QUANTUM STATISTICAL PHYSICS

Gérard G. Emch

1 INTRODUCTION

In search for the headwaters of the Missouri during their 1804–1806 expedition, Lewis and Clark decreed that the river begins at the confluence of three streams — the Jefferson, Gallatin, and Madison rivers — and ends as a main tributary to the mighty Mississippi.

Similarly, and with some of the same arbitrariness, three major headings can be used to mark the beginnings of quantum statistical physics (QSP): Planck's "quantum hypothesis" following his 1900 papers [Planck, 1900a; Planck, 1900b], Gibbs' 1902 book on "statistical mechanics" [Gibbs, 1902], and what is now known as Einstein's 1905 "Brownian motion" [Einstein, 1905b]. Pushing the metaphor into our own days, the power of QSP is manifest in the landscape of condensed matter physics (from solid state physics to astrophysics). The navigation there, albeit often tentative, has brought to shore predictions that have been confirmed with a precision impressive enough to clamor for a consistent explanation. The purpose of this chapter is to point to directions along which such explanations may be found. I begin this search by tracing briefly the course of the three tributaries mentioned above, thus by identifying the initial motivations for QSP.

Planck's long-lasting hesitations indicate how much in advance he was, not only of his own time, but perhaps even of himself; e.g., at first, he had put forward his black-body radiation law on account of the nature of the *body* — little oscillators in the walls — rather than on account of the nature of the *radiation.* As Planck was transposing to the description of electromagnetic waves the counting arguments Boltzmann used in the thermal physics of material bodies, he initially left open the question of whether this was a mere formal analogy, or whether it was one that could be justified from putative interactions between radiation and matter; or whether, yet, this speculative analogy had deeper roots. Planck's reluctance still shows through in the recommendation he wrote in 1913 to support young Einstein's early election to the Prussian Academy of Sciences: "That he may sometimes have missed the target of his speculations, as for example in his hypothesis of the light quanta, cannot really be held against him." While this may be seen as a barb directed to [Einstein, 1905a], note nevertheless that Planck's reference to a quantum *hypothesis* is not a passing accident: he was meticulous in his use of words; consider, for instance the use of "theory", "theorem", and "hypothesis"

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in the title of his 1911 address to the German Chemical Society [Planck, 1911]. Soon thereafter, the rest of the world overcame his scruples: the Nobel prize was awarded to Planck in 1918 for "his discovery of energy quanta"; and to Einstein in 1921 for "his discovery of the law of the photoelectric effect." For each of them, the *laudatio* calls attention to their respective contributions to the nascent QSP, specifically: the black body radiation for Planck and the specific heat of solids for Einstein; see subsections 2.1 and 2.3 below.

Gibbs' book [Gibbs, 1902] focuses on *classical* statistical physics. While the basic concepts had been apprehended differently by the German Clausius, the Austrian Boltzmann and the British Maxwell, the American Gibbs proposes that the field has reached the modicum of maturity necessary for a consolidation of the foundations; for axiomatization in other fields, compare with Hilbert [Hilbert, 1900; Hilbert, 1899; Hilbert, 1918], and Einstein [Einstein, 1921]. Even in the classical context, Gibbs' reluctance to invoke Boltzmann's ergodic postulate points to the persistence of unresolved issues regarding what Gibbs calls in the very title of his book "the rational foundation of thermodynamics"; for a brief presentation of those aspects of Gibbs' work that may be most relevant to my purpose here, see [Uffink, 2006, section 5]. It pertains to the present chapter to examine how much of this dichotomy persists in the quantum realm, and the extent to which whatever persists is relevant to the explanatory purposes of QSP.

Einstein's papers on Brownian motion still reside conceptually in the realm of classical physics. In spite of the neglect in which many mathematicians still held the foundations of probabilistic theories around the turn of the twentieth century (cf. e.g. [Hilbert, 1900, Problem 6]), Einstein's approach stands as a witness to the fact that stochastic arguments — i.e. arguments involving random processes — had gained currency in the physicists' marketplace. Einstein's conclusions were widely (if not universally) accepted at face value as empirical proof of the existence of molecules, as not just computationally convenient small entities or units, but as objects with definite dimensions [Einstein, 1906b]. Furthermore, Einstein's papers were not the isolated manifestation of a singular genius that the cumbersome title of his first paper might suggest [Einstein, 1905b]. On the one hand, from the physicist's perspective, it must be noted that Einstein begins his second paper in the sequence with an ackowledgment that he had ignored the earlier contributions of Siedentopf and Gouy who had interpreted the "so-called Brownian motion" [Einstein *dixit*] as caused by the irregular thermal motions of the molecules [Einstein, 1906c; Gouy, 1888]. On the other hand, the modern mathematician will recognize, with the hindsight of practitioners such as Kac and Chandrasekhar, that Smolukowski simultaneously distilled from the same empirical sources the mathematical intuition allowing him to post a claim on what was to become the theory of stochastic processes [Smolukowski, 1906a; Smolukowski, 1916]. Yet, it was only in 1933 that Kolmogorov made precise the essentials of the underlying syntax, namely the mathematical theory of probability [Kolmogorov, 1933]. Even so, an unresolved issue remains to this day as to the proper semantics: von Mises' collectives [von Mises, 1928] or de Finetti's subjec-

tive assignments [de Finetti, 1937]. I post my stakes — see subsection 3.1 — on the latter issue when considering the extension of the theory of probability to the quantum realm, with special regard to the specific demands of QSP.

As this essay opens, the question arises as to whether the confluence of three streams of interest compounds the foundational problems of each of them or, on the contrary, whether they can be brought to inform one another. I aim my argument towards the latter view, although I am not oblivious to such ubiquitous problems as questioning what elements of reality should — or should not — be ascribed to individual microscopic quantum systems. As part of the larger problem of the reduction of thermodynamics by statistical mechanics, I consider specifically the question whether and how QSP can claim to explain the collective properties of many-body systems: it does postulate a quantum description at the microscopic level, while it has not obtained as yet an ontological grasp of the individual components of these systems. In my presentation I follow Einstein's admonition: "If you want to find out anything from the theoretical physicists about the methods they use ... don't listen to their words, fix your attention on their deeds." [Einstein, 1933].

2 EARLY SUCCESSES

In [Jammer, 1966] Max Jammer provides much of the specific historical documentation pertaining to the beginnings of quantum theory; and he discusses some of the ensuing debates in [Jammer, 1974]. Here, I start with a discussion of the early pragmatic successes of QSP, with special attention to two aspects: their classical mooring in the high temperature regime; and the understanding QSP gives of the particle-wave duality. Both of these aspects illustrate the added insight gained from the contextual differences coloring the answers to the same questions when asked in QSP rather than in the quantum theories of, say, the Bohr atom or scattering processes; compare with Mara Beller's perspective on the making of the quantum revolution [Beller, 1999].

2.1 Planck's interpolating formula for black-body radiation

The *experimental evidence* available to Planck was the spectral density $\rho_T(\nu)$ of the energy per unit volume of electromagnetic radiation, as a function of its frequency ν, when electromagnetic radiation is in equilibrium with a black-body at temperature T. In [Planck, 1900a; Planck, 1900b], Planck proposes to fit these data with the formula

$$(1) \quad \rho_T(\nu) = A \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} \quad \text{with} \quad A = \frac{8\pi\nu^2}{c^3}$$

where c is the speed of light, $k = R/N_{Av}$ is the Boltzmann constant, R is the universal gas constant and N_{Av} is the Avogadro number. In addition, *a new*

constant enters the formula, h, known nowadays as the Planck constant. While Planck himself would pretend that (1) had been a "lucky guess" such a formula could not have come into existence in a conceptual vacuum.

Two qualitative laws had been identified by Wien [1894], Stefan [1879] and Boltzmann [1884]. The *Wien displacement law* states that

$$(2) \quad \rho_T(\nu) = \nu^3 \, f(\frac{\nu}{T})$$

where f is some undetermined function, satisfying the condition that the following integral converges

$$(3) \quad \frac{1}{V} E(T) = \int_o^\infty d\nu \rho_T(\nu)$$

which expresses the density, per unit volume, of the energy of the radiation at temperature T. Upon inserting (2) in (3), one receives immediately the *Stephan–Boltzmann* law:

$$(4) \quad E(T) = \sigma T^4$$

where σ is a constant. Planck's proposal complies with these laws.

Two analytic expressions (or "laws") had been proposed, which specify the function f in (2). One law, due to Wien [1896], reads:

$$(5) \quad \rho_T(\nu) = \alpha \, \nu^3 \, \exp^{-\gamma \frac{\nu}{T}} \quad .$$

With α and γ being two constants, this law had been confirmed empirically in the range where ν/T is *large.* In contrast, the other law, due to Rayleigh [1900], see also Jeans [1905a], is:

$$(6) \quad \rho_T(\nu) = \frac{8\pi}{c^3} \, \nu^2 \, kT$$

which had been confirmed empirically in the range where ν/T is *small.*

Clearly, (1) interpolates analytically between the Wien and Rayleigh–Jeans formulas; and it gives a quantitative meaning to the conditions that ν/T be "large" (resp. "small"), namely $\nu/T \gg k/h$ (resp. $\nu/T \ll k/h$). In the intermediate range, Planck's interpolating formula fits experimental results very well, both qualitatively and quantitatively.

Planck's colleagues could not fail to be impressed and Planck's triumph would have been complete had he been able to explain his formula from first principles, at least to the considerable extent with which (2) to (6) could be understood. Instead, Planck has to resort to "an act of desperation" — his own words [Jammer, 1966] — and he constructs, after several attempts, a heuristic model in which the radiation exchanges energy in discrete *quanta* with putative "resonators" in thermodynamical equilibrium within the walls. The model suffers from several shortcomings — among them Planck's adaptation of Boltzmann's counting — and much uncertainty concerning its theoretical status:

> Walter Nernst ... initially disliked quantum theory, claiming that it was 'really nothing else than an interpolation formula ... only a rule for calculations ... but has proven so fruitful by the work of Planck ... and ... of Einstein that the duty of science is to take it seriously and to subject it to careful investigations'. [Jammer, 1966, p. 59]

The consensus that later settled in the physics community is that *any* attempt — Planck's included — to derive (1) from first principles would be doomed to failure: (1) *is* a fundamental or primary law, i.e. one that is not to be explained, but the consequences of which ought to be explored.

