Classical versus Quantum Equilibrium

CIRM, Luminy, January 22, 2016

Nonequilibrium : Physics, Stochastics and Dynamical Systems

Jean BRICMONT

Université Catholique de Louvain

Where does “Probability” come from in Quantum Mechanics ?

Is is an Axiom ?

Is it “irreducible” ?

Or can it be reduced to some hypothesis on initial conditions ?

In quantum mechanics, one associates to every system a state, i.e. a vector Ψ in a Hilbert space and to each physical quantity (like energy or angular momentum) a self-adjoint operator (or a matrix) A.
If the operator has a basis of eigenvectors :

$$A\psi_k = \lambda_k \psi_k,$$

then, one decomposes the quantum state Ψ into that basis

$$\Psi = \sum_k c_k \psi_k,$$

and the results of a measurement of A yields the value λ_k with probability $|c_k|^2$ (one assumes $\|\Psi\|^2 = \sum_k |c_k|2 = 1$).

Then the quantum state jumps or “collapses” to ψ_k.

For a continuous variable, like the position, $|\Psi(x)|^2$ gives the probability density of results of measurements.
Outside of measurements, the state evolves according to a deterministic and continuous evolution, like Schrödinger’s equation.

Let us first see how probabilities work in classical statistical physics.

Given $\mathbf{x}(t) = (\mathbf{q}(t), \mathbf{p}(t))$, which is the MICRO-STATE

for a (closed) mechanical system,

$\mathbf{q}$ = the positions of the particles

$\mathbf{p}$ = the momenta of the particles,

then 'everything' follows.

In particular, macroscopic quantities, like the density or the energy density, are functions of $\mathbf{x}$.

Simple example of macroscopic equation : diffusion

$$\frac{d}{dt} u = \Delta u$$

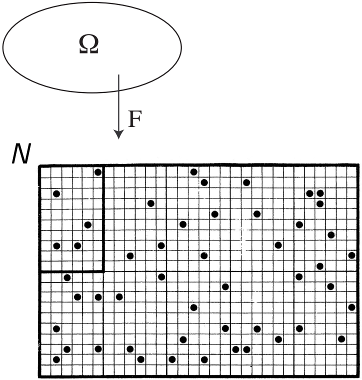
$u = u(z, t), z \in \mathbb{R}^3$.

Let $u =$ density (or energy density).

$u =$ example of ‘macroscopic’ variable.

Same idea with Navier-Stokes, Boltzmann...

Ω = PHASE SPACE $\subset \mathbb{R}^{6N}$
$N \sim$ AVOGADRO



$n << N$
Ex :

n CELLS

$F(\mathbf{x}) = (F_1(\mathbf{x}), ...; F_n(\mathbf{x})) \in \mathbb{R}^n$ = fraction of particles in each cell ;
$F(\mathbf{x})$ is the macro-state.
$u(z)$ in the diffusion equation is a continuous approximation to F.

Simple example of micro- and macro-state
Coin tossing

$\mathbf{x} \rightarrow (H, T, T, H...)$: micro-state
2^N possible values

$F(\mathbf{x}) =$ Number of heads or tails : macro-state
$= N$ possible values
$N << 2^N$.

$$\begin{array}{lll} \mathbf{x}(0) \to \mathbf{x}(t) = T^t\mathbf{x}(0) & & \text{Hamilton} \\ \downarrow \qquad\quad \downarrow & & \\ F_0 \quad \to \quad F_t & & \end{array}$$

The goal of non-equilibrium statistical mechanics is to show that the evolution of F

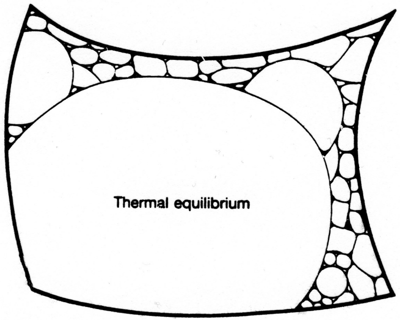
is the same for the vast majority of $\mathbf{x}(0)'s$ mapped onto F_0 (and is given by the macroscopic law). Here "vast majority" is meant relative to the Lebesgue measure on the set of micro-states $\mathbf{x}(0)$ corresponding to F_0.

