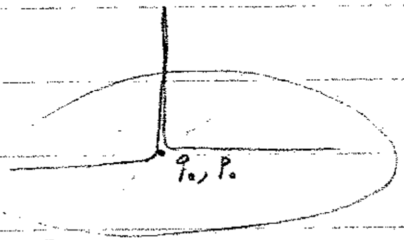
$$w_1 = \int_{R_1} dq\,dp \qquad w_2 = \int_{R_2} dq\,dp$$

clearly

$$f(q,p) = w_1 f_1(q,p) + w_2 f_2(q,p) \qquad w_1 + w_2 = 1$$

Thus, we can always think of f as a weighted sum of different f's, unless, the support R is a single point. But the only normalized distribution whose support is a single point is the Dirac distribution

$$\delta_0(q,p) = \delta(q-q_0)\,\delta(p-p_0)$$



These are the only irreducible propositions, and they are in one-to-one corresp. with the points in Ω

Moreover, every $f(q,p)$ can be uniquely decomposed as a "weighted sum" of Dirac distributions.

$$f(q,p) = \int dq_0\,dp_0\, f(q_0,p_0)\,\delta_0(q,p) \quad \times$$

Classical Mechanics

system $\longrightarrow$ phase-space Ω (canonical coordinates q, p; complex coordinate
state $\longrightarrow$ point q_0, p_0 in Ω (see homework)
observable $\longrightarrow$ function on Ω, $g(q,p)$
causality $\longrightarrow$ Hamilton equations
value of an observable $\longrightarrow$ value of function at state point q_0, p_0.
result of single measurement act $\longrightarrow$ value of function at point q_0, p_0

Classical Statistical Mechanics

preparation Π $\longrightarrow$ normalized distribution on Ω, $f_\Pi(q,p)$
value of observable $\longrightarrow$ $\langle g \rangle_\Pi = \int_\Omega g(q,p)\, f_\Pi(q,p)\, dq\, dp$ $\qquad$ $1 = \int_\Omega f_\Pi(q,p)\, dq\, dp$

$\uparrow$ normalization

statistical composition of preparations $\longrightarrow$ $f_\Pi = w_1 f_{\Pi_1} + w_2 f_{\Pi_2}$
$\Pi = w_1 * \Pi_1 + w_2 * \Pi_2$

Theorem.

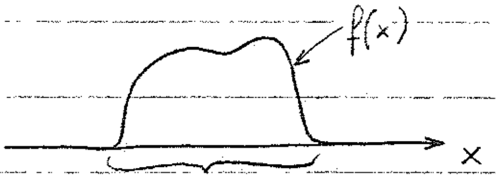
$$\langle g \rangle_\Pi = w_1 \langle g \rangle_{\Pi_1} + w_2 \langle g \rangle_{\Pi_2}$$

Question:

what distributions represent homogeneous preparations?

Π° homog. if $\Pi^\circ = w_1 * \Pi_1 + w_2 * \Pi_2 \longrightarrow \Pi_1 = \Pi_2 = \Pi^\circ$

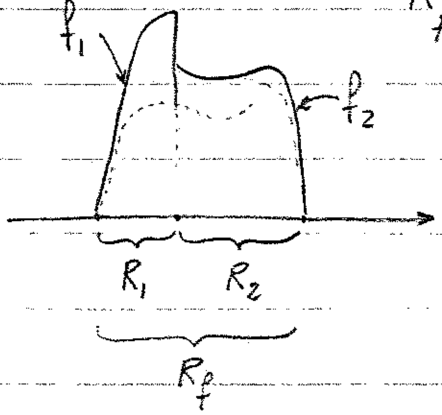
$$f_{\Pi^\circ} = w_1 f_{\Pi_1} + w_2 f_{\Pi_2} \longrightarrow f_{\Pi_1} = f_{\Pi_2} = f_{\Pi^\circ}$$



R_f = support of the function

we can almost always partition subdivide the support into two disjoint subsets ~~as~~

$$R_f = R_1 \cup R_2 \qquad R_1 \cap R_2 = \phi$$



and define functions f_1 and f_2 such that

$$f_1 = \begin{cases} 0 & \text{on } R_2 \\ \dfrac{f(x)}{\int_{R_1} f(x)\,dx} & \text{on } R_1 \end{cases}$$

$$f_2 = \begin{cases} \dfrac{f(x)}{\int_{R_2} f(x)\,dx} & \text{on } R_2 \\ 0 & \text{on } R_1 \end{cases}$$

both f_1 and f_2 qualify as functions representative of preparations and

$$f = w_1 f_1 + w_2 f_2$$

where
$$w_1 = \int_{R_1} f(x)\,dx \Big/ \int_{R_f} f(x)\,dx$$

$$w_2 = \int_{R_2} f(x)\,dx \Big/ \int_{R_f} f(x)\,dx$$

therefore any function whose support can be partitioned cannot represent a homogeneous preparation.

Only a point support cannot be partitioned.

The only normalized function with a point support is the Dirac delta "function"

$$\delta(x-x_0) = \begin{cases} 0 & \text{for} \quad x \neq x_0 \\ \infty & \text{for} \quad x = x_0 \end{cases}$$

$$\text{but such that} \quad \int \delta(x-x_0)\,dx = 1$$

$$\text{and} \quad \int g(x)\,\delta(x-x_0)\,dx = g(x_0)$$

$$\begin{tikzcd}
\text{Homogeneous preparations} \arrow[r] & \text{Dirac distributions on } \Omega \arrow[d, "\text{they are in one-to-one correspondence with points in } \Omega"] \\
\text{states} & \text{points in } \Omega \arrow[l]
\end{tikzcd}$$

This is a first consistency check of Classical Stat. M.

Question:

In how many ways can a preparation be decomposed into its homogeneous components? Correct answer should be: one and only one. Lets check it.

Decomposition of a function (preparation) into a "weighted sum" of delta functions (homog,

$$f(x) = \int w(x')\,\delta(x'-x)\,dx'$$

Assume there are two decomposition

$$f(x) = \int w_1(x')\,\delta(x'-x)\,dx' = \int w_2(x')\,\delta(x'-x)\,dx'$$

$$f(x) = w_1(x) = w_2(x)$$ decomp. is unique.

Conclude that C.S.M. ~~em~~ represents propositions consistently with the general abstract notions that we developed before this theory was presented.

Failures of C.M.

Abstraction based on new phenomena force to a major departure from classical ideas:

- the notion of individual state has to be inherently probabilistic, : ~~we must abandon~~ the idea that the result of a single measurement act is ~~p~~determined by the state of the system must be abandoned,
- the individual state determines only the probability with which a given result will obtain

The mathematical structure of the phase-space is insufficient to include these new notions, ~~the~~ ~~The point new state representatives will have to have be math. richer~~

The new representatives of observables will have to be richer.

Observable E	State
Possible outcomes of a single E-measurement act	Probability of outcome
e_1	P_{e_1}
e_2	P_{e_2}
e_3	$\vdots$
$\vdots$	
e_N	P_{e_N}

$$\sum_i^N P_{e_i} = 1$$

~~[illegible]~~

~~Every measurement act can be~~

Simplest observables : "questions" with a yes/no $(1/0)$ answer

E.g.: Is the energy e_3 ?

State

Possible outcomes	Probability of outcome
yes (1)	P_{e_3}
no (0)	$1 - P_{e_3}$

We will construct a math. description with these features.

Space $\mathcal{H}$ on $\mathbb{C}$
Points (or vectors) $\psi, \varphi, \ldots$ in $\mathcal{H}$
Scalars (complex) $a, b, \ldots$ in $\mathbb{C}$

If ψ and φ are in $\mathcal{H}$, then $a\psi + b\varphi$ is also in $\mathcal{H}$ (linear comb.)

