

Time Evolution and Stationary States of Macroscopic Systems: Classical and Quantum

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The modern search for a quantitative microscopic theory of macroscopic phenomena dates to the middle of the nineteenth century. At that time the experiments of Joule and others made it clear that phenomena like boiling and freezing, heat conduction, diffusion, etc., have their origins in the dynamics of the atoms and molecules which are the constituents of matter.

It was also soon recognized that the large disparity in the spatial and temporal scales between the world of atoms and the world of macroscopic experience not only necessitated a statistical theory but also assured, in analogy to the law of large numbers in probability theory, that such a theory will give predictions precise enough to have the force of "law", as in Fourier's law or in the second law of thermodynamics

The twentieth century saw the development of the subject into a physically very successful and mathematically very beautiful theory of statistical mechanics of systems in thermal equilibrium. Statistical mechanics explains how cooperative behavior of the atoms gives rise to emergent phenomena such as phase transitions.

The development of a comparable theory for the more complex world of nonequilibrium phenomena, including in particular those occurring in biological systems, remains a challenge for the twenty-first century. This will require “cooperative behavior” between physicists, mathematicians, biologists,

Microstates: classical

The complete microscopic (or micro) state of an isolated classical system of N point particles of unit mass is specified at any time t by a point X in its phase space Γ ,

$$X = (\mathbf{r}_1, \mathbf{v}_1, \dots, \mathbf{r}_N, \mathbf{v}_N), \quad \mathbf{r}_i \in \mathbf{V} \subset \mathbb{R}^d, \quad \mathbf{v}_i \in \mathbb{R}^d.$$

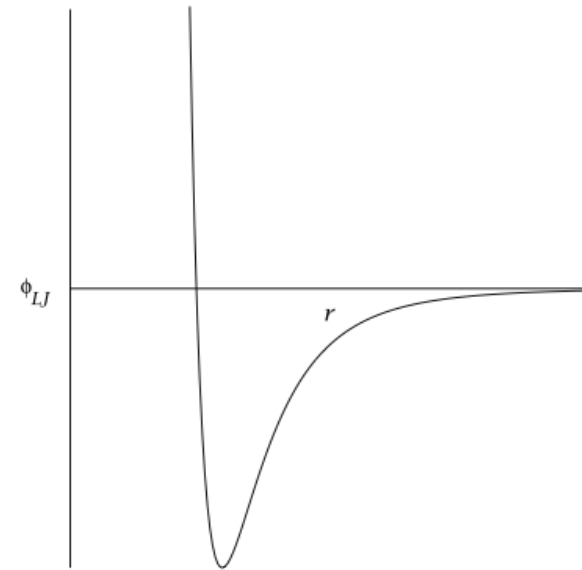
Given an X at some time t_0 , the microstate at any other time $t \in \mathbb{R}$, $X(t)$, is given (as long as the system stays isolated) by the Hamiltonian evolution which takes place on an energy surface, Γ_E , specified by $H(X) = E$.

A typical (effective, non-relativistic) Hamiltonian for a simple fluid, say Argon, has the form

$$H(X) = \frac{1}{2} \sum v_i^2 + \frac{1}{2} \sum_{i \neq j} \phi(\mathbf{r}_{ij}).$$

A representative interaction is given by the Lennard-Jones potential

$$\phi_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right].$$



The equations of motion

$$\dot{\mathbf{r}}_i(t) = \mathbf{v}_i(t), \quad \dot{\mathbf{v}}_i(t) = - \sum_{j \neq i} \frac{\partial}{\partial \mathbf{r}_i} \phi(\mathbf{r}_{ij}),$$

with appropriate boundary conditions on ∂V preserve the energy and the projection of the Liouville volume, $d\Gamma = \prod d\mathbf{r}_i d\mathbf{v}_i$, on Γ_E .

Macrostates

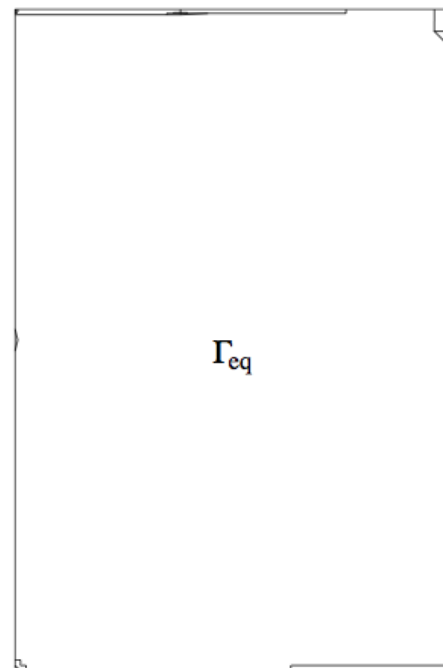
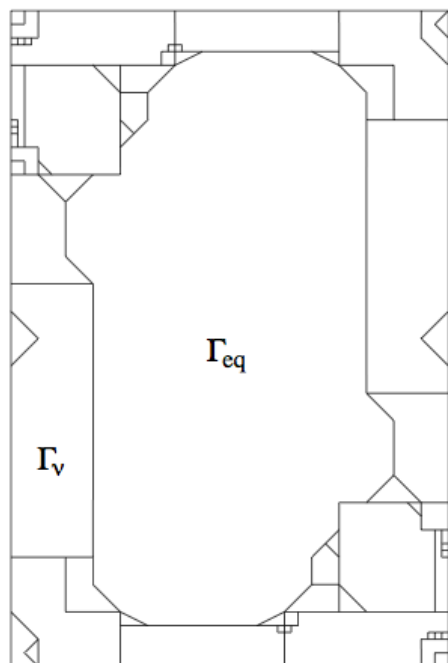
To describe the macroscopic state of a system of N atoms in a box V , say $N \gtrsim 10^{20}$, we make use of a much cruder description than that provided by the microstate X . We shall denote by M such a macroscopic description of a macrostate. As an example we may divide V into K cells, where K is large but still $K \ll N$, and specify the number of particles, the momentum and the amount of energy in each cell, with some tolerance.

Clearly there are many X 's (in fact a continuum) which correspond to the same M . Let Γ_M be the region in Γ_E consisting of all microstates X corresponding to a given macrostate M and denote by $|\Gamma_M|$ its Liouville volume projected on Γ_E . Since we are dealing with macroscopic systems, we should actually think of Γ_E as an energy shell of thickness $\delta E \ll E$.

For N large enough and any reasonable choice of M 's, there exists an equilibrium macrostate, M_{eq} , for which $|\Gamma_{M_{eq}}| \sim |\Gamma_E|$, the volume of the whole energy shell. When M specifies a nonequilibrium state, $|\Gamma_M|$ is much smaller. Thus if a dilute gas contains N atoms in a volume V then the ratio of $|\Gamma_{M_{eq}}|$ for the macrostate M_{eq} in which there are $(\frac{1}{2} \pm 10^{-10})N$ particles in the left half of the box to $|\Gamma_M|$, corresponding to a macrostate M in which all the particles are in the left half, is of order 2^N . The result is similar if we use $K \ll N$ boxes. We will still have that for N large enough $|\Gamma_{M_{eq}}| \sim |\Gamma_E|$. In fact, we expect that

$$\frac{|\Gamma_E \setminus \Gamma_{M_{eq}}|}{|\Gamma_E|} \sim e^{-cN}.$$

Pictorially



The second picture is slightly more faithful. Neither shows the topology or differences in relative sizes of the different Γ_M 's.