2.2 Einstein's fluctuation formula and the particle-wave duality

For a start, Einstein notes two shortcomings in Planck's derivation. The first is formal, but nevertheless essential: Planck's account does not conform to Boltzmann's statistical counting as closely as Planck suggests. The second is pointed out in [Einstein, 1906a]: Planck's treatment involves an inconsistency between: (a) his use of the (classical) Maxwell theory of electromagnetism to compute the average energy of a resonator in a radiation field; and (b) the assumption that the energy of a resonator can change only discontinuously. Together with other empirical problems — among which the photoelectric effect [Einstein, 1905a] — these difficulties led Einstein to propose that, while Planck's radiation formula (1) has incontestable empirical merits, the "quantization" itself is to be looked for in the radiation field rather than in a dubious mechanism of interaction with the walls. Einstein's criticism raises, in the same volley, the question of whether light is wave-like as accounted for by Maxwell's electromagnetic theory; or whether it is particle-like as Newton's theory had it before its purported falsification in interference experiments conducted in the early nineteenth century .

Einstein's fluctuation formula [Einstein, 1909a] proposes that light should be viewed *simultaneously* as *both* particle *and* wave; specifically:

SCHOLIUM 1. Let the Planck's spectral density $\rho_T(\nu)$ in (1) be interpreted as the average energy $\langle u_T(\nu)\rangle$ of quantum oscillators of frequency ν of the radiation in thermal equilibrium at temperature T. Then for all values of $h\nu/kT$, the energy fluctuation $\langle(\Delta u)^2\rangle = kT^2\partial_T\langle u_T(\nu)\rangle$ is the sum of two terms

$$\langle(\Delta u)^2\rangle = \langle(\Delta u)^2\rangle_p + \langle(\Delta u)^2\rangle_w \quad \text{where}$$

$$(7) \qquad \left\{ \begin{array}{l} \langle(\Delta u)^2\rangle_p = \langle u_T(\nu)\rangle\, h\nu \\ \\ \langle(\Delta u)^2\rangle_w = \langle u_T(\nu)\rangle^2\, \frac{c^3}{8\pi\nu^2} \end{array} \right\} \quad \text{and} \quad \langle(\Delta u)^2\rangle_p \,/\, \langle(\Delta u)^2\rangle_w = \exp^{\frac{h\nu}{kT}} - 1$$

Hence, the particle-like contribution $\langle(\Delta u)^2\rangle_p$ dominates when $h\nu/kT >> 1$, and the wave-like contribution $\langle(\Delta u)^2\rangle_w$ dominates when $h\nu/kT << 1$. In this in-

terpretation, *the particle-wave duality is thus a matter of degree,* rather than an alternative between the two mutually exclusive horns of a dilemma.

Less of a conceptual problem in QSP, this duality becomes more difficult to master in other empirical contexts where one may prefer to view a photon *either* as a particle *or* as a wave packet. Moreover, this duality has since been extended to all (sub-atomic) particles; e.g. phenomena usually associated with waves, such as diffraction of beams of light, have been observed as well with beams of electrons and then neutrons; cf. e.g. [Jammer, 1966, pp. 249-253]; or for an update [Rauch, 2005]. In other circumstances, one prefers to use a particle language, as for instance in the description of the photo-electric effect [Einstein, 1905a]; as reported in most QM textbooks, a photon impinging on a metallic surface causes an electron to be expelled; or in atomic spectroscopy, a particle — the atom — emits a beam of light; cloud- and bubble-chambers have since let us visualize interparticle collisions; and yet their description in scattering theory uses the so-called wave operator; cf. e.g. [Amrein *et al.*, 1977]. In the light of this duality, and following upon the speculations of Einstein and de Broglie, physicists have learned to adapt their language to the aspect they wish to emphasize. Yet, the persistent arguments about "self-interference" show that some residual ambiguities have yet to be resolved; cf. the long debate extending from [Taylor, 1909] to [Aichele *et al.*, 2005], and surely beyond.

Upon returning to the early manifestations of QSP, one ought to mention that the Einstein fluctuation formula (7) above, as well as the explanation of the temperature dependence of the specific heat of solids — see subsection 2.3 below — motivate the Ehrenfests' suggestion [Ehrenfest and Ehrenfest, 1911] that in statistical mechanics, quantum behaviour manifests itself mostly at low temperatures, whereas classical behaviour emerges at high temperatures. The fact is that in many expressions, such as the Planck distribution (1), the Planck constant h and the temperature T appear together in a factor h/T, or in the form used in the sequel, $\hbar\beta$; hence in these expressions the "classical limit" $h \to 0$ and the "high-temperature limit" $T \to \infty$ are included in $(\hbar\beta) \to 0$. All refer to cases where the relevant energies, or energy densities, are extremely large when measured in the scale determined by the numerical value of the Planck constant.

2.3 Debye's specific heat of solids below the classical regime

For the purpose of this subsection, the situation down in the field is that Dulong & Petit (1819) had proposed an argument to the effect that the specific heat — measured in calories per mole per degree — ought to be the same for all solids: $3R$ where R is the universal gas constant. Yet, it later became apparent that this "constant" could decrease dramatically with temperature, so much so that by the end of the nineteenth century, the experimental data led to the *conjecture* that the specific heat of solids becomes vanishingly small as the temperature approaches absolute $0\,K$. In the meantime, the discovery of X-rays by Roentgen (1895) had allowed several experimentalists — Ewald (1911), and at the suggestion of von

Laue, Friedrich and Knipping (1912) — to obtain diffraction patterns corroborating speculations that crystalline solids are regular lattices, at the vertices of which sit the atoms.

As no classical explanation of the observed drastic temperature dependence of the specific heat seemed forthcoming, Einstein and Debye offered the following model; cf. [Einstein, 1907; Einstein, 1911b; Debye, 1912].

The starting point is (1) above, the Planck formula for black-body radiation, now reinterpreted in terms of the vibrational modes of a solid at temperature T :

$$(8)\quad U(T) = \int d\nu\, g(\nu)\, U(\nu, T) \quad \text{with} \quad U(\nu, T) = \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} \quad \text{and} \quad \int_0^\infty d\nu\, g(\nu) = 3N$$

where N is the number of 3-dimensional oscillators in the solid. Where Einstein had assumed that g is concentrated on a fixed frequency ν_o , Debye chooses for g the simplest vibrational distribution that takes into account that in a crystal, say of volume V , the vibrations have a minimal wavelength of the order of the interatomic distance in the lattice:

$$(9)\quad g(\nu) = G \left\{ \begin{array}{lll} 1 & \text{if} & 0 \le \nu \le \nu_o \\ 0 & \text{if} & \nu > \nu_o \end{array} \right\} \quad \text{with} \quad G = \frac{12\pi\nu^2}{s^3} V \quad .$$

G takes into account that vibrations are now sound waves rather than electromagnetic waves — compare with $A = \frac{8\pi\nu^2}{c^3}$ in (1) — thus s is now the speed of sound, instead of the speed c of light; and the replacement of $8\pi = 2{\cdot}4\pi$ by $12\pi = (2{+}1){\cdot}4\pi$ reflects the fact that sound-waves in solids have, in addition to the two transverse polarizations also present in light, a third degree of freedom, namely longitudinal modes. These hypotheses entail the following consequence.

SCHOLIUM 2. There exists a temperature Θ , such that the specific heat satisfies

$$(10)\quad C_V \simeq \left\{ \begin{array}{ll} 3R & \text{for } T \gg \Theta \\ \\ \frac{12}{5}\pi^4 R(\frac{T}{\Theta})^3 & \text{for } T \ll \Theta \end{array} \right. \quad .$$

Hence, the Debye model differentiates between two regimes: at high temperatures it recovers the Dulong–Petit law; and it predicts that as the temperature approaches $0\,K$, the specific heat vanishes according to $C_V \sim T^3$. In this model, the temperature Θ , now called the *Debye temperature,* depends on the solid considered through the cut-off frequency ν_o , and thus on the speed of sound in that solid and on its density N/V . The numerical value of Θ gives a quantitative estimate — for details, see subsection 6.1 — of what is meant by high and low temperature regimes for the specific heat of crystalline solids. Moreover, in Debye's model, C_V decreases monotonically and continuously over the whole range of temperatures $T \in \mathbb{R}^+$.

As a last comment on the passage from (1) to (8), note that by analogy with the *photons* as the quanta of light, the elementary sound vibrations in solids are viewed as quanta, now known as *phonons*.

2.4 BE-condensation: the long haul

When taking seriously the idea that the microscopic picture of the macroscopic world may be a quantum one, the most immediate question is to obtain the corresponding description of a quantum ideal gas; this came to be known as the Bose—Einstein gas, or simply the Bose gas [Bose, 1924; Einstein, 1924]. The starting point is the grand canonical partition function $Z(\Lambda, T, \mu)$ of an assembly of identical massive particles of mass m in equilibrium at temperature T and chemical potential μ; this assembly is enclosed in a cubical box of volume $\Lambda \subset \mathbb{R}^3$, with periodic boundary conditioms. As these particles are non-interacting, the total energy is the sum of their individual energies $\epsilon_k = \hbar^2|k|^2/2m$, where $k \in Z^3$. The quantum hypothesis is that the Planck distribution (1) applies here so as to entail (with $\beta = 1/kT$) :

$$(11)\quad Z(\Lambda, T, \mu) = \prod_{k \in Z^3} (1 - \exp^{-\beta(\epsilon_k - \mu)})^{-1} \quad .$$

From this formula, one computes the specific volume v and the pressure P, according to the rules learned in classical statistical mechanics; the so-called activity is defined as $z = \exp(\beta\mu)$:

$$(12)\quad v^{-1} = z\partial_z \frac{1}{|\Lambda|} \ln Z(\Lambda, T, \mu) \quad \text{and} \quad \beta P = \frac{1}{|\Lambda|} \ln Z(\Lambda, T, \mu) \quad .$$

The problem is thus stated completely, although the consequences of (11–2.12) are not easy objects to compute directly. The solution involves a mathematical excursion through some classical analysis, and the reward is a nice physical bounty: a phase transition with the onset of a condensed phase at very low temperatures; not your classical ideal gas!