$\mathcal{H}$ space

$\psi, \varphi, \ldots$ elements of $\mathcal{H}$ ("vectors")

$a, b, \ldots$ (complex) scalars in $\mathbb{C}$ (or $\mathbb{R}$)

space: "closed" under addition and scalar multiplication, i.e.,

$$a\psi + b\varphi \quad \text{is still a vector in } \mathcal{H}$$

A Hilbert space is a space equipped with several additional properties and definitions:

complete: every sequence ψ_n converges to a ψ still in $\mathcal{H}$

metric: a "distance" $d(\psi, \varphi)$ is defined

norm: a norm $\|\psi\|$ is defined

inner product: a "scalar" product $<\psi, \varphi>$ is defined

scalar product: axioms, for every ψ, φ in $\mathcal{H}$ and a in $\mathbb{C}$:

$$<\psi, \psi> \;\geq 0$$

$$<\psi, \psi> \;= 0 \quad \text{iff} \quad \psi = 0$$

$$<\psi, \varphi>^* = <\varphi, \psi>$$

$$<a\psi_1 + b\psi_2, \varphi> = a^* <\psi_1, \varphi> + b^* <\psi_2, \varphi>$$

in terms of a scalar product
we can define a "natural" norm and metric

$$\|\psi\| = <\psi, \psi>^{1/2}$$

$$d(\psi, \varphi) = \|\psi - \varphi\|$$

~~[illegible] that scalar~~

$x = (\xi_1, \ldots, \xi_n)$, $\langle x, y\rangle = \sum_k^n \xi_k$

Examples: $\mathbb{C}^n$ or $\mathbb{R}^n$, the familiar n-dimensional euclidian space

$L^2(a,b)$, the square integrable complex functions defined on the set $a \le x \le b$, $\int_a^b |f(x)|^2 dx < \infty$

with scaler product

$$\langle f, g\rangle = \int_a^b f^*(x) g(x) dx$$

The space of absolute convergent sequences $x = (\xi_1, \xi_2, \ldots, \xi_k, \ldots)$, $\sum_{k=1}^{\infty} |\xi_k|^2 < \infty$ with scaler product

$$\langle x, y\rangle = \sum_k^{\infty} \xi_k^* \eta_k$$

Different systems will require different spaces.

Note that so far ~~we are not in~~ C. M. is contained, $\mathcal{H} = \mathbb{R}^{2N}$

Again points in $\mathcal{H}$ will represent states.
But the distinction will come with observables, ~~and~~ their values and their structure
~~So we with that~~
Again functions on $\mathcal{H}$ will represent observables.
But their values will acquire special meaning.

We start with the simplest observable; a yes/no "question"

$$Q_a \equiv \text{is observable } A \text{ equal to } a\,?$$

recall that we want to
represent in our new theory
that fact that a single outcome
will not tell the complete story

we have two possible "answers": 0 (no), 1 (yes)
The function on $\mathcal{H}$ we denote by

$$q_a(\psi) = \sum \frac{N_1}{N} \cdot 1 + \frac{N_0}{N} 0$$

we want to give it ~~a~~ a more explicit ~~?~~ structure. It will have to equal the mean value, thus

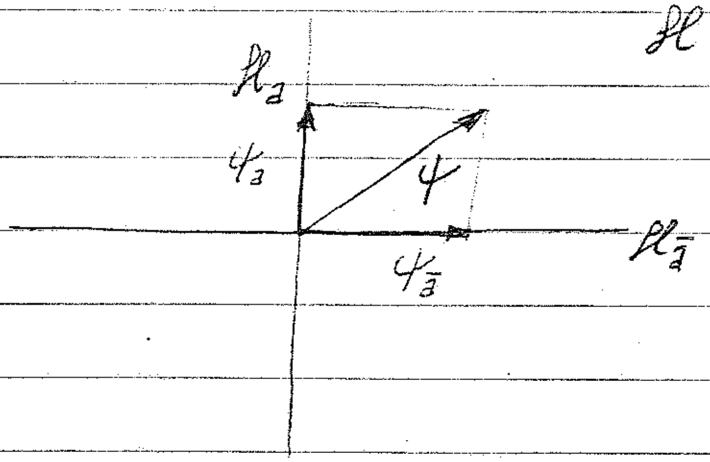
$$0 \le q_a(\psi) \le 1$$

There will be also the ~~[illegible]~~ inverse "question" $Q_{\bar a} \equiv$ is observable A different from a?
which will be answered by the same experiment and the mean value is

$$q_{\bar a}(\psi) = \frac{N_1}{N} 0 + \frac{N_0}{N} 1$$

$$q_a(\psi) + q_{\bar a}(\psi) = 1$$

Here is a way to do it (we are not proving anything!)



we define

$$\mathcal{H}_a = \{\psi_1 \mid q_a(\psi_1) = 1\}$$

$$\mathcal{H}_{\bar a} = \{\psi_0 \mid q_a(\psi_0) = 0\}$$

clearly these two subspaces of $\mathcal{H}$ will be disjoint: the value of a question cannot be simultaneously 1 and 0!

next we ~~[illegible]~~ want to conceive of states that do not have ~~such~~ a single answer and we say that generic states are of the form

$$\psi = \psi_a + \psi_{\bar a}$$

$$\mathcal{H} = \mathcal{H}_a \oplus \mathcal{H}_{\bar a}$$

The "question" has identified two disjoint subspaces of $\mathcal{H}$, one for each "answer", such that $\mathcal{H}$ is the "direct sum" of these subspaces.

$$\psi = P_{\mathcal{H}_a}\psi + P_{\mathcal{H}_{\bar a}}\psi \qquad P_{\mathcal{H}_a} = \text{projection onto } \mathcal{H}_a$$

$$= \psi_a + \psi_{\bar a}$$

note that

$$\|\psi\|^2 = \|\psi_a\|^2 + \|\psi_{\bar a}\|^2$$

Only if orthogonal

so if we define:

$$q_a(\psi) = \frac{\|\psi_a\|^2}{\|\psi\|^2}$$

[what we want to express is satisfied]

$$q_2(\psi) = \frac{\| P_{\mathcal{H}_2} \psi \|^2}{\| \psi \|^2} = \frac{\langle P_{\mathcal{H}_2} \psi , P_{\mathcal{H}_2} \psi \rangle}{\langle \psi , \psi \rangle} = \frac{\langle \psi , P_{\mathcal{H}_2} \psi \rangle}{\langle \psi , \psi \rangle}$$

Chose $\langle \psi , \psi \rangle = 1$, since it is really the direction which counts.

$$q_2(\psi) + q_{\bar{2}}(\psi) = 1$$

We are studying the representation of <u>homogeneous preparations</u> in Quantum Mechanics
(From now on heterogeneous preparations play <u>no role</u>, they do not exist!)

$\mathcal{H}$	Hilbert space
$\psi, \varphi, \ldots$	~~State~~ Vectors
$<\psi, \varphi>$	Scalar Product

"Question" Q_a: is observable A equal to a?

Possible "answers" (= outcomes of a single act of measurement of Q_a):

$$\begin{array}{lc|c} & & Q_{\bar{a}} \\ \text{yes} & 1 & 0 \\ \text{no} & 0 & 1 \end{array}$$

$$\boxed{\begin{array}{c} q_a(\psi) + q_{\bar{a}}(\psi) = 1 \\ <Q_a> + <Q_{\bar{a}}> = 1 \end{array}}$$

Functional on $\mathcal{H}$ $\quad q_a(\psi)$

~~Result~~ Arithmetic mean of Q_a-measurements on an ensemble $\quad <Q_a>$

In classical theory: $<Q_a>$ is either 1 or 0

In quantum theory: for a given homog. prep., i.e., a given state, both outcomes are possible for a single act, thus, all values

$$0 \leq <Q_a> \leq 1 \quad \text{are possible.}$$

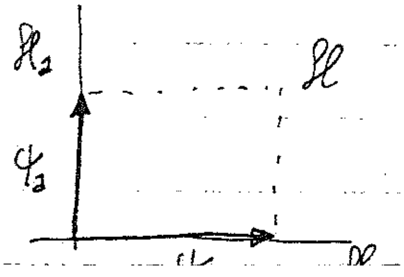
So we define two subspaces of $\mathcal{H}$

$$\mathcal{H}_a \equiv \{\psi \mid q_a(\psi) = 1\} \qquad \mathcal{H}_{\bar{a}} \equiv \{\psi / q_a(\psi) = 0\}$$

and assume that

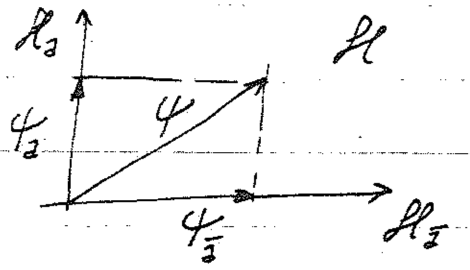
$$<\psi_a, \psi_{\bar{a}}> = 0$$

i.e., that $\mathcal{H}_a$ and $\mathcal{H}_{\bar{a}}$ are "orthogonal" subspaces



In Classical theory : only vectors in either $\mathcal{H}_1$ or $\mathcal{H}_{\bar{1}}$ would qualify as states and that would have to be true for all possible "questions".

In Quantum theory instead we want to include states for which the "answers" are not always definite.



$$\psi = \psi_1 + \psi_{\bar{1}}$$

ψ is neither in $\mathcal{H}_1$ nor in $\mathcal{H}_{\bar{1}}$ but has components in both.