The fact that $|\Gamma_{eq}| \sim |\Gamma_E|$ explains why typical properties of macroscopic equilibrium systems, i.e. those true for almost all $X \in \Gamma_{eq}$, are also typical for all $X \in \Gamma_E$ and can thus be obtained from the microcanonical ensemble. N.B. We did not have to invoke ergodicity to justify use of the microcanonical ensemble.

Approach to Equilibrium

Boltzmann (also Maxwell, Kelvin, ...) argued that given this disparity in the sizes of the Γ_M corresponding to the various macrostates, the evolution of a typical microstate X specified to be at $t = t_0$ in the phase space region Γ_M , will be such that $|\Gamma_{M(X(t))}|$ will increase for $t > t_0$ in a way which *explains* and describes the evolution towards equilibrium of macroscopic systems which start in the macrostate Γ_M , $M \neq M_{eq}$, and are kept (effectively) isolated afterwards.

Typical here means that for any Γ_M the relative volume of the set of microstates X in Γ_M for which this is false during some time period τ during which the macrostate undergoes a macroscopically noticeable change, but no bigger than the age of the universe, goes to zero exponentially in the number of atoms in the system.

Boltzmann's Entropy

To make a connection with the Second Law of Thermodynamics, enunciated by Clausius in 1855, Boltzmann defined the entropy of a macroscopic system in a microstate X as

$$S_B(X) = k \log |\Gamma_{M(X)}| = S_B(M)$$

and showed that (for a dilute gas) in an equilibrium macrostate M_{eq} , $S_B(M_{eq})$ is proportional to the thermodynamic entropy of Clausius. Following O. Penrose, I shall call $k \log |\Gamma_M(X)|$ the Boltzmann entropy of a system in the macrostate $M(X)$.

Thus calling $S(E) = k \log |\Gamma_E|$, we have the Boltzmann-Einstein formula

$$\text{Prob}(X \in \Gamma_M) \sim e^{-[S(E) - S_B(M)]} \sim e^{-[S_{eq} - S_B(M)]} \sim e^{-N\delta_M}$$

i.e., δ_M is a large deviation function (LDF) for macrostates M in the microcanonical measure.

The above heuristic argument, based on relative phase space volume, is a “believable” (and correct) explanation for the behavior observed in actual macroscopic systems. It is, however, very far from a mathematical theorem which, as Mark Kac would say, is what is necessary to convince a skeptic. (It also contains no quantitative information about time scales.)

Such a theorem would “derive” macroscopic equations to describe the time evolution of macrostates, e.g. of the hydrodynamic density profile $\xi_{X(t)}(\mathbf{x}) = (n(\mathbf{x}, t), \mathbf{u}(\mathbf{x}, t), e(\mathbf{x}, t))$, $\mathbf{x} \in V$ from the dynamics of the microstates $X(t)$. These would vary on a macroscopic space-time scale due to the local conservation laws. The derivation of such time evolution equations is a (possibly the) central open problem of nonequilibrium statistical mechanics. It is mathematically a very difficult problem already in the classical domain, let alone in the quantum one.

The best result so far is the derivation of the Euler Equations by Olla, Varadhan, and Yau in 1993. They had to cheat a bit, adding some noise and making some technical adjustment to the dynamics which however disappeared from the final equations. The derivation of Navier-Stokes equations appears to be out of sight (but not out of mind).

There is also the example of the dilute gas where Lanford proved the validity of the Boltzmann Equation in the Boltzmann-Grad Limit — at least for short times, and the (degenerate) case of point particles moving in a 2-D periodic array of convex scatterers — the Sinai Billiards — for which Bunimovich, Chernov, and Sinai proved diffusive behavior — but that is about it, as far as rigorous derivations of macroscopic equations from microscopic ones for an isolated system.

Lyapunov Function for Isolated System

We can say a bit more mathematically if we suppose (assume) that the time evolution of the macrostate M , given by M_t satisfies an autonomous deterministic equation, such as the Navier-Stokes equation or the Boltzmann equation. This means that if $M_{t_1} \rightarrow M_{t_2}$, then the microscopic dynamics Φ_t carries $\Gamma_{M_{t_1}}$ inside $\Gamma_{M_{t_2}}$, i.e. $\Phi_{t_2-t_1}\Gamma_{M_{t_1}} \subset \Gamma_{M_{t_2}}$ with negligible error. The fact that phase space volume is conserved by the Hamiltonian time evolution implies that $|\Gamma_{M_{t_1}}| \leq |\Gamma_{M_{t_2}}|$ and thus that $S_B(M_{t_2}) \geq S_B(M_{t_1})$ for $t_2 \geq t_1$. Boltzmann's argument then becomes rigorous.

We have thus derived an “ \mathcal{H} -theorem” or Lyapunov function for any deterministic evolution of the macro-variables arising from the microscopic dynamics of an isolated Hamiltonian system.

N.B. Even if there is no deterministic equation for M_t we can still expect it to be true that for any sequence of macrostates in an isolated system M_{t_i} , $S_B(M_{t_l}) \geq S_B(M_{t_k})$ for $t_l > t_k$, i.e. the second law.

Example: For spatially uniform equilibrium systems the thermodynamic entropy is extensive

$$S(E, \mathbf{N}, V) = |V|s(e, \mathbf{n}).$$

$s(e, \cdot)$ is a concave function of e .

$$\frac{\partial s}{\partial e} = \frac{1}{T}, \quad \frac{\partial}{\partial e} \left(\frac{1}{T} \right) = -\left(\frac{1}{T^2} \right) \frac{\partial T}{\partial e} \leq 0.$$

For systems in “local thermal equilibrium” (LTE) with local velocity field $\mathbf{u}(\mathbf{x})$, the Boltzmann entropy

$$\begin{aligned} S_B(n, \mathbf{u}, e) &= \int_V s(e(\mathbf{x}) - \frac{1}{2}mn(\mathbf{x})\mathbf{u}^2(\mathbf{x}), n(\mathbf{x}))d\mathbf{x} \\ &= S_{l.e} \end{aligned}$$

where $S_{l.e}$ is the local equilibrium (hydrodynamic) entropy.

Consider now an isolated system in LTE (with $\mathbf{u} = 0$ and n constant) in a region V with boundary Σ and an energy density profile $e(\mathbf{x})$ satisfying the macroscopic conservation law

$$\frac{\partial e}{\partial t} = -\nabla \cdot \mathbf{J}$$

where \mathbf{J} is the heat flux. Assume that \mathbf{J} is given by Fourier's law,

$$\mathbf{J} = -\kappa \nabla T, \quad \kappa(T : \mathbf{x}) \geq 0, \text{ a tensor}$$

We then have a deterministic evolution for the macrostate $M = \{e(\mathbf{x})\}$.