The necessary classical analysis — now widely available, cf. e.g. [Whittaker and Watson, 1927, p.280, ex. 7], [Erdélyi, 1953, I, pp. 27–30], or for some historical perspective [Truesdell, 1945] — was already known to our pioneers, and they did recognize that in the limit $\Lambda \uparrow \mathbb{R}^3$, these sums reduce to:

$$(13)\quad \left.\begin{array}{ll} v^{-1} & = 4\pi \int_o^\infty dp\, p^2\, z[\exp(\hbar^2 p^2/2mkT) - z]^{-1} \\ \beta P & = 4\pi \int_o^\infty dp\, p^2\, \ln[1 - z\, \exp(-\hbar^2 p^2/2mkT)] \end{array}\right\}$$

which are known in classical analysis as Appell integrals, namely

$$(14)\quad \left.\begin{array}{ll} v^{-1} & = \lambda^{-3} g(\frac{3}{2}, z) \\ \beta P & = \lambda^{-3} g(\frac{5}{2}, z) \end{array}\right\} \quad \text{with} \quad \left\{\begin{array}{ll} \lambda^2 & = 2\pi\hbar^2/mkT \\ g(s,z) & = \frac{z}{\Gamma(s)} \int_o^\infty dt\, \frac{t^{s-1}}{\exp^t - z} \end{array}\right. \quad .$$

For every s with $Re(s) > 0$, g defines a function of z which is analytic in the cut complex plane $C\backslash[1, \infty)$. For $|z| < 1$ and $Re(s) > 0$, one receives the well-studied Lerch zeta functions which can be expanded in power series

$$(15)\quad g(s,z) = z\,\zeta(s,z) \quad \text{with} \quad \zeta(s,z) = \sum_{n=0}^{\infty} z^n\,(n+1)^{-s} \quad .$$

For $z = 1$ and $Re(s) > 1$ the above series converges to the Riemann zeta function $\zeta(s)$. Note that the values $s = \frac{3}{2}$ and $s = \frac{5}{2}$ — which are needed in (14) — fall within this range. Moreover $g(\frac{3}{2},\cdot) : z \in (0,1) \mapsto R^+$ is smooth, strictly increasing, with $\lim_{z\to 1} g(\frac{3}{2},z) = \zeta(\frac{3}{2}) = 2.612\ldots$. The problem is thus mathematically under complete control.

Now to the physics. This divides into two steps.

The *first* step is easy: it considers the high temperature and low density regime, where $\lambda^3\,v^{-1} < g(\frac{3}{2},1) = \zeta(\frac{3}{2})$. In particular, by straightforward 1st-order power expansion:

$$(16)\quad \text{for } \lambda^3\,v^{-1} << 1 \,:\; P\,v = kT\,[1 - 2^{-5/2}(\lambda^3\,v^{-1}) + \ldots\,] \quad .$$

Hence, in this high temperature and low density regime, the quantum gas behaves asymptotically like the classical ideal gas of Boyle/Mariotte/Gay–Lussac. This is yet another confirmation of the Ehrenfests' remark according to which the classical limit obtains in QSP as a high temperature limit; note indeed that the so-called *thermal wavelength* λ that appears in (14) satisfies $\lambda \sim \hbar\,\beta^{\frac{1}{2}}$, i.e. in this problem again, the limits $T \to \infty\,(\Leftrightarrow\ \beta \to 0)$ and $\hbar \to 0$ have formally the same effect.

The *second* step in the treatment of the problem is where the bounty is to be found. The question is how to go beyond the above regime, i.e. beyond the unnatural limit

$$(17)\quad \lambda^3 v^{-1} = \zeta(\frac{3}{2}) \quad ,$$

a restriction no actual gas should be expected to respect. Mathematically, this limiting condition seems to appear as the consequence of the breakdown of analyticity in (14) that begins at $z = 1$. Physically, the problem appears because the limit $|\Lambda| \to \infty$ has been taken too carelessly.

Let us therefore return to the expression of v^{-1} when $|\Lambda| < \infty$. We have then, with $\langle n_k\rangle$ denoting the average number of particles in mode k :

$$(18)\quad \frac{1}{|\Lambda|}\sum_{k\in Z^3}\langle n_k\rangle = \frac{1}{|\Lambda|}\sum_{k\in Z^3,k\neq 0}\langle n_k\rangle + \frac{1}{|\Lambda|}\,\frac{z}{1-z} \quad .$$

As the $\langle n_k\rangle$ with $k \neq 0$ are well-behaved as $z \to 1$, the separation of (18) into two terms suggests that we take simultaneously the limits $|\Lambda| \to \infty$ and $z \to 1$ in such a manner that the second term in (18) approaches a finite limit, say ${v_o}^{-1}$, resulting in the replacement of (14) by:

$$(19)\quad \left.\begin{array}{ll} v^{-1} & = \lambda^{-3}\,\zeta(\frac{3}{2}) + {v_o}^{-1} \\ \beta\,P & = \lambda^{-3}\,\zeta(\frac{5}{2}) \end{array}\right\} \quad .$$

The above limiting procedure, interpreted as

$$(20)\quad {v_o}^{-1} = \lim_{|\Lambda|} \frac{1}{|\Lambda|} \langle n_o \rangle \quad ,$$

leads to a *macroscopic occupation of the ground state* $k = 0$; the theory does not predict the value of v_o : it may depend on the temperature. Note that the pressure P in (19) depends on temperature only (namely through λ). The state of the system described by (19) is called its *condensed phase*; the transition to this phase from the normal phase $\lambda^3 v^{-1} < \zeta(\frac{3}{2})$ is referred to as the *Bose–Einstein condensation,* (or *BEC*) and its appearance at low temperature is a prediction of purely quantum origin, one that has no equivalent in the classical world.

This begs for an instantiation in the world of the laboratory. At low temperature a superfluid phase appears in ^{4}He. The density at the onset of this phenomenon is about $\rho \simeq .178$ g/cm^3. Upon taking into account the value of the Avogadro number, one receives $v^{-1} \simeq 2.7 \cdot 10^{23}$ cm^{-3}, from which (17) gives a thermal wavelength $\lambda \simeq 4.6 \cdot 10^{-8}$ cm which is not unreasonable for a quantity that is to be interpretated as a measure of the interparticle distance. To this value corresponds, via the definition of λ in (14), a temperature $T \simeq 3.2\, K$. The experimental value of the temperature at the onset of the superfluid phase in ^{4}He is $T \simeq 2.2\, K$, a rather remarkable fit, considering how crude the model is. Moreover, the thermodynamics of the model can be worked out — cf. e.g. [Huang, 1965] — and shows that the specific heat $C_v(T)$ at first increases monotonically from $C_v(0) = 0$ to exceed the classical value $3/2$ but then experiences a sharp peak — a discontinuity in the first derivative — from which it decreases monotonically to $\lim_{T\to\infty} C_v(T) = 3/2$. The specific heat of ^{4}He also exhibits such a singularity, albeit more pronounced: it is logarithmic; hence its name $\lambda - point$, as the graph of the specific heat as a function of temperature looks like the Greek lower case letter lambda.

All this represented a great success in the the mid-1920s. The next batch of problems appeared when the theory tried to account for the fact that ^{4}He is not a gas, but a liquid; for this, the *ideal* gas assumption of the model is quite unrealistic: a liquid is not made of non-interacting particles. Putting the interactions into the theory proved to be a formidable problem, long compounded by the experimental fact that ^{4}He was the only substance recognized to exhibit Bose–Einstein condensation: theoreticians had no variable parameter to guide and adjust their speculations. Following up on a proposal made in the late 1950s, the situation changed drastically during the 1980s and 1990s with the advent of micro-Kelvin technology which allowed BEC to be observed in atomic gases in harmonic traps; for two deep, but very different, reviews, cf. [Lieb, 2001] and [Pitaevskii and Stringari, 2003]; and for a brief overview [Emch and Liu, 2002, subsection 14.2.2].

The account in this subsection was limited mostly to the macroscopic, thermodynamical aspects of BEC in its infancy; in subsection 5.2 below, a C$^*-$algebraic treatment of the Bose–Einstein model is discussed in connection with the appearance in QSP of the modular structures to be associated to the equilibrium KMS condition.

2.5 Beyond the Bohr atom: the Thomas–Fermi model

The entry in quantum mechanics of Schrödinger wave-mechanics (1926) was marked by a resounding success: the physics community could recognize immediately the application of a then already well-established method to a new realm; the theoretical explanation of the energy spectrum of the hydrogen atom was reduced to solving an eigenvalue problem in a differential equation. Every entry-level text in quantum mechanics presents this derivation.

And yet, beyond the Bohr atom, the solution of the Schrödinger equation for an atom with even a few electrons turned to be an insurmontable task: the electrons are charged particles and while the interaction between a single electron and the nucleus had been rigorously accounted for in the hydrogen atom, one could not deal analytically with the mutual electromagnetic interactions between the electrons.