ψ_1 = "projection" of ψ onto $\mathcal{H}_1$ $= P_{\mathcal{H}_1}\psi$

$\psi_{\bar{1}}$ = $= P_{\mathcal{H}_{\bar{1}}}\psi$

$$\|\psi\|^2 = \|\psi_1\|^2 + \|\psi_{\bar{1}}\|^2$$

$$1 = \frac{\|\psi_1\|^2}{\|\psi\|^2} + \frac{\|\psi_{\bar{1}}\|^2}{\|\psi\|^2}$$

one usually selects $\|\psi\|^2 = 1$

↳ note that $\psi_2 = c\psi_1$ give the same val for all questions thus, really the same state.

So, if we let

$$q_1(\psi) = \frac{\|\psi_1\|^2}{\|\psi\|^2} \quad \text{and} \quad q_{\bar{1}}(\psi) = \frac{\|\psi_{\bar{1}}\|^2}{\|\psi\|^2}$$

we have that $0 \le q_1(\psi) \le 1$ and $q_1(\psi) + q_{\bar{1}}(\psi) = 1$

Thus, the definition satisfies our requirement.

$$\|\psi_1\|^2 = \langle \psi_1, \psi_1 \rangle = \langle \psi, \psi_1 \rangle = \langle \psi, P_{\mathcal{H}_1}\psi \rangle$$

$$q_1(\psi) = \frac{\langle \psi, P_{\mathcal{H}_1}\psi \rangle}{\langle \psi, \psi \rangle}$$

Now, let us consider an observable A with a list of possible outcomes :

$$a_1, a_2, \ldots, a_j, \ldots$$

For each ~~value~~ outcome we can define a "question"

$$Q_{a_j} : \text{ is observable } A \text{ equal to } a_j ?$$

Clearly, if I make an A-measurement act, I answer simultaneously all those questions! Because the system responds with only one of them.

Associated functional : $q_{a_j}(\psi) = \langle \psi, P_{\mathcal{H}_{a_j}} \psi \rangle$

Arithmetic mean : $\langle Q_{a_j} \rangle$

What is the arithmetic mean of A in terms of those of Q_{a_j} ?

$0 \leq \langle Q_{a_j} \rangle \leq 1$ is the fraction of times the system gave answer a_j

$$\langle A \rangle = a_1 \langle Q_{a_1} \rangle + a_2 \langle Q_{a_2} \rangle + \ldots = \sum_j a_j \langle Q_{a_j} \rangle$$

Functional associated with observable A, $a(\psi)$ must equal that :

$$a(\psi) = \sum_i a_j \, q_{a_i}(\psi)$$

Hence:

$$a(\psi) = \sum_j a_j \langle \psi, P_{\mathcal{H}_{a_j}} \psi \rangle = \langle \psi, \sum_j a_j P_{\mathcal{H}_{a_j}} \psi \rangle$$

That object is an operator that we denote by

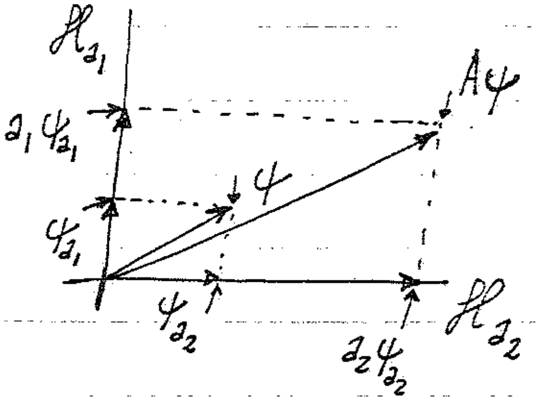
$$A \equiv \sum_j a_j P_{\mathcal{H}_{a_j}}$$

what does it do?

$$A\psi = \sum_j a_j P_{\mathcal{H}_{a_j}} \psi = \sum_j a_j \psi_{a_j}$$

e.g.,

$$A = a_1 P_{\mathcal{H}_{a_1}} + a_2 P_{\mathcal{H}_{a_2}}$$



$\mathcal{H}$	Hilbert space	
$\psi, \varphi, \ldots, \eta_i, \ldots$	vectors	$\ldots \{\eta_i\}$ an orthonormal basis
$a, b, \ldots, c_i, \ldots$	scalars	
$\langle \psi, \varphi \rangle$	scalar product	
$\alpha^*, \beta^*, \ldots, \eta_i^*, \ldots$	linear functionals	
$A, B, \ldots, P_{\eta_i}, \ldots, I, \ldots$	linear operators	

I identity operator

P_α projector onto the "direction" of α

$$P_\alpha(\ ) = \frac{\alpha \langle \alpha,\ \rangle}{\langle \alpha, \alpha \rangle}$$

$$P_\alpha P_\alpha^\dagger = P_\alpha \rightarrow \begin{cases} P_\alpha^\dagger = P_\alpha \\ P_\alpha^2 = P_\alpha \end{cases}$$

$$\psi = \sum_i c_i \eta_i \qquad c_i = \eta_i^*(\psi) = \langle \eta_i, \psi \rangle \qquad \langle \eta_i, \eta_j \rangle = \delta_{ij}$$

thus

$$I(\psi) = \psi = \sum_i \eta_i \langle \eta_i, \psi \rangle = \sum_i P_{\eta_i}(\psi)$$

so

$$I(\ ) = \sum_i P_{\eta_i}(\ )$$

completeness relation
or
resolution of the identity

$$I(\ ) = \sum_i \eta_i \langle \eta_i,\ \rangle$$

$A^\dagger$: $\langle A^\dagger(\psi), \varphi \rangle = \langle \psi, A(\varphi) \rangle$ for all ψ, φ in $\mathcal{H}$

A self-adjoint if $A^\dagger = A$

Is P_α hermitian ? see p. 8 of this se

Eigenvalue problem of ~~a~~ a linear self-adjoint operator A

$$A(\alpha) = a\alpha$$

The scalars $a_1, a_2, \ldots, a_k, \ldots$ for which there is a solution are called eigenvalues of A.

The vectors in the set $\{\alpha \,/\, A(\alpha) = a_k\alpha\}$ are called eigenvectors of A belonging to eigenvalue a_k.

A linear → the set $\{\alpha \,/\, A(\alpha) = a_k\alpha\}$ is a space (a subspace of $\mathcal{H}$). We denote it by $\mathcal{H}_{a_k}$ and call it the eigenspace belonging to eigenvalue a_k

Let $\{\alpha_{kd}\}$ for $d = 1, 2, \ldots, D_k$ be ~~the~~ an orthonormal basis for $\mathcal{H}_{a_k}$
~~and~~ (D_k, the dimensionality of $\mathcal{H}_{a_k}$ is also called the degeneracy of eigenvalue a_k)

$A^\dagger = A \rightarrow$

The set $\{\alpha_{kd}\}$ for all k and d is an orthonormal basis for $\mathcal{H}$

The eigenvalues are real. $\left.\begin{array}{l} \langle A(\alpha), \alpha\rangle = \langle a\alpha, \alpha\rangle = a^*\langle\alpha,\alpha\rangle \\ \langle \alpha, A(\alpha)\rangle = \langle\alpha, a\alpha\rangle = a\langle\alpha,\alpha\rangle \end{array}\right\} a = a^*$

Eigenspaces $\mathcal{H}_{a_k}$ are orthogonal

$$P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{a_j}} = \delta_{ij} P_{\mathcal{H}_{a_i}}$$

$$\mathcal{H} = \mathcal{H}_{a_1} \oplus \mathcal{H}_{a_2} \oplus \cdots \oplus \mathcal{H}_{a_k} \oplus \cdots$$

Two operators are identical if they have the same eigenvalues <u>and</u> the same eigenspaces.

Let α_i be in $\mathcal{H}_{a_i}$.

$$P_{\mathcal{H}_{a_k}}(\alpha_i)=0 \quad \underset{k\neq i}{} \qquad P_{\mathcal{H}_{a_i}}(\alpha_i)=\alpha_i \Rightarrow \boxed{P_{\mathcal{H}_{a_k}}(\alpha_i)=\delta_{ik}\,\alpha_i}$$

↑ note that this is itself an eigenvalue problem

let

$$A(\;)=\sum_j a_j\, P_{\mathcal{H}_{a_j}}(\;)$$

$$A(\alpha_i)=\sum_j a_j\, P_{\mathcal{H}_{a_j}}(\alpha_i)=\sum_j a_j\,\delta_{ij}\,\alpha_i=a_i\,\alpha_i$$

These two are the same operator.