Computing the change in S_B :

$$\begin{aligned} \frac{dS_{l.e}}{dt} &= \frac{d}{dt} \int_V s d\mathbf{x} = - \int_V \frac{1}{T} (\nabla \cdot \mathbf{J}) d\mathbf{x} \\ &= - \int_{\Sigma} \frac{1}{T} \mathbf{J} \cdot d\Sigma + \int_V \mathbf{J} \cdot \left(\nabla \frac{1}{T} \right) d\mathbf{x} = \int_V \left(\frac{1}{T^2} \right) \nabla T \cdot \kappa \cdot \nabla T d\mathbf{x}, \end{aligned}$$

since for the isolated system $\mathbf{J} \cdot d\Sigma = 0$. This satisfies the second law iff $\kappa \geq 0$.

Warning: Do not buy any material claiming to have a negative heat conductivity.

We have thus shown that $S_B = S_{l.e}$ is indeed a Lyapunov functional for the heat equation with Neumann (no flux) or periodic boundary conditions

$$\frac{\partial e(\mathbf{x}, t)}{\partial t} = \nabla \cdot [\mathbf{D}\nabla e], \quad \mathbf{D} = \kappa \partial T / \partial e = \mathbf{D}(T : \mathbf{x}) \geq 0$$

Note: If there is more than one system having the same \mathbf{D} but different $s(e)$ we can use any of them as Lyapunov functions. In fact for the heat equation with Neumann or periodic boundary conditions, any concave function of e is a Lyapunov function.

This is useful for certain non-linear diffusion equations with non-uniform Dirichlet b.c. where the stationary state is one with currents. The entropy is then no longer a Lyapunov function, but the LDF computed from the zero range process does serve as a Lyapunov functional.

Going Beyond LTE: Dilute Gases

It is clear that the choice of the macro-variables M is essential for the computation of $S_B(X)$. For systems in LTE, those are specified by the locally conserved and hence microscopically slowly varying quantities—precisely those for which one has hydrodynamic type autonomous equations. For systems not in LTE one has to find appropriate macro-variables M for the system under consideration: if possible those which satisfy autonomous time evolution equations.

Following Boltzmann, we refine the thermodynamic M used for systems in LTE by noting that the microstate $X = \{\mathbf{r}_i, \mathbf{v}_i\}$, $i = 1, \dots, N$, can be considered as a set of N points in six dimensional μ -space. We then divide up this μ -space into \tilde{J} cells $\tilde{\Delta}_\alpha$, centered on $(\mathbf{r}_\alpha, \mathbf{v}_\alpha)$, of volume $|\tilde{\Delta}_\alpha|$. A macrostate \tilde{M} is then specified by the (coarse grained) number of particles in each $\tilde{\Delta}_\alpha$,

$$\tilde{M} = \{N_\alpha\}, \quad \alpha = 1, \dots, \tilde{J} \ll N.$$

For dilute gases one can *neglect*, for typical configurations, the existence of interactions between the particles. The coarse grained energy of the system in the state \tilde{M} is given by

$$\frac{1}{2}m \sum_{\alpha} N_{\alpha} v_{\alpha}^2 = E$$

$$\sum N_{\alpha} = N$$

The phase space volume associated with such an \tilde{M} is then readily computed to be

$$|\Gamma_{\tilde{M}}| = \prod_{\alpha} (N_{\alpha}!)^{-1} |\tilde{\Delta}_{\alpha}|^{N_{\alpha}}$$

Stirling's formula gives

$$S_B(\tilde{M}) \sim -k \left\{ \sum_{\alpha} \left(\frac{N_{\alpha}}{|\tilde{\Delta}_{\alpha}|} \log \frac{N_{\alpha}}{|\tilde{\Delta}_{\alpha}|} \right) |\tilde{\Delta}_{\alpha}| - N \right\}.$$

Using \widetilde{M} we can associate with a typical X a coarse grained density $f_X \sim N_\alpha/|\widetilde{\Delta}_\alpha|$ in μ -space, i.e. such that $N_\alpha = \int_{\widetilde{\Delta}_\alpha} d\mathbf{x}d\mathbf{v}f_X(\mathbf{x}, \mathbf{v})$. The Boltzmann entropy is then given by

$$S_B(X) = S_{\text{gas}}(f) = -k \int_V d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{v} f(\mathbf{x}, \mathbf{v}) \log f(\mathbf{x}, \mathbf{v})$$

The maximum of $S_{\text{gas}}(f)$ over all f which satisfy the constraints,

$$\int_V d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{v} f(\mathbf{x}, \mathbf{v}) = N$$

$$\int_V d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{v} \frac{1}{2} m \mathbf{v}^2 f(\mathbf{x}, \mathbf{v}) = E$$

is given by the equilibrium distribution

$$f_{eq} = \frac{N}{V} (2\pi kT/m)^{-3/2} \exp[-m\mathbf{v}^2/2kT]$$

where $kT = 2/3(E/N)$.

In this case S_B coincides with the Clausius entropy

$$S_{\text{gas}}(f_{eq}) = S(E, N, V) = Nk \left[\frac{3}{2} \log T - \log(N/V) + \text{Const.} \right]$$

When $f \neq f_{eq}$ then f and consequently $S_{\text{gas}}(f)$ will change in time. The second law, now says that for *typical* $X \in \Gamma_{\tilde{M}}$ at the initial time $t = 0$, will have an $\tilde{M}_t = \tilde{M}(X_t)$ such that $S_B(\tilde{M}(X_t)) \geq S_B(\tilde{M}(X_{t'}))$, for $t \geq t'$. This means that $S_{\text{gas}}(f_t) \geq S_{\text{gas}}(f_{t'})$, for $t \geq t'$. This is exactly what happens for a dilute gas described by the Boltzmann equation for which

$$\frac{d}{dt} S_{\text{gas}}(f_t) \geq 0, \text{ Boltzmann's } \mathcal{H}\text{-theorem}$$

i.e. $S_{\text{gas}}(f)$ (the LDF for the \tilde{M} in the microcanonical ensemble) is a Lyapunov function.

As put by Boltzmann: “In one respect we have even generalized the entropy principle here, in that we have been able to define the entropy in a gas that is not in a stationary state”.

Quantum systems: microstates

Let me turn now to the quantum world, which is, to the best of our knowledge, the world we live in. The first question to answer is: what takes the place of the point $X \in \Gamma$ as the microstate of a macroscopic system?

Sad to say there is not, at the present time (almost a century after the Bohr atom), a satisfying generally accepted answer to this question. What "everyone" does agree on is that the wave function Ψ , $\Psi \in \mathcal{H}$, the Hilbert space of the system, is an important ingredient of the microstate. Let us assume for the present that Ψ is a sufficiently good description, i.e. it will give, via the usual rules, the properties of our isolated system.