Very soon thereafter, Thomas [1927] and Fermi [1927] came up with a semi-classical model in which two ingredients enter. The first is the ground state electron density ρ which is assumed to be spherically symmetric and normalized by the condition

$$(21)\quad 4\pi \int_o^\infty dr r^2 \rho(r) = Z$$

where eZ is the charge of the nucleus. The second is the average electric potential $\Phi(r)$ in the atom. These two ingredients are assumed to satisfy the *classical* equation, the Poisson equation of electrostatics

$$(22)\quad \Delta\Phi \equiv \frac{1}{r}\frac{d^2}{dr^2}(r\Phi) = 4\pi e\rho \quad \text{with} \quad \lim_{r\to 0}\Phi(r) = eZ \quad .$$

And yet the model has a quantum aspect to account for the Pauli exclusion principle; this is the so-called Fermi–Dirac statistics that had been proposed just the previous year [Fermi, 1926]. Here, this shows up in:

$$(23)\quad n(r,p) = \begin{cases} 2h^{-3} & \text{if} \quad \epsilon := \frac{1}{2m} - e\Phi < \epsilon_o \\ 0 & \text{if} \quad \epsilon > \epsilon_o \end{cases} \quad .$$

from which one gets, by integration over p (upon putting $\epsilon_o = 0$), that ρ satisfies

$$(24)\quad \rho(r) = \begin{cases} \frac{8\pi}{3h^3}(2me\Phi)^{3/2} & \text{if} \quad \Phi > 0 \\ 0 & \text{if} \quad \Phi < 0 \end{cases} \quad .$$

Clearly, the model is conceptually inconsistent, with stakes in each of the classical and the quantum realms. Yet, in my student days this model was a routine staple of the quantum mechanics curriculum [Schiff, 1955; Landau and Lifshitz, 1958a; Messiah, 1960] as it can be solved without any further assumptions than those listed above; the solution is exact up to the fact that it requires a numerical computation well within the realm of a controllable approximation.

Upon using the numerical values of the Planck constant h, the charge e and the mass m of the electron, the model predicts that the radius of the atom, taken

to be the radius of the sphere that contains all the electrons but one increases monotonically from $2.2 \cdot 10^{-8}$ cm for $Z = 25$, to $2.8 \cdot 10^{-8}$ cm for $Z = 100$. The order of magnitude is correct. This can be counted therefore as an early success of quantum theory.

However, one should expect that such a crude model does not tell the whole story. Indeed: (1) the predicted increase stops at $Z = 55$ (corresponding to the cesium atom) after which the radius decreases, albeit slowly; (2) when looked at more closely, the model yields an electron density that has unreasonable properties both very close and very far from the nucleus. Besides, the model needs serious reconsiderations to explain the existence of stable molecules or to accommodate a relativistic treatment. These problems never completely left the scene of theoretical physics, but remained somewhat in the background for about half-a-century, until rigorous analytic methods clarified the sense in which the model is asymptotically exact and may be used to study the stability of atoms, molecules and even stars; cf. [Lieb and Simon, 1977; Lieb, 1982a; Lieb, 1990]; see also [Catto *et al.*, 1998; Le Bris and Lions, 2005].

2.6 White dwarfs: the Chandrasekhar bound

Returning to the quantum ideal gas discussed in subsection 2.4, let us examine now the Fermi gas. Instead of (11), start with the partition function

$$(25)\quad Z(\Lambda, T, \mu) = \prod_{k \in Z^3} (1 + \exp^{-\beta(\epsilon_k - \mu)})$$

which now entails in the limit $\Lambda \uparrow Z^3$, instead of (13):

$$(26)\quad \left.\begin{array}{ll} v^{-1} & = 4\pi \int_o^\infty dp\, p^2\, z[\exp(\hbar^2 p^2/2mkT) + z]^{-1} \\ \beta\, P & = 4\pi \int_o^\infty dp\, p^2\, \ln[1 + z\, \exp(-\hbar^2 p^2/2mkT)] \end{array}\right\} \quad .$$

In the high temperature and low density regime — $\lambda^3 v^{-1} \ll 1$ — one recovers again an asymptotic expansion, the leading term of which is the classical ideal gas:

$$(27)\quad for\ \lambda^3\, v^{-1} << 1 :\ P\, v \simeq kT\, [1 + 2^{-5/2}(\lambda^3\, v^{-1}) + \dots\,] \quad .$$

Again, up to the sign of the correction, this is very similar to the Bose–Einstein result (16): it also coincides asymptotically with the classical ideal gas as T becomes large.

In the low temperature and high density regime — $\lambda^3 v^{-1} \gg 1$ — the situation differs drastically from what it was in subsection 2.4: whereas bosons tend to congregate, no two fermions are allowed in the same state on account of the Pauli exclusion principle. Recall that in chemistry, this is the principle that underpins a quantum explanation for the Mendeleev table of elements. In QSP the Pauli principle is visible through (26): in the ground state of the system, the fermions occupy the lowest possible energy states up to a finite energy, called the Fermi–energy

$$(28)\quad \epsilon_F = \frac{\hbar^2}{2m}\left[(3\pi^2)\,v^{-1}\right]^{\frac{2}{3}} \quad .$$

For temperatures such that $kT \ll \epsilon_F$ the momentum distribution will be

$$(29)\quad < n_p >= \begin{cases} 1 & \text{for} \quad (|p|^2/2m) \overset{\sim}{<} \epsilon_F \\ 0 & \text{for} \quad (|p|^2/2m) \overset{\sim}{>} \epsilon_F \end{cases}$$

with a steep sigmoid of narrow breadth kT around ϵ_F. This regime is called the *degenerate Fermi gas.* To characterize this regime, rewrite $kT \ll \epsilon_F$, with ϵ_F as in (28), as:

$$(30)\quad \beta\, v^{-\frac{2}{3}} \gg \left[\frac{\hbar^2}{2m}(3\pi^2)^{\frac{2}{3}}\right]^{-1}$$

which gives a quantitative meaning to the expression *low temperature and high density* regime; for instance, this yields a useful first approximation for the gas of electrons in metals at usual temperatures. The condition $kT \ll \epsilon_F$ corresponds to $\lambda^3 v^{-1} \gg 1$ and in this regime (26) entails

$$(31)\quad Pv \simeq \frac{2}{5}\epsilon_F\left[1 + \frac{5\pi^2}{12}(\frac{kT}{\epsilon_F})^2 + \ldots\right] \quad \text{i.e.} \quad \lim_{\frac{kT}{\epsilon_F}\to 0} Pv^{\frac{5}{3}} = \frac{2}{5}(3\pi^2)^{\frac{2}{3}}\frac{\hbar^2}{2m} \quad .$$

Hence, at fixed density, the pressure approaches a strictly positive constant as $T \to 0$, in marked contrast with the behaviour of the classical ideal gas (see (27)) where $T \to 0$ implies $P \to 0$.

Less mundane examples are provided by celestial objects, white dwarfs and neutron stars. With a temperature similar to that of the sun, i.e. $10^7 K$ to $10^8 K$ in the center, and a mass of the same order of magnitude as the sun, the white dwarfs have a very high density, about 10^6 to 10^7 times that of the sun. They are stars where all the hydrogen fuel has been burned, and thus they are constituted of completely ionized helium atoms. From these hypotheses on the composition and condition of a white dwarf, one computes the density of the electron gas, and then from (28) the corresponding Fermi energy ϵ_F which, when expressed in terms of $T_F = \epsilon_F/k$, turns out to give $T_F \simeq 10^{11} K$. Hence $T \ll T_F$ and it is consistent to assume — as R.H. Fowler did already in 1926 [Fowler, 1926] — that the electron assembly in the white dwarfs may be described as a degenerate Fermi gas, and that it is the enormous pressure in such a gas that prevents the star from gravitational collapse. It is however true that at such density and pressure, electrons must be treated relativistically, i.e. $\epsilon = \sqrt{(pc)^2 + (mc^2)^2}$ instead of $\epsilon = p^2/2m$. This brings about all sorts of analytic difficulties, among which is a change from 5/3 towards 4/3 in the power of v in (31). In the course of his computations of this effect, Chandrasekhar [1931a] remarked that since the gravitational pressure is governed by the mass of the star, the latter would collapse if the mass were to become too large; he actually evaluated this critical mass M_{max} to be

$$(32)\quad M_{max} \simeq (3\pi)^{\frac{1}{2}}(\frac{\hbar c}{G})^{3/2}(\mu m_N)^{-2} \simeq 1.4\, M_\odot$$

where (in cgs units) $\hbar = h/2\pi$ with $h \simeq 6.62 \times 10^{-27}$ ergs cm is the Planck constant, $c \simeq 3 \times 10^{10}$ cm/sec is the speed of light, $G \simeq 6.67 \times 10^{-8}$ dyn cm^2 g^{-2} is Newton's gravitational constant, $m_N \simeq 1.66 \times 10^{-24}$ g, μ is the number of nucleons per electron; here $\mu = 2$ since the star is supposed to have used its hydrogen supply, and be made of $^4_2$He. Finally, to reduce the result in astronomic units, $M_\odot \simeq 1.99 \times 10^{33}$ g is the mass of the sun. Astronomers today refer to the maximum mass M_{max} as the *Chandrasekhar limit* [where mathematicians would speak of a "bound"].

Chandrasekhar's original derivation is mathematically correct, yet somewhat cumbersome. Already by the end of 1932, L.D. Landau [1932] presented a more elementary argument, *and* in addition, upon hearing of the discovery of the neutron, he applied the above formula to then putative neutron stars.

To have included these predictions here among the early "successes" of QSP may be justified only by hindsight. When they appeared in the early 1930s they and their consequences caused quite a wave, on the crest of which rode A.S. Eddington, an astronomer of commanding authority, who spoke of a *reductio ab absurdum* calling for the interposition of an as yet unknown fundamental theory: for him a massive star ($M > M_{max}$) collapsing to a black hole was heresy, and he was in a position not to mince his words about it. Eddington's fierce attack on a junior colleague did not cause Chandrasekhar to recant; unconvinced, Chandra nevertheless decided to turn to other astronomical problems until the late 1950s [Chandrasekhar, 1958] and early 1960s, when his speculations, and Landau's, found observational confirmations.