The basis of Boltzmann's approach to irreversibility is that the map F is many to one in a way that depends on value taken by F.

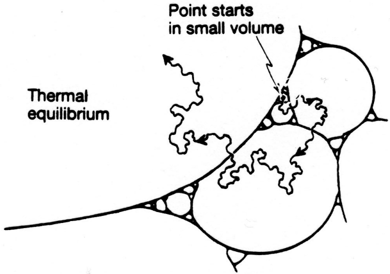
Think of coin tossing

$F = N \to$ one 'configuration'

$F = \frac{N}{2} \to \simeq \frac{2^N}{\sqrt{N}}$ 'configurations'



A coarse-graining of phase space Ω into regions corresponding to states that are macroscopically indistinguishable from one another.



As time evolves, the phase-space point enters compartments of larger and larger volume.

$\Omega_0 = F^{-1}(F_0)$, given F_0

$\overline{\Omega_0} \subset \Omega_0$ "good" configurations, meaning that

$\forall\ \mathbf{x} \in \overline{\Omega_0}$

$F_0 = F(\mathbf{x}) \longrightarrow F_t$

ACCORDING TO THE MACROSCOPIC LAW.

THE GOAL IS TO SHOW THAT THE LEBESQUE MEASURE OF $\Omega_0 \setminus \overline{\Omega_0}$ IS SMALL FOR N LARGE.

THIS IS A LAW OF LARGE NUMBER TYPE OF RESULT. F IS LIKE AN AVERAGE OF MANY MORE OR LESS INDEPENDENT RANDOM VARIABLES ;
IT TAKES A CONSTANT VALUE “ALMOST EVERYWHERE”.
THE “GOOD” CONFIGURATIONS ARE SOMETIMES CALLED “TYPICAL”.

WHY LEBESGUE MEASURE ? $\longrightarrow$INDIFFERENCE PRINCIPLE (LAPLACE).

Misleading ‘solution’

Appeal to ergodicity

(Almost) every trajectory in the ‘big’ phase space Ω will spend in each region of that space a fraction of time proportional to its ‘size’ (i.e. Lebesgue volume).

Shows too much and too little !

Too much : we are not interested in the time spent in every tiny region of the phase space Ω !

Too little : ergodicity, by itself says nothing about time scales. We want the *macroscopic* quantities (and only them !) to 'reach equilibrium' reasonably fast.

DOES THIS EXPLAIN

IRREVERSIBILITY

AND THE SECOND LAW ?

WHAT DO YOU MEAN BY “EXPLAIN”?

IN A DETERMINISTIC FRAMEWORK :

IF THE LAWS IMPLY THAT A STATE A AT TIME ZERO YIELDS A STATE B AT TIME T,

THEN B AT TIME T IS "EXPLAINED" BY THE LAWS AND BY A AT TIME ZERO.

OF COURSE, IT REMAINS TO EXPLAIN A.

IN A PROBABILISTIC FRAMEWORK :

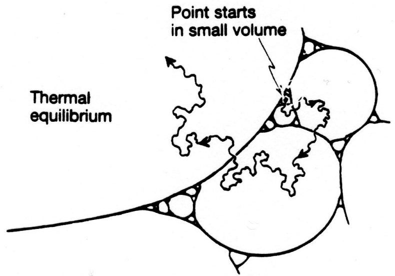
IF F_0 IS A MACROSTATE AT TIME ZERO, THEN THERE IS A "NATURAL" MEASURE (HERE THE LEBESGUE MEASURE; IN GENERAL, THE ONE WITH MAXIMAL ENTROPY) ON THE CORRESPONDING SET $F^{-1}(F_0)$ OF MICROSTATES $\mathbf{x}_0$.

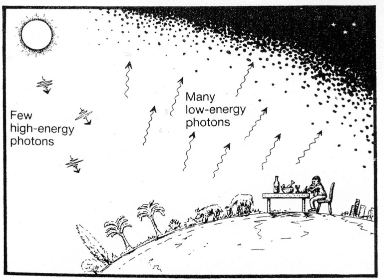
IF, WITH LARGE PROBABILITY WITH RESPECT TO THAT MEASURE, THE MACROSTATE $F(\mathbf{x}_t)$ OBTAINED FROM THE EVOLUTION OF THE MICROSTATE $\mathbf{x}_t$ EQUALS F_t, THEN F_0 AND THE LAWS "EXPLAIN" F_t.