Macrostates: quantum

The next question then is: what takes the place of the $\Gamma_M \subset \Gamma$. The answer, as given by von Neumann, is to first "round" the operators corresponding to the macro variables so they all commute, then let \mathcal{H}_ν be the linear subspace of \mathcal{H} specified by their simultaneous eigenvalues, ν . Thus $\Psi \in \mathcal{H}_\nu$ corresponds to the system being in the macrostate M_ν . We then have

$$\mathcal{H}_E = \bigoplus \mathcal{H}_\nu$$

with the \mathcal{H}_ν forming an orthogonal decomposition of the very large but still finite dimensional Hilbert space \mathcal{H}_E , with a basis given by the energy eigenstates $|\phi_\alpha\rangle$ with $E_\alpha \in [E, E + \delta E]$.

To what extent this “rounding” can actually be done mathematically is still an open problem. For example, for a macroscopic system of Heisenberg spins on a lattice,

$$\underline{\sigma}_a = (\sigma_i^x, \sigma_i^y, \sigma_i^z), i = 1, \dots, N,$$

how well can we find three commuting operators $m_N^\alpha, \alpha = x, y, z$, such that

$$\left\| m_N^\alpha - \frac{1}{N} \sum_i \sigma_i^\alpha \right\| \rightarrow 0$$

as $N \rightarrow \infty$ in a suitable norm? Physically, it certainly seems very reasonable that we can specify simultaneously all three spin components $\frac{1}{N} \sum_i \sigma_i^\alpha$ with arbitrary small error, $\epsilon_N \rightarrow 0$, as $N \rightarrow \infty$.

There is a very recent proof of this by a Japanese mathematical physicist but I have not read it yet.

Accepting this rounding, the orthogonal decomposition of \mathcal{H} corresponds to the classical decomposition of the energy shell Γ_E into regions Γ_M with $\Gamma_E = \cup \Gamma_M$. The analog to the Liouville volume $|\Gamma_M|$ is the dimension of \mathcal{H}_ν , denoted by $|\mathcal{H}_\nu|$. The Hamiltonian time evolution preserving Liouville volume now corresponds to the unitary evolution, obtained from the solution of the Schrödinger equation, which preserves the dimension of subspaces of \mathcal{H} .

The linear subspace, \mathcal{H}_{eq} , corresponding to the equilibrium macrostate is again (like in the classical case) characterized by the fact that its dimension is, for a macroscopic system, almost the same as the dimension of the whole (microcanonical) Hilbert space,

$$|\mathcal{H}_{eq}| \approx |\mathcal{H}_E|.$$

All other $|\mathcal{H}_\nu|$ are much, much smaller.

The analog of the Boltzmann entropy for the system with a wave function $\Psi \in \mathcal{H}_\nu$ would then be, according (more or less) to von Neumann*, given by

$$S_B(\nu) = \log |\mathcal{H}_\nu|.$$

Using this prescription, the reasoning of Boltzmann about the approach to equilibrium and the microscopic origin of the second law for classical systems goes through, essentially unchanged, also for macroscopic quantum systems.

The only "fly in the ointment" in this analysis is that while for classical systems the microstate X uniquely specifies the macrostate $M(X)$ (with possible exceptions of Lebesgue measure zero which can generally be ignored) this is no longer true in quantum mechanics:

A "typical" wave function Ψ will (in general) not be just in one linear subspace but will have projections $P_\nu|\Psi\rangle \neq 0$, for essentially all ν .

*One always talks of von Neumann's Gibbs entropy $S_G = -\text{tr}(\rho \log \rho)$ which gives zero entropy to a pure state and never of his Boltzmann entropy discussed in chapter 5 of his book Foundations of Quantum Mechanics.

Thus, giving Ψ does not uniquely specify the macrostate of the system. This is the paradox of Schrödinger's cat, where the Ψ of the cat clearly corresponds to a superposition of incompatible macrostates: one in which the cat drank the milk and one in which it did not.

My only answer to this, at the moment, is that there is always a “fact of the matter” about macrostates, i.e. of whether the cat has drunk its milk or has not. How this “fact of the matter” for macrostates is to be understood or reconciled with the autonomous Schrödinger evolution of the wave function is still very much (as far as I am concerned) an unsettled matter. I quote from J. S. Bell's talk in 1989 on the occasion of Julian Schwinger's 70th birthday celebration.

”After Einstein and Bohr the most famous person [in the foundations of quantum mechanics] is Schrödinger’s cat (Fig. 2). Now Schrödinger’s cat is a quantum cat. It is like the traditional or classical cat in that it has nine lives; but unlike the traditional classical cat it can have all of these lives at the same time. This is a consequence of the superposition principle of quantum mechanics. If a state A is possible and a state B , then a state $A + B$ is also possible, and so on. This particular cat is at the same time thin and fat - it has had supper *and* it has not had supper. Now this is not just an academic possibility - it happens all the time, and Schrödinger pointed out that it could be realized under controlled laboratory conditions.”

Schrödinger's cat 1935

QUANTUM

(empty) + (full)