Eigenvalue problem of a projection operator onto the ~~one~~ subspace $\mathcal{H}_\gamma$

$$P_{\mathcal{H}_\gamma}(x)=p\,x$$

$$P^2=P \qquad P(x)=P^2(x)=P(P(x))=P(p\,x)=$$

$$=p\,P(x)=p^2x=p\,x$$

$$\boxed{p^2=p\ \begin{array}{l}\nearrow 0\\ \searrow 1\end{array}}$$

Function of an s.a. operator

let $F(x)$ be an analytic function of the real variable x

$$F(x) = \sum_n c_n x^n$$

we define

$$F(A) \equiv \sum_n c_n A^n$$

A^n ?

$$A^0 = I$$
$$A^1 = A$$

$$A^2(\ ) = A(A(\ )) = \Big(\sum_i a_i P_{\mathcal{H}_{a_i}}(\ )\Big)\Big(\sum_j a_j P_{\mathcal{H}_{a_j}}(\ )\Big) = \sum_{ij} a_i a_j P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{a_j}} =$$

$$= \sum_{ij} a_i a_j \delta_{ij} P_{\mathcal{H}_{a_i}} = \sum_i a_i^2 P_{\mathcal{H}_{a_i}}(\ )$$

$$A^n = \sum_k a_k^n P_{\mathcal{H}_{a_k}}$$

$$F(A) = \sum_k F(a_k) P_{\mathcal{H}_{a_k}}$$

Commutator of two s.a. operators

$$[A, B] \equiv AB - BA$$

i.e.

$$[A,B](\ ) = A(B(\ )) - B(A(\ ))$$

when do two operators commute? i.e., when is $[A,B] = 0$?

$$A = \sum_i a_i P_{\mathcal{H}_{a_i}} \qquad B = \sum_j b_j P_{\mathcal{H}_{b_j}}$$

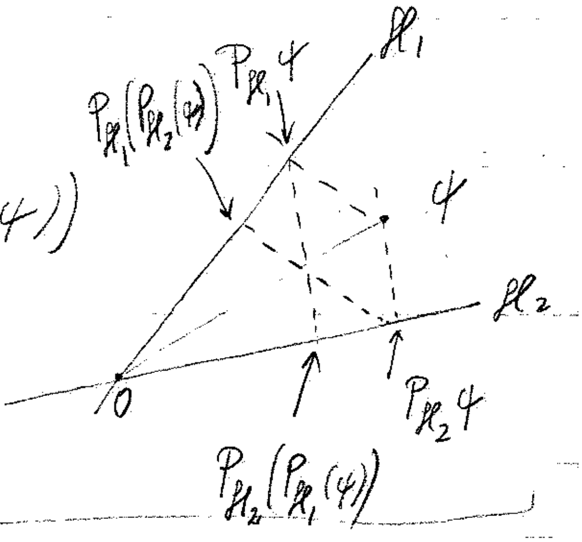
$$[A,B] = \sum_{ij} a_i b_j \left(P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{b_j}} - P_{\mathcal{H}_{b_j}} P_{\mathcal{H}_{a_i}} \right) = \sum_{ij} a_i b_j \big[P_{\mathcal{H}_{a_i}}, P_{\mathcal{H}_{b_j}}$$

so when do two projectors commute?

$$P_{\mathcal{H}_1} P_{\mathcal{H}_2} \overset{?}{=} P_{\mathcal{H}_2} P_{\mathcal{H}_1}$$

$$P_{\mathcal{H}_1}\left(P_{\mathcal{H}_2}(\psi)\right) = P_{\mathcal{H}_2}\left(P_{\mathcal{H}_1}(\psi)\right)$$

if $\mathcal{H}_1 \perp \mathcal{H}_2$ or $\mathcal{H}_1 = \mathcal{H}_2$



See Messiah p. 200 for proof

$[A,B]=0$ iff there exists a basis for $\mathcal{H}$ which is simultaneously an eigenbasis of both A and B.

i.e., if A and B share a common eigenbasis

Problem: if $[A,B]=0$ and $[A,C]=0$, is $[B,C]=0$?

Matrix representation of operators

Let $\{\eta_j\}$ be an orthonormal basis for $\mathcal{H}$. Fix it

$$P_{\eta_j} = \eta_j \langle \eta_j , \ \rangle$$

$$I = \sum_j P_{\eta_j} = \sum_j \eta_j \langle \eta_j , \ \rangle$$

$$A = IAI = \sum_j \eta_j \langle \eta_j , \ \rangle \left(A \sum_k \eta_k \langle \eta_k , \ \rangle \right) =$$

$$= \sum_{jk} \eta_j \underbrace{\langle \eta_j , A \eta_k \rangle}_{a_{jk}} \langle \eta_k , \ \rangle$$

Since $\{\eta_j\}$ is fixed, the coeff a_{jk} fully specify A.

$$\mathrm{Tr}(A) = \sum_j \langle \eta_j , A \eta_j \rangle \overset{?}{=} \sum_j \langle \gamma_j , A \gamma_j \rangle \quad \text{for all bases.}$$

$$= \sum_j a_{jj}$$ sum of the diagonal elements of the matrix representation

same for all representations.

SKIP

Dirac notation based on representation theorem

$$\alpha^*(\ \ ) = <\alpha,\ \ >$$

vectors $|\psi>, |\varphi>, \ldots$ $\qquad$ $|\psi>$ "ket vector"

functionals $<\alpha|, <\beta|, \ldots$ $\qquad$ $<\alpha|$ "bra vector"

scalar product

$$\alpha^*(\psi) = <\alpha, \psi> = <\alpha|\psi>$$

$$A(\psi) = |A(\psi)> = A|\psi>$$

$$<\varphi, A(\psi)> = <\varphi|A|\psi> = <A^\dagger(\varphi), \psi> = <A^\dagger\varphi|\psi>$$

$$<A^\dagger(\varphi)| = <\varphi|A$$

Eigenvalue problem (notation)

$$A|\alpha_{kd}> = a_k|\alpha_{kd}>$$

foundations $\longrightarrow$

$$A|kd> = a_k|kd>$$

remember with only one index n running over eigenvectors (degeneracy will show up as many a_n being equal in value)

$$A|\alpha_n> = a_n|\alpha_n>$$

$$A|n> = a_n|n>$$

$$P_\alpha^2(\psi) = P_\alpha(P_\alpha(\psi)) = \alpha\langle\alpha, P_\alpha(\psi)\rangle = \alpha\langle\alpha, \alpha\langle\alpha,\psi$$

$$= \alpha\langle\alpha,\psi\rangle = P_\alpha(\psi)$$

$$P_\alpha = \alpha\langle\alpha,\ \rangle \quad , \quad P_\alpha^{+}\ ?$$

$$\langle\psi, P_\alpha(\varphi)\rangle = \langle P_\alpha^{+}(\psi), \varphi\rangle$$ for all ψ and φ

linear in second factor; conj. lin.

$$\hookrightarrow \langle\psi, \alpha\langle\alpha,\varphi\rangle\rangle = \langle\psi,\alpha\rangle\langle\alpha,\varphi\rangle = \langle\alpha\langle\psi,\alpha\rangle^*, \varphi\rangle$$

if $\langle x,\varphi\rangle = \langle y,\varphi\rangle\ \forall\varphi \rightarrow x=y$

$$P_\alpha^{+}(\psi) = \alpha\langle\psi,\alpha\rangle^* = \alpha\langle\alpha,\psi\rangle = P_\alpha(\psi)$$

$\boxed{\text{yes: hermitian}}$

Summary

$\mathcal{H} = \{ \varphi, \psi, \dots \} = \{ |\varphi\rangle, |\psi\rangle, \dots \}$ Hilbert space

$\mathcal{H}^* = \{ \alpha^*(\ ), \beta^*(\ ), \dots \} = \{ \langle\alpha|, \langle\beta|, \dots \}$ Dual space

scalar product $\langle \alpha, \varphi \rangle = \langle \alpha | \varphi \rangle = \alpha^*(\varphi)$

bases for $\mathcal{H}$: $\{ \eta_j \}$: $\langle \eta_j, \eta_k \rangle = \langle \eta_j | \eta_k \rangle = \delta_{jk}$

$\{ \varepsilon_i \}$ $\langle \varepsilon_i, \varepsilon_\ell \rangle = \langle \varepsilon_i | \varepsilon_\ell \rangle = \delta_{i\ell}$

$$I(\ ) = \sum_j \eta_j \langle \eta_j, \ \rangle = \sum_j |\eta_j\rangle\langle\eta_j| \ \rangle = I$$

$$= \sum_i \varepsilon_i \langle \varepsilon_i, \ \rangle = \sum_i |\varepsilon_i\rangle\langle\varepsilon_i|$$

$$P_{\eta_j}(\ ) = \eta_j \langle \eta_j, \ \rangle = |\eta_j\rangle\langle\eta_j| \ \rangle$$

representation of a vector

$$\psi = \sum_j c_j \eta_j = |\psi\rangle = \sum_j c_j |\eta_j\rangle \qquad c_j = \langle \eta_j,$$

of an operator

$$A = \sum_{jk} A_{jk} \eta_j \langle \eta_k, \ \rangle = \sum_{jk} A_{jk} |\eta_j\rangle\langle\eta_k| \qquad A_{jk} = \langle \eta_j, A$$

$$= \langle \eta_j | A | \eta_k$$

representation of a vector with respect to a basis.