For the unfolding of the resolution of the Chandrasekhar–Eddington conflict, cf. e.g. [Shapiro and Teukolsky, 1983], the title of which already indicates the complete extent to which Chandrasekhar was ultimately vindicated. A pristine, yet non-technical presentation of the physics of the Chandrasekhar bound may be read in [Thorne, 1994, chapter 4]; the story of the neutron stars, albeit more involved is also told there in [Thorne, 1994, chapter 5]; for the fundamental technical support, cf. [Weinberg, 1972, chapter 11].

3 AXIOMATIC PRUNINGS

Usually, either one of two reasons prompts the process of axiomatization. The first is the search for the soul — some would say the skeleton — hidden inside the aleatory appearances of the body: a ritual of purification. The second is the need for fundamental changes when a theory faces increasingly insuperable limitations. Both of these reasons motivate the developments I retrace in the present section; as I write this I am reminded of the essential tensions described elsewhere in [Segal, 1990].

It is an interesting coincidence that the early 1930s saw the almost simultaneous — albeit independent — axiomatizations of two of the ingredients of QSP:

Quantum mechanics with von Neumann's treatise [von Neumann, 1932c]; and *Statistics,* a.k.a. probability and stochastic processes, with Kolmogorov's paper [Kolmogorov, 1933]. As both of these belong to other chapters of this Handbook, only a few words will suffice here.

3.1 Kolmogorov's and von Neumann's formalisms compared

In a nutshell, Kolmogorov's syntax for probability starts with a seminal description of measure theory: a triple $\{\Omega, \mathcal{E}, \mu\}$ is given where $\mathcal{E}$ is a $\sigma-$algebra of measurable subsets of a set Ω, and μ is a countably additive function

$$(33)\quad \mu : E \in \mathcal{E} \mapsto \mu(E) \in \mathbb{R}^+ \quad \text{with} \quad \mu(\Omega) = 1$$

i.e. μ is a *probability measure* on $\{\Omega, \mathcal{E}\}$. μ naturally extends to a functional on the algebra $\mathcal{A} = \mathcal{L}^\infty(\Omega, \mathcal{E}, \mu)$ of all essentially bounded functions $A : \Omega \to \mathbb{C}$:

$$(34)\quad \mu : A \in \mathcal{A} \mapsto \mu(A) = \iint_\Omega d\mu(\omega)\, A(\omega) \in \mathbb{C}\ .$$

Hereafter, I will refer to this extension as a *classical state.*

Similarly, von Neumann's syntax involves a triple: $\{\mathcal{H}, \mathcal{P}, \psi\}$ where $\mathcal{P}$ is the orthomodular lattice of all closed subspaces of a Hilbert space $\mathcal{H}$, ψ is a countably additive positive function

$$(35)\quad \left.\begin{array}{ll} \psi : P \in \mathcal{P} \mapsto \psi(P) \in \mathbb{R}^+ & \text{with} \quad \psi(I) = 1 \quad \text{and} \\ \psi(\sum_n P_n) = \sum_n \psi(P_n) & \forall\, \{P_n\} \subset \mathcal{P} \text{ such that } n \neq m \models P_n \perp P_m \end{array}\right\}\ .$$

I shall refer to any such funtion ψ as a quantum state. Gleason's theorem asserts in particular — see below for a complete statement — that for every quantum state ψ there exists a density operator, i.e. a positive operator ρ of unit trace, such that ψ extends to the W^*-algebra $\mathcal{B} = \mathcal{B}(\mathcal{H})$ of all bounded linear operators from $\mathcal{H}$ into itself:

$$(36)\quad \psi : B \in \mathcal{B} \mapsto \psi(B) = \mathrm{Tr}\rho\, B \in \mathbb{R}\,.$$

When working within the von Neumann formalism, I will identify any closed subspace $P \subseteq \mathcal{H}$ and the projector $P \in \mathcal{B}(\mathcal{H})$ on this subspace; I will indifferently refer to ψ or to ρ as a *state* on $\mathcal{B}$; and I will refer to the restriction of ψ to $\mathcal{P}$ as a quantum measure. I will also follow the physicist's custom of referring to ρ as a *density matrix,* thus ignoring the mathematician's distinction between an operator and its expression in a specified (orthonormal) basis.

The mathematical similarities and differences between the classical and quantum realms are emphasized by the Koopman formalism of classical mechanics; cf. e.g. [Emch and Liu, 2002, pp. 255, 267]. This formalism — actually a precursor of the GNS construction — associates to $\{\Omega, \mathcal{E}, \mu\}$ the Hilbert space $\mathcal{H} = \mathcal{L}^2(\Omega, \mathcal{E}, \mu)$ of all functions $\Psi : \omega \in \Omega \to \Psi(\omega) \in \mathbb{C}$ that are square-integrable with respect to μ. Every element $A \in \mathcal{A} = \mathcal{L}^\infty(\Omega, \mathcal{E}, \mu)$ is then viewed as an element of $\mathcal{B} = \mathcal{B}(\mathcal{H})$,

namely under the identification of the function $A : \omega \in \Omega \mapsto A(\omega) \in \mathbb{C}$ with the multiplication operator $A : \Psi \in \mathcal{H} \mapsto A\Psi \in \mathcal{H}$ where $(A\Psi)(\omega) = A(\omega)\Psi(\omega)$. Under this identification $\mathcal{A}$ becomes a maximal abelian W^*- subalgebra of $\mathcal{B}$; while the center of $\mathcal{B}$, namely $\{C \in \mathcal{B} \,|\, \forall\, B \in \mathcal{B} : [B, C] = 0\}$ is trivial, i.e. consists of the multiples of the identity operator. Note further that every element $B \in \mathcal{B}(\mathcal{H})$ can be viewed as a continuous linear functional on the Banach space $\mathcal{T}(\mathcal{H})$ of all trace-class operators, spanned by the countably additive states; namely $B : T \in \mathcal{T}(\mathcal{H}) \mapsto \mathrm{Tr}\, TB \in \mathbb{C}$; conversely every norm-continuous linear functional on $\mathcal{B}(\mathcal{H})$ obtains in this manner; i.e. $\mathcal{B}(\mathcal{H})$ is the Banach space *dual* of $\mathcal{T}(\mathcal{H})$; equivalently, $\mathcal{T}(\mathcal{H})$ is the *predual* of $\mathcal{B}(\mathcal{H})$. Similarly, the predual of $\mathcal{L}^\infty(\Omega, \mathcal{E}, \mu)$ is the Banach space of $\mathcal{L}^1(\Omega, \mathcal{E}, \mu)$, spanned by the probability distributions which are absolutely continuous with respect to μ.

The interpretation of a quantum state ψ in terms of classical probabilities obtains upon reading (35) separately for each family $\{P_n\}$ of mutually compatible quantum events. The bijective equivalence between the objects described by (35) and (36) is the pragmatic content of Gleason's theorem; cf. e.g. [Emch and Liu, 2002, p. 225]: every quantum state can be uniquely written in the form (36), and every density operator ρ defines through (36) a function ψ satisfying (35), i.e. a quantum state ψ. For the semantic, i.e. the empirical (frequentist vs. subjective) interpretations of states, first in classical probability theories, and then in quantum theories, cf. e.g. [Jaynes, 1967; Emch and Liu, 2002; Emch, 2005]; in particular, see [Uffink, 2006] for the evolution in CSP of the primacy of one over the other of these interpretations of probabilities.

Again in a nutshell, I believe that it serves my purpose well, in most of this essay, to espouse the 'subjective' rather than their 'frequentist' interpretation, namely *to view the state of a physical system* — be it classical or quantum, macroscopic or microscopic — *as a faithful summary of the knowledge one has of the process by which this system has been prepared.* In particular, this semantic view of the quantum state shall translate well from the case of systems with *finitely many degrees of freedom* considered in von Neumann's quantum mechanics, to the systems *with infinitely many degrees of freedom* to be considered in QSP; see subsections 3.4 to 6.3. In particular, while von Neumann's beams or 'ensembles', of independent, identically prepared systems — [von Neumann, 1932c, note 156] — are adequate to describe scattering experiments or the atomic spectroscopy of his time, the view of quantum states that I choose to adopt here accomodates better the description of single macroscopic systems — such as a cup of coffee or a measuring apparatus.

3.2 QSP in von Neumann's formalism

The centerpiece of equilibrum QSP in von Neumann's formalism is the following result [von Neumann, 1932c]:

THEOREM 3. *Let $\mathcal{H}$ be a Hilbert space, H be a self-adjoint operator acting in $\mathcal{H}$ and such that for all $\beta > 0$: the partition function $Z := \mathrm{Tr} \exp(-\beta H)$ be finite. And, with $k > 0$ fixed, let for any state ρ on $\mathcal{B}(\mathcal{H})$*

(37) $S[\rho] = -k\,\mathrm{Tr}\rho\log\rho$.

As H has discrete spectrum and is bounded below, let ϵ_o be its smallest eigenvalue; and let s denote either the largest eigenvalue of H if H is bounded above, or ∞ if it is not. Then, for any given $\epsilon_o < E < s$, the maximum of $S[\rho]$, subject to the constraint $\mathrm{Tr}\rho H = E$ is reached on the state

(38) $\rho = Z^{-1}\,e^{-\beta H}$ with $Z = \mathrm{Tr}e^{-\beta H}$

where the value of β is determined by the value E of the constraint.

The first part of the proof consists in showing that the maximum occurs on the class of states of the form $\rho = \sum_n \lambda_n P_n$ where $\sum_n \epsilon_n P_n$ is the spectral resolution of H. After this, the result follows from the classical argument using Lagrange multipliers with respect to the collection of variables $\Lambda = \{\lambda_n\} \subset \mathbb{R}^+$, namely from determining the maximum of the function $S[\Lambda] = -k\sum_n \lambda_n \log\lambda_n$ subject to the simultaneous constraints $\sum_n \lambda_n\epsilon_n = E$ and $\sum_n \lambda_n = 1$.