CLASSICAL

A
B

A+B

Superposition
principle of QM

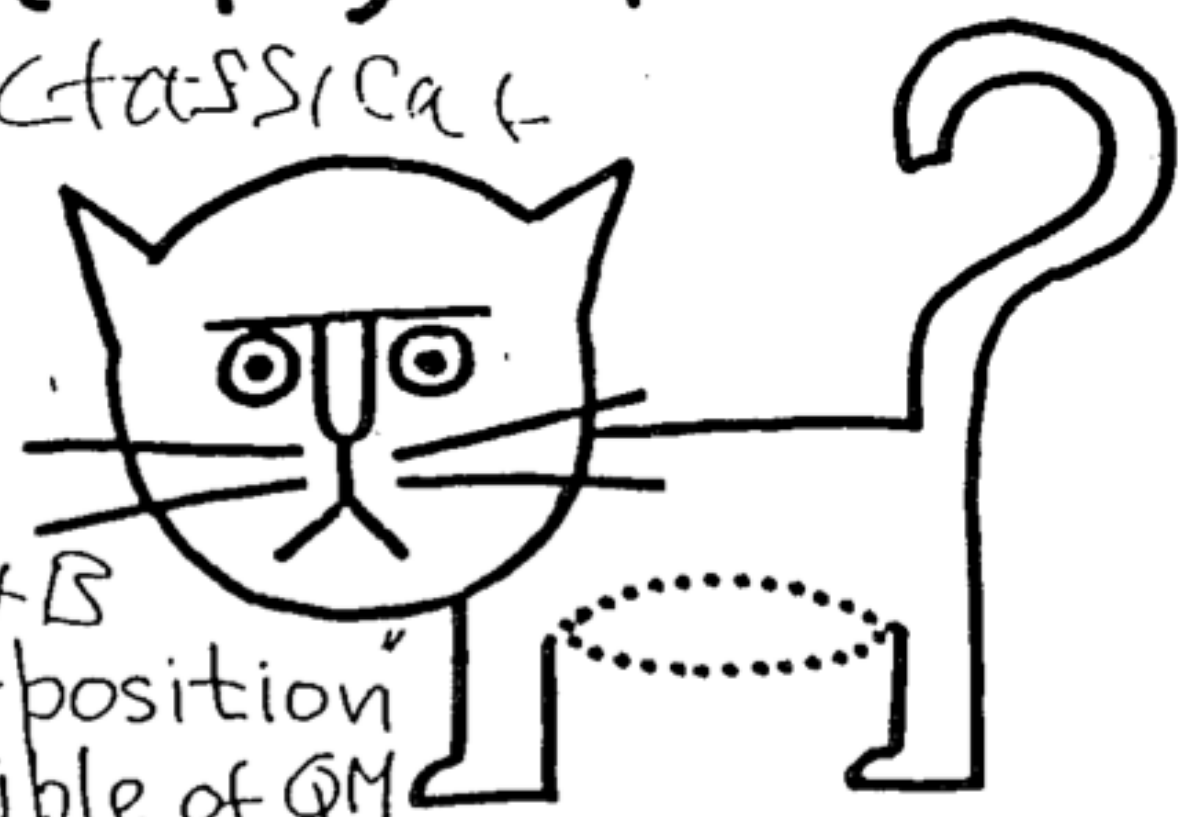


Fig. 2

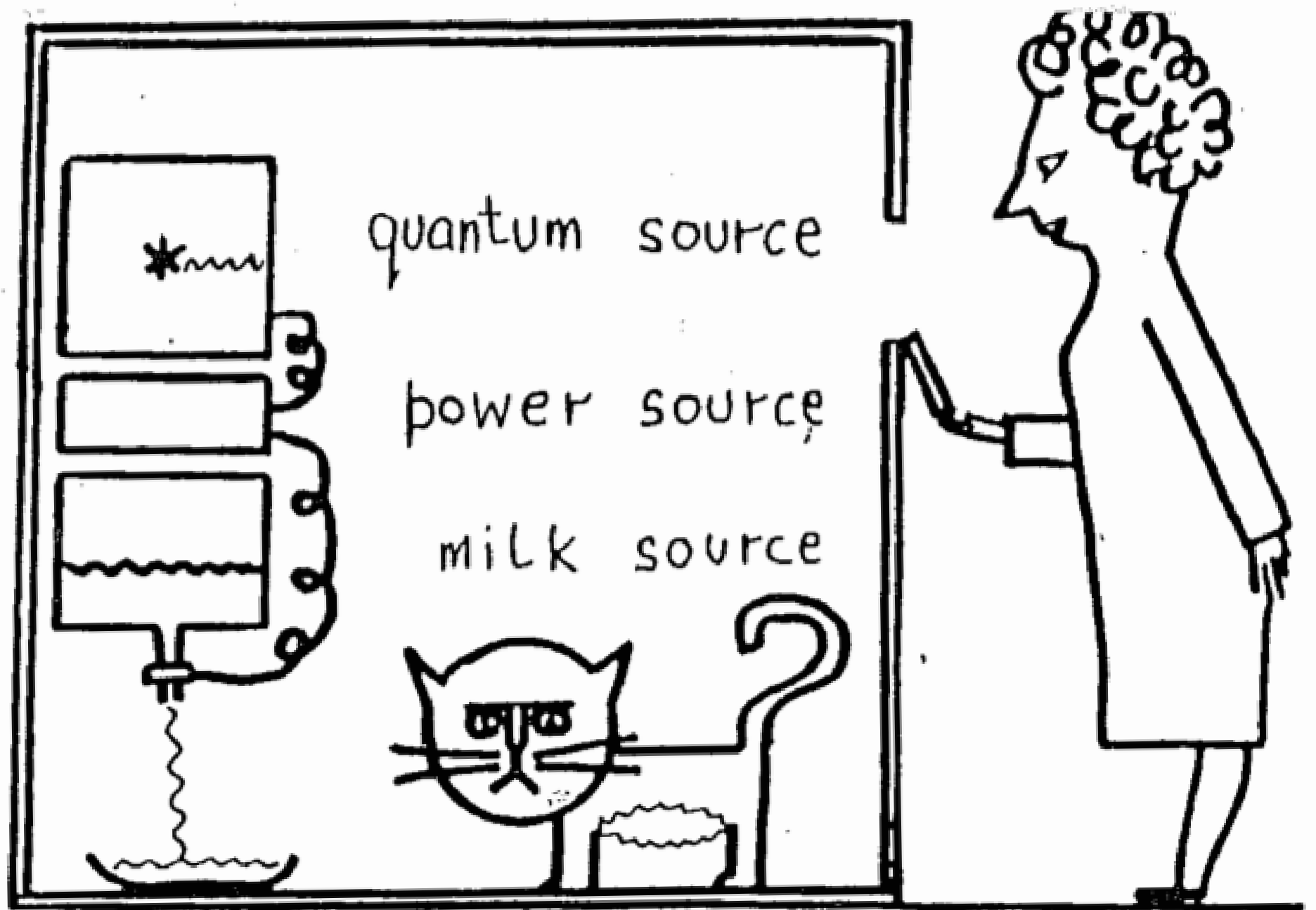


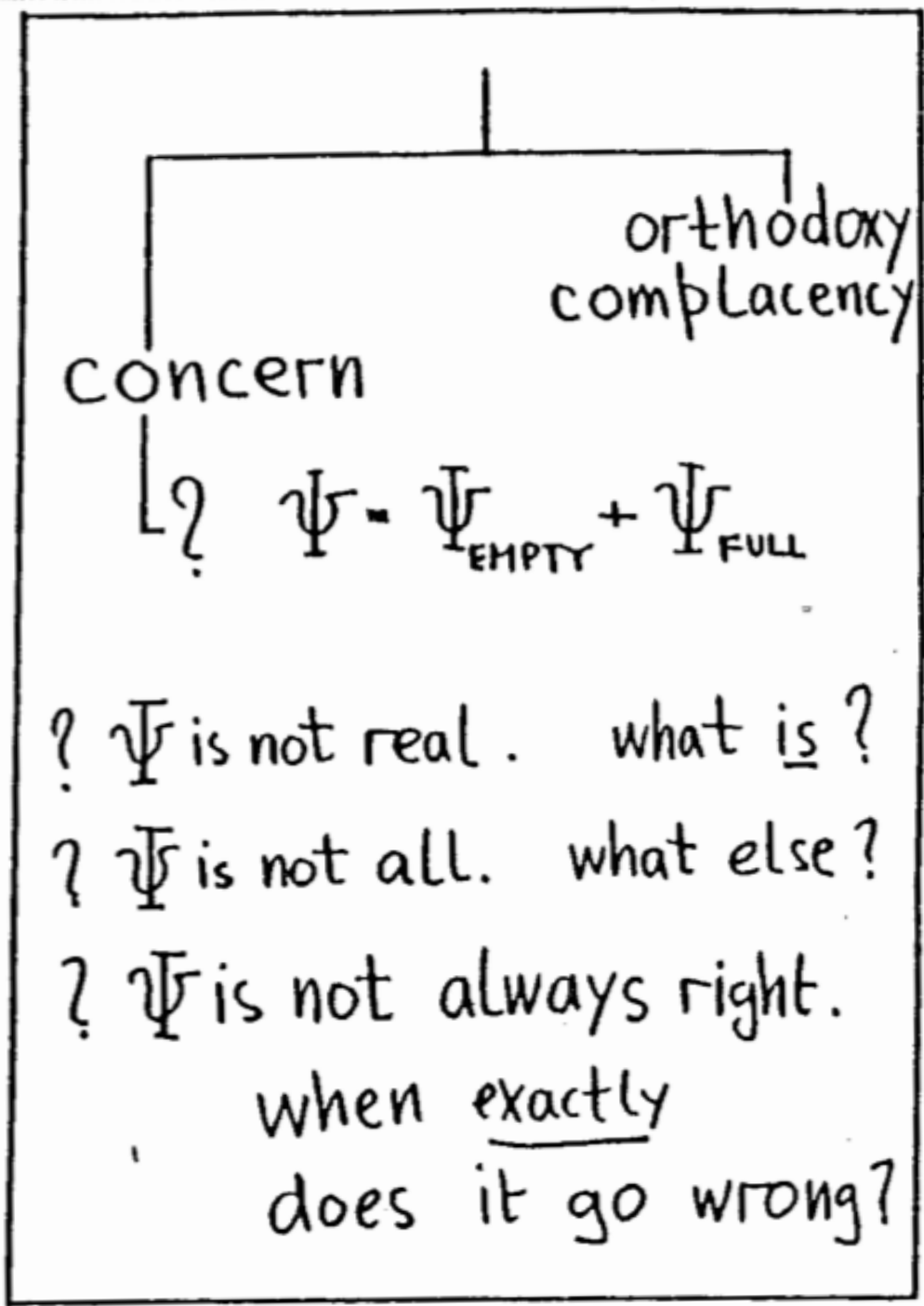
Fig. 3

Fundamental ambiguity:
Nobody knows what
quantum mechanics says
exactly about any situation.

For nobody knows where
the boundary really is,
between wavy quantum
system and the world of
particular events.

THIS IS THE PROBLEM OF QUANTUM MECHANICS

It is no problem
in practice – because
practice is not accurate
enough – and maybe never
will be.



orthodoxy
complacency

S.U.A.C.

CONCERN

? $\Psi = \Psi_{\text{EMPTY}} + \Psi_{\text{FULL}}$

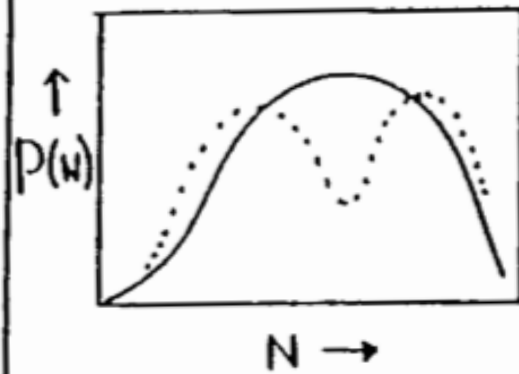
? Ψ is not real. what is?

? Ψ is not all. what else?

? Ψ is not always right.
when exactly
does it go wrong?

Fig. 7

ψ not real ? what is ?
information ? what about ?



} soldiers
} horses
} kicks

Ψ ?

} ? "allowed states"
} ? jumps

picture good only for
weakly interacting
system

Fig. 8

Ψ is not all | what else?

allowed states? jumps?

$\{\psi(t, r, \dots), x(t), \dots\}$

de Broglie Bohm 1926, 1952

x 's are particle pos

'pilot-wave picture'

$$m \dot{x}(t) = \frac{\partial}{\partial x} \ln \log \psi(t, x(t))$$

no jumps $\rho(0, x) = |\psi(0, x)|^2$

rational, clear, exact

agrees with experiment

Lorentz-invariance?

Bohmian QM: (\mathbf{Q}, ψ)

$$ih \frac{\partial \psi(q_1, \dots, q_N; t)}{\partial t} = - \sum_{k=1}^N \frac{\hbar^2}{2m_k} \nabla_k^2 \psi + V(\mathbf{q})\psi$$
$$\frac{dQ_k(t)}{dt} = \frac{\hbar}{m_k} \operatorname{Im} \frac{\nabla_k \psi(Q_1, \dots, Q_N; t)}{\psi}$$

“No one can understand this theory until (s)he is willing to think of ψ as a real objective field rather than just a ‘probability amplitude.’ Even though it propagates not in 3-space but in 3^N -space.”
... “for instantaneous macroscopic configurations the pilot-wave theory gives the same distribution [of configurations] as the orthodox theory insofar as the latter is unambiguous.”

J.S. Bell, QM for Cosmologists

I do not think that too much has changed in the basics although there is much interesting work going on, e.g. by R. Tumulka on GRW, since then. Most important the experiments are pushing us closer to having to face these questions.

[Large Quantum Superpositions and Interference of Massive Nanometer-Sized Objects](#)

O. Romero-Isart, A. C. Pflanzer, F. Blaser, R. Kaltenbaek, N. Kiesel, M. Aspelmeyer, and J. I. Cirac