$$|\psi\rangle = \sum_j |\eta_j\rangle\langle\eta_j|\psi\rangle = \sum_j |\eta_j\rangle c_j$$

$$= \sum_i |\varepsilon_i\rangle\langle\varepsilon_i|\psi\rangle = \sum_i |\varepsilon_i\rangle e_i$$

$$c_j = \langle\eta_j|\psi\rangle = \sum_i \langle\eta_j|\varepsilon_i\rangle\langle\varepsilon_i|\psi\rangle = \sum_i \langle\eta_j|\varepsilon_i\rangle e_i$$

$$e_i = \langle\varepsilon_i|\psi\rangle = \sum_j \langle\varepsilon_i|\eta_j\rangle\langle\eta_j|\psi\rangle = \sum_j \langle\varepsilon_i|\eta_j\rangle c_j$$

define the matrix

$$[U]_{\varepsilon\leftarrow\eta} = [\langle\varepsilon_i|\eta_j\rangle]$$

unitary transformation

$$[U]_{\eta\leftarrow\varepsilon} = [\langle\eta_k|\varepsilon_\ell\rangle] = [U]^{\dagger}_{\varepsilon\leftarrow\eta}$$

$$= [U]^{-1}_{\varepsilon\leftarrow\eta}$$

$\dagger$ = Hermitian conjugate = complex conjugate every term and transpos

$$[\psi]_\eta = [U]_{\eta\leftarrow\varepsilon}[\psi]_\varepsilon$$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \langle\eta_1|\varepsilon_1\rangle & \langle\eta_1|\varepsilon_2\rangle & \cdots \\ \langle\eta_2|\varepsilon_1\rangle & \langle\eta_2|\varepsilon_2\rangle & \\ \vdots & & \ddots \end{bmatrix}\begin{bmatrix} e_1 \\ e_2 \\ \vdots \end{bmatrix}$$

$$[\psi]_\varepsilon = [U]_{\varepsilon\leftarrow\eta}[\psi]_\eta$$

$$[U]_{\eta\leftarrow\varepsilon}[U]_{\varepsilon\leftarrow\eta} = [I]$$

$$[I] = \begin{bmatrix} 1 & 0 & 0 & \\ 0 & 1 & 0 & \\ 0 & 0 & 1 & \\ & & & \ddots \end{bmatrix}$$

Representation of an <u>operator</u> with respect to a basis

$$A(\ ) = A|\ \rangle = A = \sum_{jk} |\eta_j\rangle\langle\eta_j|A|\eta_k\rangle\langle\eta_k| = \sum_{jk} A^{\eta}_{jk} |\eta_j\rangle\langle\eta_k|$$

$$= \sum_{i\ell} |\varepsilon_i\rangle\langle\varepsilon_i|A|\varepsilon_\ell\rangle\langle\varepsilon_\ell| = \sum_{i\ell} A^{\varepsilon}_{i\ell} |\varepsilon_i\rangle\langle\varepsilon_\ell|$$

$$A^{\eta}_{jk} = \langle\eta_j|A|\eta_k\rangle = \sum_{i\ell} \langle\eta_j|\varepsilon_i\rangle \underbrace{\langle\varepsilon_i|A|\varepsilon_\ell\rangle}_{A^{\varepsilon}_{i\ell}} \langle\varepsilon_\ell|\eta_k\rangle$$

$$[A]_\eta = [U]_{\eta\leftarrow\varepsilon}\,[A]_\varepsilon\,[U]_{\varepsilon\leftarrow\eta}$$

<u>Identity operator</u>: I

$$I^{\eta}_{jk} = \langle\eta_j|I|\eta_k\rangle = \langle\eta_j|\eta_k\rangle = \delta_{jk}$$

$$[I]_{\text{any basis}} = \begin{bmatrix} 1 & 0 & \\ 0 & 1 & \\ & & \ddots \end{bmatrix}$$

<u>Adjoint of an operator A</u>: A^{+}

$$A^{+\eta}_{jk} = \langle\eta_j|A^{+}|\eta_k\rangle = \langle\eta_j, A^{+}(\eta_k)\rangle$$

$$= \langle A^{+}(\eta_k), \eta_j\rangle^{*} = \langle\eta_k, A\eta_j\rangle^{*} =$$

$$= \langle\eta_k|A|\eta_j\rangle^{*} = \left(A^{\eta}_{kj}\right)^{*}$$

the matrix of the adjoint of A is
the transpose of the conjugate of the matrix of A

Self-Adjoint operator : $A = A^{\dagger}$

$$A^{\eta}_{jk} = <\eta_j|A|\eta_k> = <\eta_k|A^{\dagger}|\eta_j>^* =$$

$$= <\eta_k|A|\eta_j>^* = \left(A^{\eta}_{kj}\right)^*$$

the matrix is Hermitian, i.e.,

Unitary operator : $U^{\dagger} = U^{-1}$

$$U = \exp(iG) \quad \text{where} \quad G = G^{\dagger}$$

$$U^{-1} = \exp(-iG)$$

$$U^{\dagger} = \exp(-iG^{\dagger}) = \exp(-iG)$$

$\|U(\varphi)\| = \|\varphi\|$ norm preserving

$<U(\psi), U(\varphi)> = <\psi, \varphi>$ scalar product preserving

example: $U = \sum_k |\varepsilon_k><\eta_k|$ $\quad U^{\dagger} = \sum_k |\eta_k><\varepsilon_k|$

$$UU^{\dagger} = \sum_{ij} |\varepsilon_i>\underbrace{<\eta_i|\eta_j>}_{\delta_{ij}}<\varepsilon_j| = \sum_i |\varepsilon_i><\varepsilon_i| = I$$

$$U^{\eta}_{jk} = <\eta_j|U|\eta_k> = <\eta_j|\varepsilon_k> = \left([U]_{\eta \leftarrow \varepsilon}\right)_{jk}$$

Eigenvalue problem of self-adjoint operator

$$A(\alpha) = a\,\alpha \qquad \text{or} \qquad (A - aI)(\alpha) = 0$$

$$A|\alpha\rangle = a|\alpha\rangle \qquad\qquad (A - aI)|\alpha\rangle = 0$$

representation of the eigenvalue problem with respect to a basis. To be the zero vector it has to ~~be~~ have all zero coordinate

$$\langle \eta_j | (A - aI) | \alpha \rangle = 0$$

$$0 = \sum_k \langle \eta_j | (A - aI) | \eta_k \rangle \langle \eta_k | \alpha \rangle = \sum_k \left(A^{\eta}_{jk} - a\,\delta_{jk} \right) c^{\eta}_k$$

$$\left([A]_\eta - a[I] \right) [\alpha]_\eta = 0$$

$$\begin{bmatrix} A_{11} - a & A_{12} & \cdots \\ A_{21} & A_{22} - a & \\ \vdots & & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix} = 0$$

a system of linear homogeneous equations

it has a solution only if the det is zero.

$$\det\left([A]_\eta - a[I] \right) = 0$$

with respect to another basis ? $\{\varepsilon\}$

$$[A]_\varepsilon = [U]_{\varepsilon \leftarrow \eta} [A]_\eta [U]_{\eta \leftarrow \varepsilon} \qquad [U]_{\varepsilon \leftarrow \eta} [U]_{\eta \leftarrow \varepsilon} = [I]$$

Thus

$$[A]_\varepsilon - \lambda[I] = [U]_{\varepsilon\leftarrow\eta}\left([A]_\eta - \lambda[I]\right)[U]_{\eta\leftarrow\varepsilon}$$

but

$$\det[X][Y][Z] = \det[X]\det[Y]\det[Z] = \det[Y]\det\underbrace{[X][Z]}_{I}$$

Thus

$$\det\left([A]_\varepsilon - \lambda[I]\right) = \det\left([A]_\eta - \lambda[I]\right)\cancel{\det I}\to 1$$

so it is invariant, and we define

$$\det(A-\lambda I) \equiv \det\left([A]_{\text{any basis}} - \lambda[I]\right)$$

$$\det(A-\lambda I) = (-1)^n\lambda^n + (-1)^{n-1}(\operatorname{Tr}A)\lambda^{n-1} + \dots + \det A = \text{Characteristic Polynomial of } A$$

The coefficients do not depend on the representation

$$\operatorname{Tr}A \equiv \sum_i A_{ii}^{\text{any basis}} = \sum_j \lambda_j$$

← eigenvalues of A

j ← sum over the indexes of an eigenbasis

The coefficient of λ^{n-k} is the sum of all principal minors of order k taken with the sign $(-1)^{n-k}$.