Note that this variational principle could have been rephrased as defining the state ρ in (38) as the state that minimizes — now under the single constraint $\mathrm{Tr}\rho = 1$, i.e. $\sum_n \lambda_n = 1$ — the Helmholtz free-energy defined as $F := E - TS$ with E and S as in the theorem, and $\beta = kT$ where k is known as the Boltzmann constant (see below).

Note also that, in either of these two forms, this variational principle has its root in the classical statistical physics (CSP) of Boltzmann and Gibbs; cf. [Uffink, 2006]. Conceptually, and very much as in CSP, the von Neumann QSP result involves a consensus on two questions. The first question is to justify the interpretation of S as an entropy. There are two ways to do this.

(i) Firstly, as in CSP, one may identify S with the equilibrium entropy of macroscopic thermal physics upon computing S for well-controlled model(s), such as the ideal gas and finding — for in each of the specific cases considered — that the value of S_{max} obtained through the above theorem coincides with the value of the thermodynamical entropy. It is only at that stage that k may be identified with the universal Boltzmann constant $k \simeq 1.3810^{-23}$ J/deg ; note the units, namely [energy]/[temperature], as is proper for the thermal entropy where T is the integrating factor that allows one to pass from the "heating" differential η to the exact differential $dS = \eta/T$. As fine as that may be for equilibrium CSP/QSP, this identification leaves open the interpretation of S as entropy in non-equilibrium situations.

(ii) The second route to an interpretation of S is to show that $I(\rho) = -S(\rho)$ is a measure of the information content of the state ρ, namely to find empirically meaningful conditions that express the intuitive concept of "information content" and to show that — up to a multiplicative constant — there exists exactly one S that satisfies these conditions. The argument offered by Khinchin [1957] for classical probability distributions involves — *inter alia* — the axiom of consistency under refinements. This argument was transposed to the quantum case by Thirring [1983b] to give:

THEOREM 4. *$S[\rho] = -k\,\mathrm{Tr}\rho\log\rho$ is the only functional satisfying:*

1. *$S[\rho]$ is continuous in ρ, in the sense that it is a continuous function of the eigenvalues of ρ.*
2. *For every finite probability distribution $P = \{p_n \,|\, n = 1, 2, \ldots, N\}$ and every finite collection of states $\{\rho_n \,|\, n = 1, 2, \ldots, N\}$ on a finite collection of Hilbert spaces $\{\mathcal{H}_n \,|\, n = 1, 2, \ldots, N\}$, let ρ be the state defined on $\mathcal{H} = \oplus_{n=1}^{N}\mathcal{H}_n$ by $\rho = \oplus_{n=1}^{N} p_n\rho_n$. One has then: $S[\rho] = S[P] + \sum_{n=1}^{N} p_n S[\rho_n]$ where $S[P]$ is the value of the Khinchin functional for the probability distribution P.*
3. $S\left[\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}\right] = k\log 2.$

The first of the three conditions of theorem 4 is clear: an arbitrarily small change in the state should result in an arbitrarily small change in the information it conveys. The second condition expresses refinement under a particular class of partitionings; while the third is only a normalization. Just as in CSP, the *quantum information content* $(-S)$, uniquely specified by these conditions, is formally used to define the *quantum entropy* S.

The second question concerning the conceptual relevance of theorem 3 is to justify the very use of a *variational principle;* compare with [Uffink, 1995]. In my view, for both the classical and the quantum cases, this comes most naturally when one opts for the subjective interpretation of states rather than the frequentist interpretation. Indeed, if one wants the state to account for the knowledge one has of the system, it seems consistent to select for ρ the state that assumes no more information than that expressed explicitly by the constraint.

When the operator H in theorem 3 is taken to represent the energy of the system, the state (38) is called — by analogy to the Gibbs canonical equilibrium state of CSP — the quantum canonical equilibrium state for the natural temperature $\beta = 1/kT$. Note in particular that, in the Schrödinger picture, the evolution generated by H, namely:

$$(39)\quad \forall\, t \in \mathbb{R}: \quad \rho(t) = U(t)\rho U(-t) \quad \text{with} \quad U(t) = \exp^{-i\frac{1}{\hbar}Ht}$$

leaves the canonical equilibrium state invariant, as is to be expected when one wishes to identify the energy-operator with the Hamiltonian of the system.

At first sight, the von Neumann formalism affords a good start for the development of a quantum ergodic theory. To keep things as simple as possible, consider the Hilbert space $\mathcal{L} = \{X \in \mathcal{B}(\mathcal{H}) \,|\, \mathrm{Tr}\, X^*X < \infty\}$ equipped with the scalar product $(X, Y) = \mathrm{Tr}\, X^*Y$. This space is known to mathematicians as the space of Hilbert–Schmidt operators acting on $\mathcal{H}$. In particular, every density matrix is an element of $\mathcal{L}$; and thus this space is also known to physicists as the Liouville space of the quantum system described on $\mathcal{H}$. The advantage of restricting attention to this space is that (39) extends to a unitary action on $\mathcal{L}$:

$$(40)\quad V : (t, X) \in \mathbb{R} \times \mathcal{L} \mapsto V(t)[X] = U(t)XU(-t) \in \mathcal{L} \quad .$$

In the same way as the self-adjoint generator H of the continuous unitary group $\{U(t)|t \in \mathbb{R}\}$ is called the Hamiltonian of the quantum system considered, the self-adjoint generator L of the continuous unitary group $\{V(t)|t \in \mathbb{R}\}$ is called the *Liouvillian* of this system. One has then

THEOREM 5. *Let $H \in \mathcal{B}$ have purely discrete spectrum, i.e. H can be written in the form $H = \sum_n \epsilon_n P_n$ where the P_n are mutually orthogonal projectors adding to I. Then the following limit exists*

$$(41)\quad E_{erg}[X] = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, V(t)[X] \quad \text{with} \quad X \in \mathcal{L} \quad ;$$

and

$$E_{erg}[X] = \sum_n P_n X P_n \quad \text{and} \quad \forall\, t \in \mathbb{R} \;: V(t)[E_{erg}[X]] = E_{erg}[X].$$

In particular, the ergodic average $E_{erg}[\rho]$ of a density matrix ρ exists, is again a density matrix, and is time-invariant.

It is tempting to try and consider theorem 5 as proper quantum version of the classical ergodic theorems of Birkhoff [1931] or von Neumann [1932a]. Indeed, the *conclusions* of these classical theorems and of theorem 5 are similar when one reads them in terms of (countably additive) 'states' respectively defined as:

- $A \in \mathcal{L}^\infty(\Omega, \mu) \mapsto \int_\Omega d\mu\, f A \in \mathbb{C}$ where $f \in \mathcal{L}^1(\Omega, \mu)$, f positive with f normalized by $\int_\Omega d\mu\, f = 1$ (for the classical case);
- $A \in \mathcal{B}(\mathcal{H}) \mapsto \mathrm{Tr}\,\rho A \in \mathbb{C}$ where ρ is a density matrice, i.e. a positive trace-class operator with ρ normalized by $\mathrm{Tr}\rho = 1$ (for the quantum case);

and similarly for their respective time-averages.

Note that while the classical theorems are usually followed by a corollary involving the (quasi-)ergodic hypothesis and some discussion of the relevance of the results for the foundations of CSP — for a critical presentation see e.g. [Uffink, 2006, section 6.1] — I do not intend to try and follow suit here, in view of theorems 7 and 8 below which, for the purposes of QSP, cast a shadow on the adequacy of the *assumptions* theorem 5 makes on the Hamiltonian H. For a quantum ergodic theorem better adapted to the needs of QSP, see theorem 25 below.

Nevertheless, two related interesting comments may be made about theorem 5.

(i) If, in this theorem, H is non-degenerate, i.e. if $\forall\, n : \dim P_n = 1$, then $E_{erg}[\rho]$ coincides with

$$(42)\quad Q_o[\rho] = \sum_n \mathrm{Tr}(\rho P_n) P_n = \sum_n (\rho\Psi_n, \Psi_n) P_n$$

where $P_n\Psi_n = \Psi_n$ with $(\Psi_n, \Psi_m) = \delta_{mn}$, and where $Q_o[\rho]$ is thus the density matrix resulting from the von Neumann quantum measuring process [von

Neumann, 1932c, p. 351]; see also subsection 6.3 below. In particular, if ρ is a pure state, i.e. is a projector P_Ψ on some vector $\Psi = \sum_n c_n \Psi_n$, then $Q_o[P_\Psi] = \sum_n |c_n|^2 P_n$ has lost all the information encoded in the relative phases of the coefficients c_n.

(ii) In [von Neumann, 1932c, pp. 380 ff] von Neumann shows that the entropy S of a state does not decrease — and in the generic case does increase — as the result of a measurement, whereas it is constant under the unitary evolution (40). He thus sees in

(43) $S[Q_o[\rho]] \geq S[\rho]$

a confirmation that quantum measurements are generically *irreversible* processes. Similarly then, the information encoded in a (non-degenerate) density matrix ρ may only decrease as a result of taking its time-average, a reasonable feature indeed.

Yet, while theorem 5 could have been regarded as the germ of a quantum ergodic theory, the occurrence of monotonic irreversibility in QSP is significantly more elusive, as the next subsection demonstrates.

3.3 Some reasons to go beyond von Neumann's formalism

Some of the problems non-equilibrium QSP has to face are illustrated in a simple spin-lattice model that was originally suggested to me by an actual experiment, the so-called nuclear free-induction relaxation; cf. [Emch and Liu, 2002, section 15.3].