ANOTHER WAY TO SAY THIS, IS THAT ONE EXPLAINS F_t, IF, BY A BAYESIAN REASONING, ONE WOULD HAVE PREDICTED F_t, KNOWING ONLY F_0 AT TIME 0.

REAL PROBLEM

ORIGIN of the LOW ENTROPY STATES





The sun and the cycle of life

" God " choosing the initial conditions of the universe, in a volume of size $10^{-10^{123}}$ of the total volume (according to R. Penrose).
There is no good answer to *that* problem.

WHAT ABOUT QUANTUM PROBABILITIES ?

We can either regard them as a *deus ex machina* or consider them as arising from a deeper deterministic theory.

(We are NOT talking here about probability distributions on quantum states ; that is more or less similar to classical probabilities).

We are interested in the probabilistic meaning of quantum states.

The deterministic theory cannot be ordinary quantum mechanics, even though the time evolution of the quantum state is deterministic (OUTSIDE OF MEASUREMENTS), since the quantum state only determines probabilities (OF RESULTS OF MEASUREMENTS).

Moreover, ordinary quantum mechanics only speaks of *probabilities of results of measurements* and is silent about what goes on outside of laboratories.

To tell something about what goes on outside of laboratories and to "explain" the origin of probabilities, we need a theory that goes beyond ordinary quantum mechanics.

THE DE BROGLIE-BOHM THEORY

In the de Broglie-Bohm's theory, the state of system is a pair $(\mathbf{X}, \Psi)$, where $\mathbf{X} = (X_1, \ldots, X_N)$ denotes the actual positions of all the particles in the system under consideration, and $\Psi = \Psi(x_1, \ldots, x_N)$ is the usual quantum state.

The dynamics of the de Broglie-Bohm's theory is as follows : both objects Ψ and $\mathbf{X}$ evolve in time :

1. SCHRÖDINGER'S EQUATION : for the quantum state, at all times, and whether one measures something or not

$\Psi_0 \to \Psi_t = U(t)\Psi_0$

$i\hbar\partial_t\Psi(x_1, \ldots, x_N, t) = (H\Psi)(x_1, \ldots, x_N)$

$\mathcal{H} = -\frac{1}{2}\Delta + V$ where H is the Hamiltonian and V the potential.

THE QUANTUM STATE NEVER COLLAPSES.

2. PILOT EQUATION The evolution of the positions is guided by the quantum state : writing $\Psi = Re^{iS}$

$$\dot{X}_k(t) = \frac{\hbar}{m_k} \nabla_k S(X_1(t), \ldots, X_N(t))$$

for $k = 1, \ldots, N$, where $X_1(t), \ldots, X_N(t)$ are the actual positions of the particles at time t.

Double slit experiment : numerical solution in the de Broglie-Bohm theory.

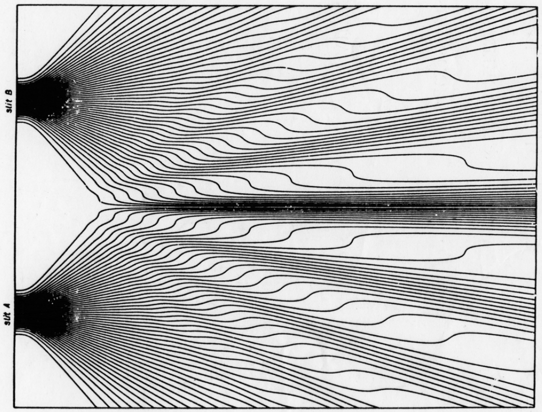


Figure 9.3 Trajectories for two Gaussian slits with a Gaussian distribution of initial positions at the slits.