The Char-Pol. has n roots: the eigenvalues.
Once you find them, you can ~~[illegible]~~ construct the eigenvectors.

$$\operatorname{Tr}A \equiv \operatorname{Tr}[A]_{\substack{\text{any}\\\text{basis}}} = \sum_i A_{ii}^{\text{any basis}} = \sum_j \lambda_j \quad \text{eigenvalues (repeated)}$$

$$\operatorname{Tr}AB \equiv \operatorname{Tr}[A][B] = \operatorname{Tr}[B][A] = \operatorname{Tr}BA$$

$$\boxed{\operatorname{Tr}|\eta\rangle\langle\varepsilon| = \langle\varepsilon|\eta\rangle}$$

Operator space

$\mathcal{L}(\mathcal{H})$: the set of all linear operators A, B, ... on $\mathcal{H}$ such that

$$\mathrm{Tr}\,A^\dagger A < \infty$$

$$\mathcal{L}(\mathcal{H}) \equiv \{ A \mid A : \mathcal{H} \rightarrow \mathcal{H},\ \mathrm{Tr}\,A^\dagger A < \infty \}$$

with the scalar product $(A, B) \equiv \mathrm{Tr}\,A^\dagger B = (\mathrm{Tr}\,B^\dagger A)^* = (B, A)^*$

$\therefore$ $\mathcal{L}(\mathcal{H})$ is a Hilbert space

So every thing we know about Hilbert spaces applies

For example: the linear <u>functionals</u> on $\mathcal{L}(\mathcal{H})$

denote them by

$$a^*(\ \ ) : \mathcal{L}(\mathcal{H}) \longrightarrow \mathbb{R}$$

they are maps, or functions, from $\mathcal{L}(\mathcal{H})$ to $\mathbb{R}$

So

$$a^*(B) \quad \text{is a number}$$

Representation theorem: to every $a^*(\ \ )$ there corresponds a <u>unique</u> element, say A, in the space $\mathcal{L}(\mathcal{H})$ such that

$$a^*(\ \ ) = (A,\ \ )$$

thus

$$a^*(B) = (A, B) = \mathrm{Tr}\,A^\dagger B$$

Orthonormal basis for $\mathcal{L}(\mathcal{H})$

$$\{T_\alpha\} \qquad (T_\alpha, T_\beta) = \delta_{\alpha\beta}$$

$$\alpha = 1, 2, \dots$$

so that

$$A = \sum_\alpha c_\alpha T_\alpha$$

Example: let $\{\eta_j\}$ be a basis for $\mathcal{H}$, then

$$T_\alpha \equiv |\eta_j\rangle\langle\eta_k| \qquad \alpha \equiv j, k \qquad \beta \equiv i, l$$

is a dyadic basis for $\mathcal{L}(\mathcal{H})$

in fact

$$A = \sum_{jk} A_{jk} |\eta_j\rangle\langle\eta_k| = \sum_\alpha c_\alpha T_\alpha \qquad c_\alpha = A_{jk}$$

and

$$(T_\alpha, T_\beta) = \mathrm{Tr}\, \overbrace{|\eta_k\rangle\langle\eta_j|}^{T_\alpha^\dagger}\, \overbrace{|\eta_i\rangle\langle\eta_l|}^{T_\beta} = \delta_{ij}\, \mathrm{Tr}\, |\eta_k\rangle\langle\eta_l| =$$

$$= \delta_{ij} \langle\eta_l|\eta_k\rangle = \delta_{ij}\delta_{lk} = \delta_{\alpha\beta}$$

Real linear functionals defined on self-adjoint operators $B^\dagger = B$

$$a^*(B) = \mathrm{Tr}\, A^\dagger B$$

if $a^*(\ )$ is real

$$[a^*(B)]^* = [\mathrm{Tr}\, A^\dagger B]^* = \mathrm{Tr}\, B^\dagger A = \mathrm{Tr}\, BA = \mathrm{Tr}\, AB$$

$$= a^*(B) = \mathrm{Tr} A^\dagger B$$ for every B

$$(A, B) = (A^\dagger, B)$$ for every $B^\dagger = B$ implies $A = A^\dagger$.

Self-adjoint operator A on $\mathcal{H}$

Eigenvalue problem $A(\alpha) = a\,\alpha$

Solution : eigenvalues a_k (real)

eigenspaces $\mathcal{H}_{a_k}$ (orthogonal and complete)

$$\mathcal{H} = \mathcal{H}_{a_1} \oplus \cdots \oplus \mathcal{H}_{a_k} \oplus \cdots$$

$\psi = \alpha_1 + \cdots + \alpha_k + \cdots$ for every ψ in $\mathcal{H}$

where $\alpha_k = P_{\mathcal{H}_{a_k}}(\psi)$

$$P_{\mathcal{H}_{a_i}} P_{\mathcal{H}_{a_j}} = \delta_{ij} P_{\mathcal{H}_{a_i}}$$

Two operators A and B are equal iff they have the same eigenvalues and eigenspaces.

Consider operator

$$B(\ ) \equiv \sum_j a_j P_{\mathcal{H}_{a_j}}(\ )$$

you can check that $B = A$

Examples:

$\mathcal{H} = L^2_{2\pi}$: continuous, square integrable, complex periodic functions $\varphi(x)$ of period 2π

a basis $\quad \eta_n = \exp(inx)$

$$\varphi(x) = \sum_{n=-\infty}^{\infty} \exp(inx)\, c_n$$

$$\eta_n^*(\ ) = \frac{1}{2\pi}\int_0^{2\pi} \exp(-inx)(\ )\,dx$$

$$\langle \psi, \varphi \rangle \equiv \int_0^{2\pi} \overline{\psi}(x)\, \varphi(x)\, dx$$

note that

$$\eta_n^*(\varphi) = \int_0^{2\pi} \exp(-inx)\, \varphi(x)\, dx = \langle \overline{\eta}_n, \varphi \rangle$$

$\mathcal{H} = L^{2*}$, dual of $\mathcal{H}$, functionals on $L^2_{2\pi}$ of type

$$g(\ ) = \int_0^{2\pi} f(x)(\ )\,dx$$

a basis is $\quad \eta_n^*(\ ) = \frac{1}{2\pi}\int_0^{2\pi} \exp(-inx)(\ )\,dx$

$$g(\ ) = \sum^{\infty} c_n\, \eta_n^*(\ )$$

Examples:

$\mathcal{H} = \mathbb{R}^N$: vectors of N ~~complex~~ real numbers $\alpha = \begin{vmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{vmatrix}$

a basis

$$\eta_1 = \begin{vmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{vmatrix} \quad \eta_2 = \begin{vmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{vmatrix} \quad \cdots \quad \eta_N = \begin{vmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{vmatrix}$$

$$\alpha = \sum_{i=1}^{N} \eta_i a_i$$

$$\langle \beta, \alpha \rangle = \sum_{i=1}^{N} b_i a_i$$

$\mathcal{H} = \mathbb{C}^N \times \mathbb{C}^N$; $N \times N$ complex matrices

$$\alpha = \begin{vmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \\ \vdots & & \ddots \end{vmatrix}$$

a basis

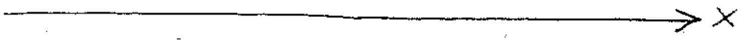
$$\eta_1 = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \\ & & & \end{vmatrix} \quad \eta_2 = \begin{vmatrix} i & 0 & \\ 0 & 0 & \\ & & \ddots \end{vmatrix} \quad \eta_3 = \begin{vmatrix} 0 & 1 & \cdots \\ 0 & 0 & \\ & & \ddots \end{vmatrix}$$

$$\alpha = \sum_{i=1}^{N^2} \eta_i a_i$$

$\dagger$ = transpose conjugate

$$\langle \beta, \alpha \rangle = \sum_{i=1}^{N^2} \bar{b}_i a_i = \mathrm{Tr}(\beta^\dagger \alpha)$$

Quantum Mechanics of a single degree of freedom



particle in one dimension

$\mathcal{H}$

$\psi, \varphi, \ldots$

position operator $\quad Q\,\chi_x = x\,\chi_x$

$$\langle \chi_x , \chi_{x'} \rangle = \delta(x-x')$$

representation of vectors $\psi, \varphi, \ldots$

$$\psi(x) \equiv \langle \chi_x , \psi \rangle \qquad \text{complex function}$$

$$\varphi(x) \equiv \langle \chi_x , \varphi \rangle$$

$$\langle \psi, \varphi \rangle = \int dx\; \psi^*(x)\,\varphi(x)$$

$$\psi = \int dx\; \chi_x\, \psi(x)$$

$$Q\psi = \int dx\; \chi_x\, x\, \psi(x)$$

$$(Q\psi)(x) = x\,\psi(x)$$

Next assume that

$$(P\psi)(x) = -i\hbar \frac{\partial}{\partial x}\psi(x)$$

$$P\psi = -i\hbar \int dx\; \chi_x \frac{\partial}{\partial x}\langle \chi_x , \psi \rangle$$

Check that $\quad [Q, P] = i\hbar I$

Further assume that

$$H = \underbrace{\frac{P^2}{2m}}_{\text{free particle energy}} + V(Q) .$$

for harmonic oscillator

$$V(Q) = \frac{1}{2} m\omega^2 Q^2$$

representation

$$(H\psi)(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2} m\omega^2 x^2 \psi(x)$$

Want to solve the eigenvalue problem:

$$H\nu = e\nu$$

$\mathcal{H}$

$\psi, \varphi, \cdots$

Q position operator

Let χ_x be the eigenvectors of Q : $Q\chi_x = x\chi_x$

the eigenvalues $-\infty \le x \le +\infty$ are continuous.