The system consists of a linear chain of N interacting spins $\{\sigma_k = (\sigma_k^x, \sigma_k^y, \sigma_k^n) \; | k = 1, \ldots, N\}$ with N even (and large, in a sense to be specified later on), and let

$$(44)\quad \sigma_k^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_k^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_k^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

be the Pauli matrices acting on $\mathcal{H}_k \simeq C^2$. The Hilbert space of the system is then $\mathcal{H} = \otimes_k \mathcal{H}_k \simeq \mathbb{C}^{2^N}$. In this chain, two spins on sites k and $k+n$ interact with an energy $-J_n \sigma_k^z \sigma_{k+n}^z$, with $J_n > 0$ so that a lower energy is ascribed to configurations in which the $z-$components of these spins are parallel rather than anti-parallel. The whole system is plunged in a homogeneous magnetic field B in the direction z. The total Hamiltonian is chosen to be

$$(45)\quad H_N = -B \sum_{k=1}^{N} \sigma_k^z - \sum_{k=1}^{N} \sum_{n=1}^{N/2} J_n \sigma_k^z \sigma_{k+n}^z \quad \text{with} \quad J_n = 2^{-n} J_o > 0 \; .$$

The system is initially prepared in the state

$$(46)\quad \rho_N = Z_N^{-1} \exp^{-\beta B \sum_{k=1}^{N} \sigma_k^x} \quad \text{with} \quad Z_N = \mathrm{Tr} \exp^{-\beta B \sum_{k=1}^{N} \sigma_k^x} \; .$$

For the three "macroscopic" observables

$$(47)\quad S_N^\alpha = \frac{1}{N}\sum_{k=1}^{N}\sigma_k^\alpha \quad \text{with} \quad \alpha \ \text{ standing for } \ x, y, z$$

one computes easily from (39–40) with $H = H_N$ given by (45):

$$(48)\quad \left.\begin{array}{ll} \mathrm{Tr}\,(V_N(t)[\rho_N]\,S_N^x) & = \mathrm{Tr}\,(\rho_N\,S_N^x)\cos(2Bt) f_N(t) \\ \mathrm{Tr}\,(V_N(t)[\rho_N]\,S_N^y) & = \mathrm{Tr}\,(\rho_N\,S_N^y)\sin(2Bt) f_N(t) \\ \mathrm{Tr}\,(V_N(t)[\rho_N]\,S_N^z) & = \mathrm{Tr}\,(\rho_N\,S_N^z) \end{array}\right\}$$

where

$$(49)\quad \left.\begin{array}{c} f_N(t) = f(t)/W_N(t) \quad \text{with} \\ f(t) = \left[\frac{\sin(J_o t)}{J_o\, t}\right]^2 \quad \text{and} \quad W_N(t) = \left[\frac{\sin(2^{-N/2} J_o t)}{2^{-N/2} J_o\, t}\right]^2 \end{array}\right\} \ .$$

REMARKS 6.

1. For the purpose of discussing the putative irreversibility of the model, the (conservative) Larmor precession $\{\cos(Bt), \sin(Bt)\}$ of the magnetization around the direction z of the magnetic field B is of little or no interest.

2. In favour of the "irreversibility" of the model, one first notes that

   $$(50)\quad \forall\, t \text{ with } |t| << T_N = 2^{N/2}\pi J_o^{-1} \ : \quad f_N(t) \simeq f(t)$$

   and then the decay of $|\mathrm{Tr} V_N(t)[\rho]\, S_N^\alpha|$ is governed by t^{-2}. Therefore, *in this time frame,* the magnetization (48) exhibits an apparent approach to equilibrium.

3. However, against the statement that the model would show an irreversible approach to equilibrium, one observes that

   $$(51)\quad \lim_{t\to T_N} f_N(t) = 1 = f_N(0)$$

   and thus, over the long run the system is periodic in time. This quantum model therefore would seem to confirm the classical Zermelo recurrence objection, or *Wiederkehreinwand*; for the latter, see [Uffink, 2006, section 4.5].

4. The saving grace, nevertheless, is that the period T_N increases exponentially with the size N of the system; see (50). This exponential behaviour is already encountered is CSP, as demonstrated by the Ehrenfest dog-flea model briefly mentioned in subsection 6.1 below. Thus, a modern Galileo would have his *Simplicio* argue that for macroscopically large systems, unaccountable perturbations would set in before T_N is approached, thus irremediably masking this periodicity; compare this to Boltzmann's responses to the Zermelo objection; see again [Uffink, 2006, section 4.5].

5. Upon taking stock of this objection *Salviati* would invoke some modern version of the apocryphal commandment to the effect that "*Thou shalt not interchange limits*" since:

   (52) $\lim_{N\to\infty}\lim_{t\to\infty} f_N(t)$ does not exist but $\lim_{t\to\infty}\lim_{N\to\infty} f_N(t)$ exists and is 0 .

6. The present model presents also a quantum manifestation of the classical Loschmidt reversibility objection, or *Umkehreinwand* — cf. [Uffink, 2006, section 4.3] — as one has, here also:

   (53) $f_N(-t) = f_N(t)$ and even $f(-t) = f(t)$

   confirming the classical *Janus* dictum according to which the security of a *postdiction* is the same as that of a *prediction*. Hence, this model indicates that, if the Umkehreinwand were indeed a genuine objection to QSP — which I do not believe it is — the thermodynamical limit would not avoid it, whereas remarks (4) and (5) above show how it may respond to the Wiederkehreinwand.

7. Finally, one serious shortcoming of the present model — not as a model of the particular experiment considered above, but as a model for the approach to equilibrium in a QSP accounting for transport coefficients — is that, even in the limit of $N \to \infty$, the evolution is monitored by an inverse power law in time, rather than an exponential law, as would be required for the type of behaviour encountered in such macroscopic situations as described by Newton's cooling law, Fourier's heat equation, or more generally any macroscopic differential transport equation with linear coefficients.

The model illustrates explicitly some of the essential limitations of the von Neumann formalism for QSP, as manifested in the following two general results. The main assumption of theorems 3 and 5, namely that the Hamiltonian operator H has discrete spectrum, though seemingly innocuous — and actually necessary — when dealing with equilibrium QSP, has one potentially disastrous consequence when one attempts to extend the formalism to non-equilibrium situations: metastases of the classical objections spread into the quantum realm, as we shall now see.

The first result is a quantum version of the classical recurrence theorem of Zermelo. To be mathematically precise recall, in the words of Besicovitch's standard text [Besicovitch, 1954], that a function $f : t \in \mathbb{R} \mapsto f(t) \in \mathbb{C}$ is said to be *almost periodic* in the sense of Harald Bohr, if $f(t+T)$ is approximately equal to $f(t)$ — with an arbitrary degree of accuracy — for infinitely many values of T, these values being spread over the whole real line, in such a way as not to leave empty intervals of arbitrarily great length.

THEOREM 7. *If the Hamiltonian $H = H^* \in \mathcal{B}(\mathcal{H})$ has purely discrete spectrum, i.e. if $H = \sum_n \epsilon_n P_n$; and if $\{V(t) \,|\, t \in \mathbb{R}\}$ is the unitary action in the Liouville space $\mathcal{L}$ defined in (40), then*

(54) $\forall X, Y \in \mathcal{L} : f_{X,Y}(t) = \mathrm{Tr}\,(V(t)[X]\,Y)$

is an almost periodic function in t *in the sense of H. Bohr.*

Proof. $f(t)$ is a Fourier series $\sum_{n,m} a_{n,m} \exp^{-i\frac{1}{\hbar}(\epsilon_n - \epsilon_m)t}$ with $a_{n,m} = \mathrm{Tr}(\,P_n X\, P_m\, y)$; by the Schwartz inequality in $\mathcal{L}$: $\sum_{n,m} |a_{n,m}|^2$ converges and thus — cf. [Besicovitch, 1954] — f is an almost periodic function of t in the sense of H. Bohr. ■

One might then attempt to get rid of recurrences by assuming — as is certainly allowed in the von Neumann formalism of quantum mechanics, provided $\dim\mathcal{H} = \infty$ — that the spectrum of the Hamiltonian is purely continuous. From the point of view of QSP, however, this cure would raise the following new difficulty, namely that ergodic states may not be countably additive, i.e. may not be representable by density matrices.

To describe this phenomenon, consider the Banach space $\mathcal{B} = \mathcal{B}(\mathcal{H})$ equipped with its usual operator norm; and denote by $\mathcal{B}^*$ its dual, i.e. the Banach space of all continuous, linear functionals on $\mathcal{B}$. Then

(55) $\mathcal{B}^* = \mathcal{A}^* \oplus \mathcal{A}^\perp$

where

i. $\mathcal{A}$ is the space of compact operators on $\mathcal{H}$, i.e. $\mathcal{A} = \{A \in \mathcal{B}(\mathcal{H}) \mid \Psi_n \rightharpoonup \Psi \;\Rightarrow\; A\Psi_n \to A\Psi\}$; here, $\rightharpoonup$ and $\to$ respectively denote weak- and strong-convergences in $\mathcal{H}$. When the $^*-$algebra $\mathcal{A}$ is equipped with the operator norm it inherits from $\mathcal{B}(\mathcal{H})$, $\mathcal{A}$ is closed in $\mathcal{B}(\mathcal{H})$ and thus is a Banach space on its own; in fact $\mathcal{A}$ is the only non-trivial closed two-sided $^*-$ideal of $\mathcal{B}$.

ii. For every $\varphi \in \mathcal{A}^*$, the dual of $\mathcal{A}$, there exists a unique trace-class operator $R \in \mathcal{T} = \{B \in \mathcal{B} \mid \mathrm{Tr}\,(B^*B)^{\frac{1}{2}} < \infty\}$ such that $\forall\, A \in \mathcal{A}:\ \varphi(A) = \mathrm{Tr}(R\,A)$. In particular, to every positive, continuous linear functional ψ on $\mathcal{A}$ such that $\sup_{A\in\mathcal{A},\|A\|\leq 1} \|\psi(A)\| = 1$ there corresponds a unique density matrix, and conversely.

iii. $\mathcal{A}^\perp = \{\varphi \in \mathcal{B} \mid A \in \mathcal{A} \Rightarrow \varphi(A) = 0\}$.

Note that each of the inclusions $\mathcal{T} \subseteq \mathcal{L} \subseteq \mathcal{A} \subseteq \mathcal{B}$ is strict iff $\mathcal{H}$ is infinite-dimensional, a condition that is required whenever one wants to avoid recurrences, since $\dim\mathcal{H} < \infty$ obviously entails that the spectrum of H is purely discrete, and then theorem 7 applies.