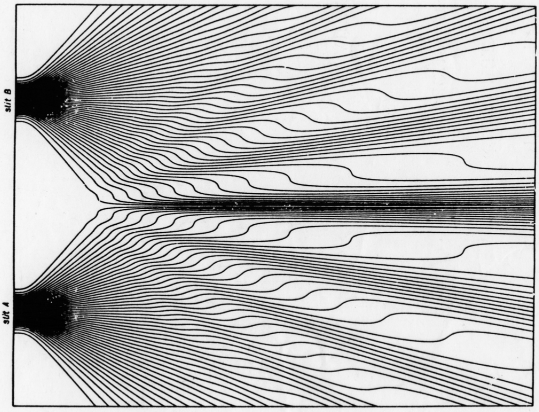
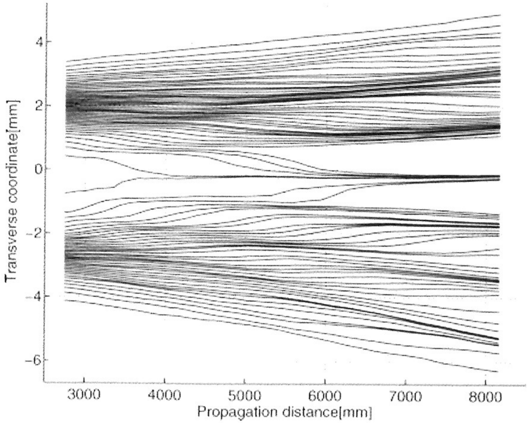


Figure 9.3 Trajectories for two Gaussian slits with a Gaussian distribution of initial positions at the slits.

Motion *in vacuum* highly *non classical*!!

Note that one can determine a posteriori through which hole the particle went!

Experiment-indirect, “weak” measurement (Science, june 2011).



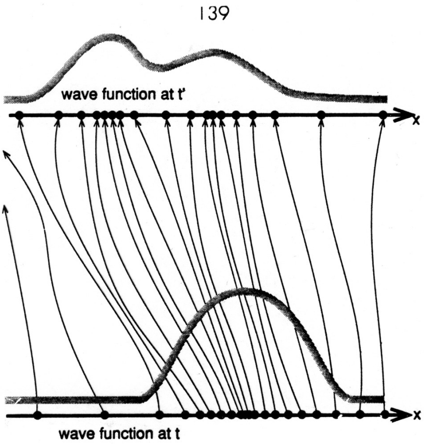
It is not clear from the smallness of the scintillation on the screen that we have to do with a particle? And is it not clear, from the diffraction and interference patterns, that the motion of the particle is directed by a wave? De Broglie showed in detail how the motion of a particle, passing through just one of two holes in the screen, could be influenced by waves propagating through both holes.

And so influenced that the particle does not go where the waves cancel out, but is attracted to where they cooperate. This idea seems to me so natural and simple, to resolve the wave-particle dilemma in such a clear and ordinary way, that it is a great mystery to me that it was so generally ignored.

J. BELL

HOW DOES THE THEORY OF DE BROGLIE-BOHM ACCOUNT FOR THE STATISTICAL PREDICTIONS OF QUANTUM MECHANICS ?

THANKS TO EQUIVARIANCE :



We have $t' > t$.
With $\rho_t = |\Psi_t|^2 \to \rho_{t'} = |\Psi_{t'}|^2$
where $\Psi_{t'}$ comes from Schrödinger's equation
$i\hbar\partial_t\Psi = \mathcal{H}\Psi$
and $\rho_{t'}$ from the pilot equation $(m_k = 1,$
$\hbar = 1)$
$\dot{X}_k = \nabla_k S$, with $\Psi = Re^{iS}$.

SO, IF WE ASSUME THAT $\rho_{t_0} = |\Psi_0|^2$ AT SOME INITIAL TIME t_0, IT WILL HOLD AT ALL TIMES $t > t_0$.
THE STATISTICAL PREDICTIONS OF QUANTUM MECHANICS ARE RECOVERED, AT LEAST AS FAR AS POSITIONS OF PARTICLES ARE CONCERNED.

WHAT ABOUT OTHER "OBSERVABLES". CONSIDER THE SPIN FOR EXAMPLE :

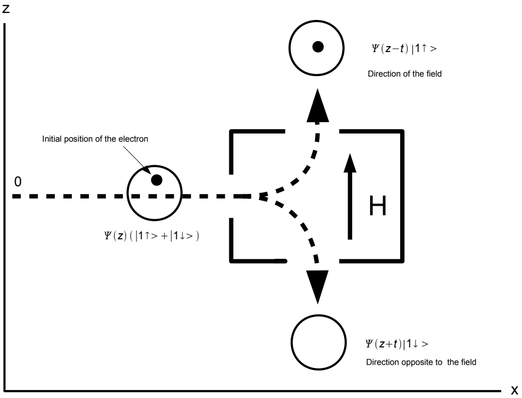
Consider a quantum state of the form

$$\Psi(z)\big(c_1|1\uparrow\rangle + c_2|1\downarrow\rangle\big) \ ,$$

with $|c_1|^2 + |c_2|^2 = 1$ and $\int |\Psi(z)|^2 dz = 1$. Consider an ensemble of particles distributed at the initial time according to the empirical density distribution $\rho(z) = |\Psi(z)|^2$.