[Phys. Rev. Lett. 107, 020405 \(2011\)](#)

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A fundamental feature of quantum physics is superposition of states, such as the double slit experiment in which a particle passes through both slits at the same time to interfere downstream. This kind of spatially separated quantum superposition has been observed for particles from electrons to complex molecules, but what about larger macroscopic systems?

The biggest obstacle is decoherence—preparing and measuring a superposition of so many atoms requires minimizing environmental interactions that would otherwise rapidly destroy this fragile state. Writing in *Physical Review Letters*, Oriol Romero-Isart from the Max Planck Institute for Quantum Optics in Garching, Germany, and colleagues propose a method for creating and observing quantum superpositions of objects with millions of atoms.

Romero-Isart *et al.* consider the case of a nanometer-size dielectric sphere, trapped and cooled in an optical cavity, which prepares an initially pure quantum state of the center of mass. The sphere can then be released from the first trap to enter a second cavity, in which a carefully designed laser pulse creates a superposition of the two distinct spatial positions (similar to a double slit). As the superposition evolves in time, measurement of the particle's center of mass reveals the interference pattern of the two wave functions centered at different locations. The authors note that the achievement of a large superposition of such massive objects should enable more stringent tests of quantum mechanics, especially of theories predicting a spontaneous collapse of the wave function. – *David Voss*

Anyway let me leave this open and assert that the second law of non-decrease in (Boltzmann) entropy will apply to any time sequence of macrostates with a typical Ψ_{t_1} . That is, if a system in a macrostate ν_1 at time t_1 , evolves into a macrostate ν_2 at time t_2 , $t_2 > t_1$, then the entropy cannot decrease, i.e. if

$$\langle \Psi_{t_1} | P_{\nu_1} | \Psi_{t_1} \rangle \sim 1 \quad \text{and} \quad \langle \Psi_{t_2} | P_{\nu_2} | \Psi_{t_2} \rangle > \varepsilon,$$

then

$$S_B(\nu_2) \gtrsim S_B(\nu_1), \quad \text{i.e.} \quad |\mathcal{H}_{\nu_2}| \gtrsim |\mathcal{H}_{\nu_1}|$$

where ε is a very small number, $\varepsilon \rightarrow 0$ as $N \rightarrow \infty$.