Theorem: Q is self-adjoint. $\{\chi_x\}$ for $-\infty \le x \le \infty$ forms a basis for $\mathcal{H}$ and satisfies:

$$I(\;) = \int dx\, \chi_x \langle \chi_x, \;\rangle$$

orthonormality

$$I(\chi_{x'}) = \int dx\, \chi_x \underbrace{\langle \chi_x, \chi_{x'} \rangle}_{\delta(x-x')} = \chi_{x'}$$

Any other φ in $\mathcal{H}$ may be represented with respect to the position eigenvectors by the coordinates $\langle \chi_x, \varphi \rangle$ [illegible] a set of $\overset{\text{complex}}{\text{functions}}$ of the variable

let $\varphi(x) \equiv \langle \chi_x, \varphi \rangle$

$$\varphi = \int dx\, \chi_x \langle \chi_x, \varphi \rangle = \int dx\, \chi_x\, \varphi(x)$$

$$\psi = \int dx'\, \chi_{x'} \langle \chi_{x'}, \psi \rangle = \int dx'\, \chi_{x'}\, \psi(x')$$

$$\langle \varphi, \psi \rangle = \langle \int dx\, \chi_x \varphi(x), \int dx'\, \chi_{x'} \psi(x') \rangle =$$

$$= \iint dx\, dx'\, \varphi^*(x)\, \psi(x') \underbrace{\langle \chi_x, \chi_{x'} \rangle}_{\delta(x-x')} = \int dx\, \varphi^*(x)\, \psi(x)$$

so we see that

$$\langle \chi_x, \mathcal{H} \rangle = L^2(-\infty, \infty)$$

the Hilbert space is isomorphic with L^2 space of square integrable complex functions

$$Q\varphi = Q\int dx\, \chi_x\, \varphi(x) = \int dx\, Q\chi_x\, \varphi(x) = \int dx\, \chi_x\, x\varphi(x)$$

so

$$Q\varphi(x) = x\varphi(x)$$

Similarly, starting with $[Q, P] = i\hbar I$ as a postulate, necessary to include the uncertainty relation, we can show that

$$(P\varphi)(x) = -i\hbar \frac{\partial \varphi(x)}{\partial x}$$

<u>Single-degree of freedom</u> (e.g., one-dimensional harmonic oscillator)

~~Particle in a one-dimensional box~~

$$\mathcal{H} \equiv L^2(-\infty, \infty) \qquad \longrightarrow x$$

$$\psi = f(x), \ \varphi = g(x), \ldots$$

$$\langle \psi, \varphi \rangle = \int_{-\infty}^{\infty} f^*(x)\, g(x)\, dx \qquad \longrightarrow \ \underline{\text{construct ladder}}$$

position operator $Q(\ ) = x(\ )$

momentum operator $P(\ ) = -i\hbar \frac{\partial}{\partial x}(\ )$

$$[Q, P] = i\hbar I$$

Hamiltonian (energy) operator

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 Q^2$$

motivated by direct analogy with classical harmonic oscillator.

$$H(\psi) = \frac{P(P(\psi))}{2m} + \frac{1}{2} m\omega^2 Q(Q(\psi))$$

$$H(\ ) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}(\ ) + \frac{1}{2} m\omega^2 x^2$$

Eigenvalue problem for H

$$H(\varepsilon) = e\,\varepsilon \qquad \varepsilon = h(x)$$

is a vector in $\mathcal{H}$, i.e., a function in $L^2(-\infty, \infty)$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2\right] h(x) = e\, h(x)$$

Method to solve

Define operator

$$Z \equiv \sqrt{1/2\hbar\omega}\,(\omega Q + iP)$$

$$Z^{\dagger} = \sqrt{1/2\hbar\omega}\,(\omega Q - iP)$$

check that $$[Z, Z^{\dagger}] = I$$

and

$$H = \hbar\omega\left(Z^{\dagger}Z + \frac{1}{2}\right)$$

let

$$N \equiv Z^{\dagger}Z = N^{\dagger}$$

check that

$$NZ = Z(N - I)$$
$$NZ^{\dagger} = Z^{\dagger}(N + I)$$

Let

$$N(\nu) = n\nu$$

be the eigenvalue problem for operator N.

If ν_n is an eigenvector of N belonging to eigenvalue n, then

$$NZ(\nu_n) = Z(N-I)(\nu_n) = (n-1)\,Z(\nu_n)$$

$Z(\nu_n)$ is an eigenvector belonging to eigenvalue $n-1$

similarly

$Z^{\dagger}(\nu_n)$ is an eigenvector belonging to eigenvalue $n+1$

Thus:

eigenvectors	...	$Z(Z(\nu_n))$	$Z(\nu_n)$	ν_n	$Z^\dagger(\nu_n)$	$Z^\dagger(Z^\dagger(\nu_n))$	...
eigenvalues	...	$n-2$	$n-1$	n	$n+1$	$n+2$	

Now we show that n can only be zero or a positive integer.

$$\|\nu_n\|^2 = \langle \nu_n , \nu_n \rangle \geq 0 \qquad = 0 \text{ iff } \nu_n = 0_V$$

$$\|Z(\nu_n)\|^2 = \langle Z(\nu_n), Z(\nu_n) \rangle = \langle \nu_n , Z^\dagger Z(\nu_n) \rangle =$$

$$= \langle \nu_n , N(\nu_n) \rangle = n \langle \nu_n , \nu_n \rangle$$

$$\Rightarrow n \geq 0$$

If $n=0$, $\|Z(\nu_n)\|^2 = 0$, $\nu_n = 0_V$, $Z(0_V) = 0_V$ [illegible] ?

if $n \neq 0$, $\|Z^k(\nu_n)\|^2 = n(n-1)\cdots(n-k+1)\langle \nu_n , \nu_n \rangle$ would become negative for $k < n+$ unless n is integer.

So we have Normalization only

eigenvectors	$\nu_0 = 0_V$,	$\nu_1 = Z^\dagger(0_V)$,	... ,	$\nu_n = \frac{1}{\sqrt{n!}} Z^{\dagger^n}(0_V)$	, ...	
eigenvalues	0 ,	1 ,	... ,	n	, .	

To summarize:

$$N(\nu_n) = n\,\nu_n \qquad n \text{ integer } \geq 0$$

$$Z(0_V) = 0_V$$

$$\langle \nu_{n'} , \nu_{n''} \rangle = \delta_{n'n''}$$

$$Z(\nu_n) = \sqrt{n}\;\nu_{n-1}$$

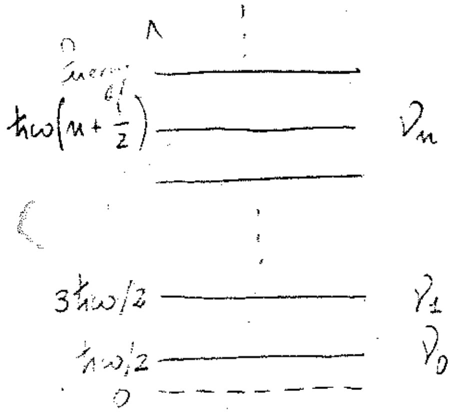
$$Z^\dagger(\nu_n) = \sqrt{n+1}\;\nu_{n+1} \qquad I(\;) = \sum_n \nu_n \langle \nu_n ,\;\rangle$$

So, we found the eigenvalues without explicitly giving the eigenvectors

$$H = \hbar\omega\left(N + \frac{1}{2}\right)$$

$$H\,\nu_n = \underbrace{\hbar\omega\left(n + \frac{1}{2}\right)}_{e_n = \hbar\omega\left(n+\frac{1}{2}\right)}\nu_n \qquad n = 0, 1, \ldots, \infty$$

Interpretation



One can think of this system as a collection of non-interacting quanta, each with energy $\hbar\omega$ plus a vacuum state with energy $\hbar\omega/2$.