We get from Schrödinger's equation

$$\Psi(z-t)c_1|1\uparrow\rangle + \Psi(z+t)c_2|1\downarrow\rangle \ ,$$



And, by equivariance, the empirical density distribution of the particle positions will be given by $|\Psi(z-t)c_1|^2 + |\Psi(z+t)c_2|^2$. Thus, equivariance implies that a fraction approximately equal to $|c_1|^2$ of the particles will go upwards and a fraction approximately equal to $|c_2|^2$ of them will go downwards, so that the usual quantum predictions ("Born's rule") are recovered in the de Broglie–Bohm theory.

THE SAME HOLDS FOR ALL "OBSERVABLES".
THE ASSUMPTION THAT $\rho_0 = |\Psi_0|^2$ IS CALLED QUANTUM EQUILIBRIUM.
HOW CAN IT BE JUSTIFIED ?

Through a Law of Large Numbers argument : consider N independent quantum systems with the same wave-function $\psi(x_i)$, $i = 1, \ldots, N$.

Then, the wave-function of the “Universe” (composed of those N systems) is : $\Psi(x_1, \ldots, x_N) = \prod_{i=1}^{N} \psi(x_i)$.

In Quantum Equilibrium, the distribution of $X_1, \ldots, X_N$ is $|\Psi(X_1, \ldots, X_N)|^2 = \prod_{i=1}^{N} |\psi(X_i)|^2$.
So, the variables $X_1, \ldots, X_N$ are independent random variables with identical distribution $|\psi(X)|^2$.

So, by the Law of Large Numbers, the vast majority of configurations $X_1, \ldots, X_N$ (relative to the measure $|\Psi(X_1, \ldots, X_N)|^2 \prod_{i=1}^{N} dX_i$) will yield an "empirical density" $\rho(x) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - X_i)$ approximately (namely, if it is "smoothed") equal to $|\psi(x)|^2$.

IMPORTANT REMARK :

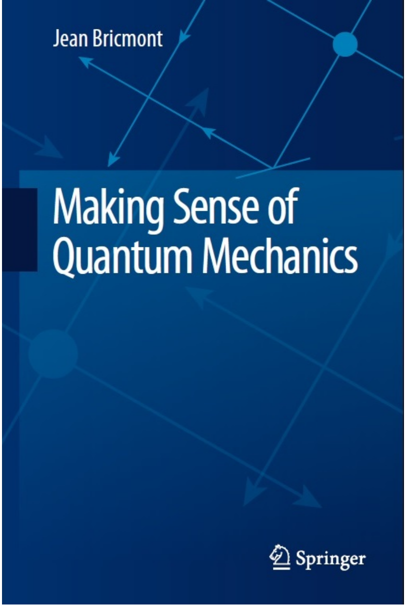
Since we have no evidence of a non-(quantum) equilibrium situation, we may assume that the world started in Quantum Equilibrium.

No need to invoke special initial conditions, as we have to do classically to account for a non-equilibrium world.

So, in some ways, Classical and Quantum Equilibrium are similar :
In both cases, one appeals to the Law of Large Numbers (or typicality) to account for observed statistical regularities.

BUT the initial measure is different and its justification is different also.
In the classical case, one appeals to the indifference principle, but the initial macro-state is "mysterious".
In the quantum case, one appeals to equivariance.

The quantum case is in some sense, easier or more natural, since we do not have to "explain" the occurrence of extremely improbable initial conditions, and there is no need to prove convergence to equilibrium.
BUT the quantum equilibrium has consequences for the limits of our knowledge (for example, Heisenberg's uncertainty relations).


Jean Bricmont
Making Sense of
Quantum Mechanics
Springer