By typical here I mean with respect to some appropriate measure on wave functions, as I shall soon discuss.

I will now describe some recent work in which the difference between the classical $X \in \Gamma$ and $\Psi \in \mathcal{H}$ plays a central role.

Canonical Typicality

Consider an isolated system consisting of two parts. Call them system 1 and 2 or system and reservoir. Then,

Theorem 1. Let H be the Hamiltonian of the whole system and let the number of particles in system 1 and 2 be $N_1 \ll N_2$. Let $\mathcal{H}_E \subset \mathcal{H}_1 \otimes \mathcal{H}_2$ be an energy shell. Then for most $\Psi \in \mathcal{H}_E$ with $\|\Psi\| = 1$,

$$\rho_1^\Psi \equiv \text{tr}_2 |\Psi\rangle\langle\Psi| \approx \text{tr}_2 \rho_{mc},$$

where ρ_{mc} is the microcanonical density matrix of the whole system at energy E , i.e. equal weight to all energy eigenstates in \mathcal{H}_E .

There is no analog to this for a classical system where any subsystem of a composite system in state $X^{(1,2)}$ is also in a unique state $X^{(2)}$.

When the interaction between systems 1 and 2 is weak, $H \approx H_1 \otimes I_2 + I_1 \otimes H_2$, then, as is well known,

$$\text{tr}_2 \rho_{mc} \approx \frac{1}{Z} e^{-\beta H_1},$$

for $\beta = \beta(E) = dS_{eq}(E)/dE$.

Typicality

When I say “for most Ψ ” of the composite system, I mean with respect to a uniform measure on the unit sphere in \mathcal{H}_E . This measure on “wave functions” for a system described by a microcanonical density matrix was considered already by Schrödinger and particularly Felix Bloch. It is analogous to the microcanonical measure on Γ_E .

What about measures on Ψ for other density matrices?

GAP or Scrooge Measure

Given any density matrix there are many measures μ giving rise to that density matrix

$$\rho^\mu \equiv \int \mu(d\Psi) |\Psi\rangle\langle\Psi|.$$

We (Goldstein, L, Tumulka, Zanghi) have singled out one of these, called the GAP measure as an appropriate physical one. This measure can be characterized as follows:

Given ρ , define a Gaussian measure $\mu_G^\rho(d\Psi)$ whose covariance is ρ . Then, before projecting on the unit sphere, $\mathbb{S}(\mathcal{H})$, adjust it by multiplying $\mu_G^\rho(d\Psi)$ by $|\Psi|^2$. Then after projection $\mu_{GAP}^\rho(d\Psi)$ still has ρ as its covariance matrix.

We gave various arguments for preferring it over other measures for the same ρ , e.g. if we start with Ψ for the composite system then there is a “natural” way to associate a Ψ_1 to the subsystem whose density matrix is ρ_1^Ψ , and for most Ψ w.r.t. the uniform measure on \mathcal{H}_E , Ψ_1 will be approximately $\text{GAP}(\rho_1)$ distributed for sufficiently large $|\mathcal{H}_2|$.

Recently we found out, thanks to a referee, that $\text{GAP}(\rho)$ was discovered already in 1994 by Jozsa, Robb, and Wootters who called it the Scrooge Measure; it is, for a given ρ , the measure which will give the least reduction in the Shannon entropy, $-\sum_i p_i \log p_i$, where p_i is the probability of being in a state Ψ_i , after making an arbitrary quantum measurement on the system.

Other results, more closely related to the approach to (or at least prevalence of) equilibrium in an isolated macroscopic quantum system are two theorems, "essentially" due to von Neumann in 1929.

Theorem 2: "Approach to equilibrium."

Let $H|\phi_\alpha\rangle = E_\alpha|\phi_\alpha\rangle$ and let $|\mathcal{H}| < \infty$, $\mathcal{H}_{\text{eq}} \subset \mathcal{H}$, P_{eq} projection to \mathcal{H}_{eq} . Assume that

$$1.) \text{ the energy levels are non – degenerate,} \quad (1)$$

and

2.) "eigenstate thermalization"

$$\langle \phi_\alpha | P_{\text{eq}} | \phi_\alpha \rangle > 1 - 2\varepsilon^2 \quad \forall \alpha = 1, \dots, \dim \mathcal{H}, \quad (2)$$

then any $\Psi_0 \in \mathcal{H}$ with $\|\Psi_0\| = 1$ will, in the "long run," spend most of the time in thermal equilibrium, i.e.,

$$\liminf_{T \rightarrow \infty} \frac{1}{T} \left| \left\{ 0 < t < T : \langle \Psi_t | P_{\text{eq}} | \Psi_t \rangle > 1 - \varepsilon \right\} \right| > 1 - \varepsilon,$$

for all $\varepsilon > 0$.

Proof. (simple)

$$\text{Time average } \overline{f(t)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(t) dt$$

$$\psi_0 = \sum_{\alpha=1}^{\dim \mathcal{H}} c_\alpha |\phi_\alpha\rangle, \quad \psi_t = \sum_{\alpha=1}^{\dim \mathcal{H}} e^{-iE_\alpha t} c_\alpha |\phi_\alpha\rangle$$

$$\begin{aligned} \overline{\langle \psi_t | P_{\text{eq}} | \psi_t \rangle} &= \sum_{\alpha, \beta} \underbrace{e^{i(E_\alpha - E_\beta)t}}_{\delta_{\alpha\beta}} c_\alpha^* c_\beta \langle \phi_\alpha | P_{\text{eq}} | \phi_\beta \rangle \\ &= \sum_{\alpha} |c_\alpha|^2 \langle \phi_\alpha | P_{\text{eq}} | \phi_\alpha \rangle \end{aligned}$$

(3)

Thus, $\langle \psi_t | P_{\text{eq}} | \psi_t \rangle > 1 - \varepsilon$ for $(1 - \varepsilon)$ of the time. □

Condition (1) can be relaxed while Condition (2), "eigenstate thermalization" (Srednicki), seems very strong but it is clear that if it does not hold then there will be initial states of the isolated system, namely energy eigenstates, which are out of equilibrium and will never change.

Of course one can argue that macroscopic quantum systems are never in pure eigenstates but have initial states which do lead to thermal equilibrium (Reimann).

Be that as it may there is another theorem which says that if we consider a sufficiently large class of Hamiltonians, and give them a "uniform" weight, then "most" of them will indeed have the property of "eigenstate thermalization."