N becomes the operator representing the number of quan

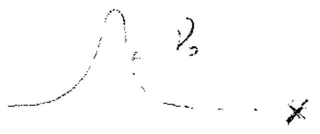
Z the annihilation and $Z^\dagger$ the creation

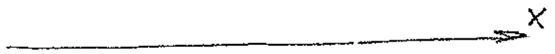
All quanta are in the same "state". They are called photon

Position representation of the eigenvectors

$$\langle \chi_x, \nu_n \rangle \equiv \nu_n(x)$$

$$\nu_0(x) = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(\frac{-\omega x^2}{2\hbar}\right)$$





Structureless Particle in One Dimension

(differentiable indefinitely in the sense of distribution theory)

$\mathcal{H}$ on $\mathbb{C}$ $\equiv$ the space of "functions" on $\mathbb{R}$;

vectors in $\mathcal{H}$ are the functions: $\psi(x), \varphi(x), \ldots$ (e.g., e^{ix}, $|x|^{-\frac{1}{2}}$, $\delta(x), \ldots$)

Scalar product (of two functions)

$$<\psi(\cdot), \varphi(\cdot)> = \int dx\, \psi^*(x)\varphi(x)$$

An "orthonormal" basis is formed by the set of "functions" $\{\delta_q(\cdot) : \delta_q(x) = \delta(x-q)\ \forall q \in \mathbb{R}\}$

In fact,

$$\psi(\cdot) = \sum\!\!\!\!\!\!\int_q \delta_q(\cdot) <\delta_q(\cdot), \psi(\cdot)> = \int dq\, \delta_q(\cdot)\psi(q)$$

$$<\delta_q(\cdot), \psi(\cdot)> = \int dx\, \delta(x-q)\psi(x) = \psi(q)$$

Position Operator Q defined as

$$Q\psi(x) = x\psi(x) \quad \text{for every } x \in \mathbb{R}$$

Momentum Operator P defined as

$$P\psi(x) = -i\hbar\psi'(x) \quad \forall x \in \mathbb{R} \left[\psi'(x) = \frac{d\psi(x)}{dx}\right]$$

Hamiltonian (Energy Operator), H constructed by analogy with classical hamiltonian

$$h(q,p) = \frac{p^2}{2m} + V(q)$$

$$H = \frac{P^2}{2m} + V(Q)$$

$$P\psi(\cdot) = -i\hbar\psi'(\cdot)$$

$$P^2\psi(\cdot) = -\hbar^2\psi''(\cdot)$$

Examples:

Harmonic Oscillator $V(q) = \frac{1}{2} m\omega^2 q^2 \rightarrow V(Q) = \frac{1}{2} m\omega^2 Q^2$

Particle in a 1-D Box $V(q) = \begin{cases} 0 & \text{if } 0 \leq q \leq L \\ \infty & \text{if } q<0 \text{ or } q>L \end{cases}$

$V(Q)\psi(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq L \\ \infty & \text{if } x<0,\ x>L \end{cases}$

Eigenvalue Problems:

Position, find $\psi(x)$ such that $Q\,\psi(\cdot) = q\,\psi(\cdot)$

or $Q\,\psi(x) = q\,\psi(x) \quad \forall x$

i.e. $x\,\psi(x) = q\,\psi(x) \quad \forall x$

Eigenvalues, any $q \in \mathbb{R}$

Eigen"functions", $\delta_q(\cdot)$ i.e. $\delta(q-x)$

Momentum, find $\psi(x)$ such that $P\psi(\cdot) = p\,\psi(\cdot)$

or $P\psi(x) = p\,\psi(x) \quad \forall x$

i.e. $-i\hbar\,\psi'(x) = p\,\psi(x) \quad \forall x$

Eigenvalues, any $p \in \mathbb{R}$

Eigenfunctions, $\psi_p(x) = e^{i\,px/\hbar}$

Energy, find $\psi(x)$ such that $H\psi(\cdot) = E\psi(\cdot)$

or $H\psi(x) = E\psi(x) \quad \forall x$

i.e.

Particle in 1-D box $-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x) \quad \forall\ 0 \leq x \leq L$

→ boundary condition $\psi(x) = 0 \quad x<0 \text{ or } x>L$

$$\psi''(x) + \frac{2m}{\hbar^2}E\psi(x) = 0 \qquad \psi(0) = \psi(L) = 0$$

$$\psi(x) = e^{i\Omega x} \qquad \psi''(x) = -\Omega^2 e^{i\Omega x}$$

so it is a solution if $\frac{2m}{\hbar} E = \Omega^2$

but satisfies boundary conditions only if $\Omega L = n\pi$, $n = 1, 2, \ldots$

So, eigenvalues

$$E_n = \frac{\pi\hbar^2}{2m} \frac{n^2}{L^2} \qquad \frac{2m}{\hbar^2} E_n = \frac{n^2\pi^2}{L^2}$$

Eigenfunctions

$$\psi_n(x) = e^{in\pi x/L}$$

Question: what is the probability of getting E_n if particle is in state $\psi(\cdot)$?

$$q_{E_n}(\psi) = \langle \psi, P_{\mathcal{H}_{E_n}} \psi \rangle$$

note, at this stage, this is just a guess! Later we will confirm that it is O.

$$\mathcal{H}_{E_n} = \{ \psi \mid \psi = c\,\psi_n \}$$ one-dimensional subspace of $\mathcal{H}$

$$P_{\mathcal{H}_{E_n}} = \psi_n \langle \psi_n, \quad \rangle \qquad P_{\mathcal{H}_{E_n}} \psi = \psi_n \langle \psi_n, \psi \rangle$$

$$q_{E_n}(\psi) = \langle \psi, \psi_n \rangle \langle \psi_n, \psi \rangle = |\langle \psi_n, \psi \rangle|^2 =$$

$$= \left| \int dx\, \psi_n^*(x) \psi(x) \right|^2 = \left| \int dx\, e^{-in\pi x/L} \psi(x) \right|^2$$

for example let $\psi(\cdot) = \psi_m(\cdot)$, i.e. let it be in an energy eigenstate,

$$q_{E_n}(\psi_m) = \left| \int dx\, e^{-in\pi x/L} e^{im\pi x/L} \right|^2 = \left| \int dx\, e^{i\frac{\pi x}{L}(m-n)} \right|^2 = \delta_{mn}$$

c Oscillator

$$H\psi(x) = \frac{P^2}{2m}\psi(x) + \frac{1}{2}m\omega^2 Q^2\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2 x^2\psi(x$$

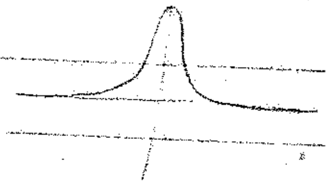
eigenvalue problem

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x)$$

eigenvalues $E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad n = 0, 1, \ldots$

eigenfunctions $\psi_n(x) = \left(\frac{\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{\omega}{\hbar}}\, x\right) e^{-\frac{1}{2}\frac{\omega}{\hbar}x^2}$

e.g., $n=0$, $E_0 = \frac{1}{2}\hbar\omega$, $\psi_0(x) = \left(\frac{\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{\omega}{\hbar}x^2}$



$H_n(\cdot)$ Hermite polynomial of order n.

Hydrogen atom

A particle in 3-D

$$\underline{P}\,\psi(x,y,z) = -i\hbar\,\underline{\nabla}\,\psi(x,y,z)$$

$$\underline{Q}\,\psi(x,y,z) = \underline{X}\,\psi(x,y,z) \qquad \underline{X} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

In spherical symmetry, one can work with coordinates r, θ, φ, and equations decouple: one in r and two in θ and φ. So write $\psi(r,\theta,\varphi) = \underline{\underline{\psi(r)}}\alpha(\theta,\varphi$

r reduced mass μ

$$\mu = \frac{mM}{m+M}$$

$$h(r,p)_{\text{classical}} = \frac{p^2}{2\mu} + V(r) \qquad V(r) = -\frac{Ze^2}{r}$$

$$P_r^2\,\psi(r) = -\hbar^2\left(\psi''(r) + \frac{2}{r}\psi'(r) - \frac{\ell(\ell+1)}{r^2}\psi(r)\right)$$

So

$$H\psi(r) = -\frac{\hbar^2}{2\mu}\left(\psi''(r) + \frac{2}{r}\psi'(r) - \frac{\ell(\ell+1)}{r^2}\psi(r)\right) - \frac{Ze^2}{r}\psi(r)$$

Eigenvalue problem, to find just eigenvalues, $H\psi(r) = E\,\psi(r)$

$$E_n = -\frac{1}{2}\mu\,\frac{Z^2e^4}{\hbar^2}\,\frac{1}{n^2} \qquad n = 1, 2, \ldots$$

E does not depend on ℓ
however ℓ accounts for part of the degeneracy.