Theorem 3. Let the energy levels E_α have non-degenerate gaps, i.e. $E_\gamma - E_{\gamma'} \neq E_\delta - E_{\delta'}$. Let $\{\phi_\alpha\}$ be a "random" orthogonal basis of \mathcal{H} with uniform distribution, and let $H = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$. Then there exists a number $D_0(\varepsilon)$ such that if $\dim \mathcal{H} > D_0(\varepsilon)$ and

$$\frac{\dim \mathcal{H}_{\text{eq}}}{\dim \mathcal{H}} > 1 - \varepsilon,$$

then condition (2) is typically satisfied, i.e.,

$$\text{Prob} \left\{ \langle \phi_\alpha | P_{\text{eq}} | \phi_\alpha \rangle > 1 - 2\varepsilon \quad \forall \alpha = 1, \dots, \dim \mathcal{H} \right\} > 1 - \varepsilon.$$

Of course this is no guarantee (in fact quite unlikely) that realistic Hamiltonians $H = K + V$ are typical in this way. The theorem (a modification of the result of von Neumann in 1929) does suggest that eigenstate thermalization may be true (at least approximately) in many systems. It presumably fails in systems with quenched randomness when the eigenstates are localized.

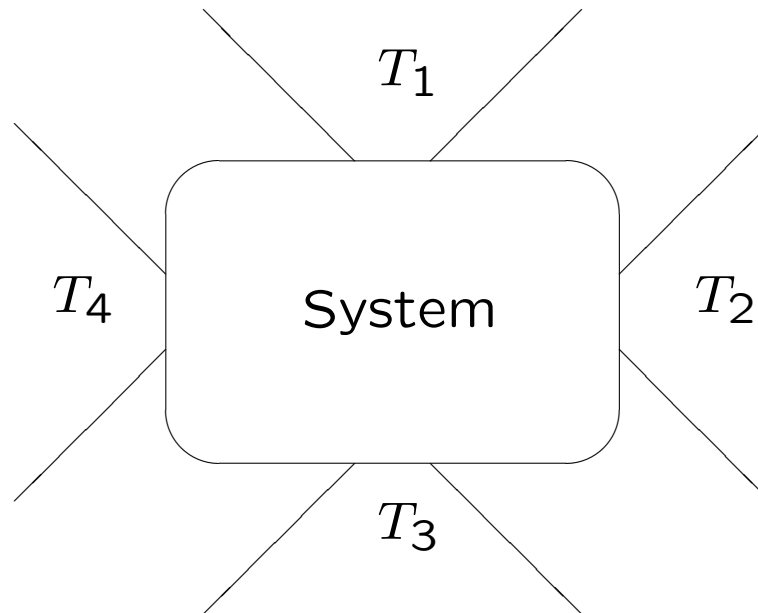
Open Systems

Consider first a classical system with Hamiltonian $H(X)$ in contact with k thermal reservoirs. It is convenient to represent the reservoirs by stochastic (boundary) terms. This is clearly an idealization: it implies in particular that there is no influence from the system on the state of the reservoirs as far as their future effect on the system goes.

The α th reservoir is at temperature $T_\alpha = \beta_\alpha^{-1}$. It acts on the system impulsively by producing “jumps” from X' to X at a rate $K_\alpha(X, X')$. The ensemble (probability) density $\mu_t(X)$ will satisfy the Markovian evolution equation

$$\frac{\partial \mu_t(X)}{\partial t} = (H, \mu_t) + \sum_\alpha \int [K_\alpha(X, X') \mu_t(X') - K_\alpha(X', X) \mu_t(X)] dX'.$$

Think of (infinite) non-interacting particle / phonon / photon reservoirs.



If there was only one reservoir at temperature T_α , then the stationary state of the system would be given by the canonical distribution

$$\mu_c \sim e^{-\beta_\alpha H(X)}.$$

Detailed balance for transitions caused by the α th reservoir then corresponds to

$$K_\alpha(X, X') = e^{-\beta_\alpha H(X)} L_\alpha(X, X'),$$

where

$$L_\alpha(X, X') = L_\alpha(X', X).$$

More generally, the requirement that

$$\int \left[K_\alpha(X, X') e^{-\beta_\alpha H(X')} - K_\alpha(X', X) e^{-\beta_\alpha H(X)} \right] dX' = 0$$

is sufficient for having the canonical (grand-canonical) ensemble density be a stationary state of the system when it is in contact with only the α th reservoir.

Entropy Production

The Gibbs entropy of the system at time t is given by

$$S(\mu_t) = - \int \mu_t \log \mu_t dX.$$

This quantity is no longer conserved by the evolution, but its change does not have a definite sign. What is true however (and easy to show) is that

$$\begin{aligned} \sigma &= \frac{dS}{dt} + \sum_{\alpha=1}^k \beta_{\alpha} J_{\alpha} \\ &= \sum_{\alpha=1}^k \iint K_{\alpha}(X, X') e^{-\beta_{\alpha} H(X')} \\ &\quad \cdot \left\{ \nu_{\alpha}(X') \left[\log \nu_{\alpha}(X') - \log \nu_{\alpha}(X) \right] + \nu_{\alpha}(X') - \nu_{\alpha}(X) \right\} dX dX' \end{aligned}$$

where J_{α} is the flux of energy to the α th reservoir from the system

$$J_{\alpha} = \int dX \mu_t(X) \int \left[H(X) - H(X') \right] K_{\alpha}(X', X) dX',$$

and

$$\nu_{\alpha}(X) = e^{\beta_{\alpha} H(X)} \mu(X).$$

The quantity $\beta_\alpha J_\alpha$ may be interpreted as the rate of entropy production in the α th reservoir and σ as the “total entropy production” in system plus reservoirs.

A similar result holds when the effect of the reservoirs is represented by Ornstein-Uhlenbeck processes.

In the stationary state

$$\frac{dS}{dt} = 0, \quad \frac{d\langle H \rangle}{dt} = -\sum J_\alpha = 0$$

and

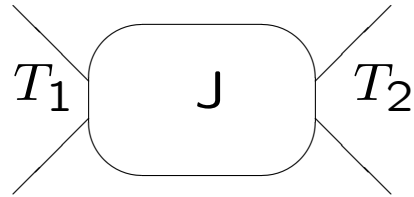
$$\sigma_{\text{st}} = \sum_{\alpha=1}^k \beta_\alpha J_\alpha \geq 0.$$

For $k = 1$, there is no net energy flow or entropy production in the stationary state. In fact, for the case of a single reservoir at temperature $T = \beta^{-1}$, σ is just the rate of change of the (negative) relative entropy w.r.t. the stationary state $\bar{\mu}$

$$\sigma = \frac{d}{dt} S(\mu_t | \bar{\mu}) \geq 0$$

where $\bar{\mu} \sim \exp(-\beta H)$.

This increase in relative entropy is true for all Markov processes, but it does not in general help very much when the stationary state $\bar{\mu}$ is unknown.



For $k = 2$,

$$J_1 = -J_2 = -J \quad \text{and so} \quad \sigma_{\text{st}} = J \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \geq 0,$$

i.e. the energy flow, if any, will be from the hotter to the cooler reservoir (from left to right for $T_1 > T_2$).

But, how will the flux depend on the system Hamiltonian H and on the K_α 's?

This is still very much an open question.