We can now make precise the above mentioned difficulty concerning the description of ergodic states within the context of countably additive states:

THEOREM 8. *Let* $H \in \mathcal{B}(\mathcal{H})$ *be the self adjoint generator of any strongly continuous unitary group* $\{U(t) \mid t \in R\}$ *acting on* $\mathcal{H}$; *and, with* t *running over* $\mathbb{R}$, *let* $\rho \in \mathcal{T} \mapsto \rho(t) = U(t)\rho U(-t) \in \mathcal{T}$ *describe the evolution of any density matrix* ρ; *further, let* ψ_t *denote the corresponding (countably additive!) state* $\psi_t : B \in \mathcal{B}(\mathcal{H}) \mapsto \psi_t(B) = \mathrm{Tr}(\rho(t)B) \in \mathbb{C}$. *Then, it follows that:*

a. *For every compact observable* $A \in \mathcal{A}$ *the ergodic limit*

$$(56)\quad \lim_{T\to\infty} \frac{1}{T}\int_o^T dt\ \psi_t(A)$$

exists and defines a positive linear functional $E_\infty[\psi]$ *on* $\mathcal{A}$.

b. *If, moreover, the spectrum of* H *is purely continous, then* $E_\infty[\psi]$ *cannot be extended to a countably additive state on* $\mathcal{B}(\mathcal{H})$.

Proof. For the part (a), the economical strategy is to take advantage of two density theorems, namely: (i) when $\mathcal{L}$ is equipped with its Hilbert-Schmidt norm, it contains $\mathcal{T}$ as a dense subspace; and (ii) when $\mathcal{A}$ is equipped with the operator norm it inherits from $\mathcal{B}(\mathcal{H})$, it contains $\mathcal{L}$ as a dense subspace. Hence, one can uniquely lift the evolution from $\mathcal{T}(\mathcal{H})$ to a unique unitary evolution on the Hilbert space $\mathcal{L}$ where one can use the classical ergodic theorem — [von Neumann, 1932a], or [Emch and Liu, 2002; Uffink, 2006] — to assert the existence of the ergodic limit for any pair $(X, Y) \in \mathcal{L} \times \mathcal{L}$, and in particular for any pair $(\rho, A) \in \mathcal{T} \times \mathcal{L}$. Upon recalling the duality $\mathcal{A} = \mathcal{T}^*$, the ergodic result is then extended by continuity from $\mathcal{T} \times \mathcal{L}$ to $(\rho, A) \in \mathcal{T} \times \mathcal{A}$.

To prove part (b), one notices that, on the one hand, this limit is given, for every $A \in \mathcal{A}$ by $E_o[\psi](A) = \mathrm{Tr}(\sum_n (P_n\, \rho\, P_n\, A)$ where $\{P_n\}$ is the set of all the projectors corresponding to the discontinuous jumps in the spectral family of H. Hence, when H has continuous spectrum, this set is empty and thus $\forall\, A \in \mathcal{A}:\ E_o[\psi](A) = 0$. On the other hand, $E_o[\psi]$ certainly extends further than $\mathcal{A}$; for instance the ergodic limit obviously exists for any $X \in \{H\}'$, i.e. for all bounded observables that are constants of the motion; in particular $E[\psi_o](I) = 1$. Hence, even if $E[\psi_o]$ could be extended to a state on $\mathcal{B}$, this state would belong to $\mathcal{A}^\perp$ and thus would have no countably additive component in the direct sum decomposition (55). ■

The proof of the theorem shows that the same objection can be raised with any Hamiltonian the spectrum of which contains even only one interval of continuity. Taking Hamiltonians that are still self-adjoint, but not bounded above would only raise more technical problems without providing a solution to the basic limitation exposed in theorem 8.

Hence, von Neumann's formalism for QSP leads non-equilibrium QSP into the horns of a dilemma: either the evolution is almost periodic or the ergodic states are not countably additive. In particular, non-equilibrium states cannot approach asymptotic states that can be described by density matrices.

To make a bad situation even worse, Zeh discovered — admittedly, long after von Neumann's treatise had appeared and yet relevant to the thrust of this section — that there are serious empirical difficulties with the concept of an isolated quantum system [Zeh, 1970; Wigner, 1984]. Could certainty be fading out? [Prigogine, 1997]. Zeh's original observation has led to the development of the concept of

decoherence; cf. Landsman [Landsman, 2006, section 7.1]. I very briefly address this and some related issues in section 6 below.

Even in equilibrium QSP, the anchor provided by von Neumann was slipping: the formalism cannot account for the coexistence of thermodynamical phases; for a response to this objection, see subsection 5.7 below.

In counterpoint to these questions, one fundamental problem needs to be addressed: namely that the von Neumann formalism is not adequate to describe typical many-body systems where an infinite number of degrees of freedom are brought into the picture. The prescribed remedy is discussed in the next subsection.

3.4 Haag–Kastler's axioms and Takeda's inductive limits

This subsection outlines a formalism proposed to deal effectively with the non-relativistic many-body problems in QSP. This formalism was born out of the axiomatic responses prompted by the diagnosis of a mid-life crisis in relativistic Quantum Field Theory [QFT] [van Hove, 1952; Friedrichs, 1953; Wightman and Schweber, 1955]; the nail in the coffin was driven by Haag [1955]; cf. e.g. the famous Haag theorem and its embalmings in [Barton, 1963, section 14], [Streater and Wightman, 1964, section IV.5], and/or [Emch, 1972a, section 3.d]. The algebraic axiomatization is presented here with sufficiently elementary details, yet with enough restraint to eschew the "imperialistic" label sometimes attached to it.

The main idea is to account for the local structure of infinitely extended systems. In their original proposal, Haag and Kastler [1964] mention several precedents in axiomatic QFT; among these [Haag, 1959a; Haag and Schroer, 1962]; see also [Haag, 1959b]. (I first heard of the algebraic approach in seminars in Geneva, where Araki presented some aspects of his Zurich lectures [Araki, 1961/2].) Segal's early advocacy of an algebraic approach [Segal, 1947] ought also to be mentioned.

This subsection is divided in two complementary parts: the first part presents a description of the general structure; the second illustrates this structure with an example, the 1-dimensional quantum spin-lattice.

Part I. The general structure.

One begins by selecting an absorbing directed net $\mathcal{F}$ of regions Λ of finite extension in space; usually, the space is the Minkowski space $\mathbb{M}^{n+1}$ for relativistic QFT, the Euclidean space $\mathbb{R}^n$ or a lattice $\mathbb{Z}^n$ for non-relativistic QSP. The case of immediate physical interest is $n = 3$, but exploratory models are often constructed with $n = 1, 2$. Recall that a directed net is a partially ordered set — here the order relation is the usual set-theoretical inclusion — such that for every pair of elements Λ_1, Λ_2 in $\mathcal{F}$ there is at least one element $\Lambda \in \mathcal{F}$ such that $\Lambda_1 \subseteq \Lambda$ and $\Lambda_2 \subseteq \Lambda$. To say that this net is absorbing is to say that for every point x in space there exists at least one element $\Lambda \in \mathcal{F}$ such that $x \in \Lambda$. The symbol $\Lambda_1 \bowtie \Lambda_2$ will be used to signify that two regions Λ_1 and Λ_2 are causally disjoint, i.e. in QFT, these

regions are spacelike to one another; and in non-relativistic QSP, they are disjoint in the set-theoretical sense, i.e. $\Lambda_1 \cap \Lambda_2 = \emptyset$. G denotes a group of rigid motions in the space, namely the inhomogeneous Lorentz group for $\mathbb{M}^{n+1}$; the Euclidean group for $\mathbb{R}^n$; or the group of lattice translations for $\mathbb{Z}^n$.

Secondly, to every $\Lambda \in \mathcal{F}$ one assigns a C^*-algebra $\mathcal{A}_\Lambda$; without loss of generality, one may assume that $\mathcal{A}_\Lambda$ has an identity I_Λ. This assignment is subject to the following three postulates.

POSTULATE 9 (Isotony). Whenever $\Lambda_1 \in \mathcal{F}$ and $\Lambda_2 \in \mathcal{F}$ satisfy $\Lambda_1 \subseteq \Lambda_2$, one is given an injective $^*-$homomorphism $i_{21} : \mathcal{A}_{\Lambda_1} \to \mathcal{A}_{\Lambda_2}$ such that

1. $i_{21}(I_{\Lambda_1}) = I_{\Lambda_2}$
2. $\Lambda_1 \subseteq \Lambda_2 \subseteq \Lambda_3 \;\Rightarrow\; i_{32} \circ i_{21} = i_{31}$.

The following result was proven by Takeda [1955].

THEOREM 10. *Let $\mathcal{F}$ be a directed net, and $\{\mathcal{A}_\Lambda \mid \Lambda \in \mathcal{F}\}$ satisfy the isotony postulate. Then there exist: a C^*-algebra $\mathcal{A}$ with unit I; and a family of injective $*-$homomorphisms $\{i_\Lambda : \mathcal{A}_\Lambda \to \mathcal{A} \mid \Lambda \in \mathcal{F}\}$ such that*

1. $\forall\, \Lambda \in \mathcal{F} \;:\; i_\Lambda(I_\Lambda) = I$;

2. $\Lambda_1 \subseteq \Lambda_2 \;\Rightarrow\; i_{\Lambda_1}(\mathcal{A}_{\Lambda_1}) \subseteq i_{\Lambda_2}(\mathcal{A}_{\Lambda_2})$;

3. $\bigcup_{\Lambda\in\mathcal{F}} i_\Lambda(\mathcal{A}_\Lambda)$ *is a norm-dense sub$-^*$algebra of* $\mathcal{A}$.

The C^*-algebra $\mathcal{A}$ is called the C^*-*inductive limit* of the net $\{\mathcal{A}_\Lambda \mid \Lambda \in \mathcal{F}\}$. We will use hereafter the notations

$$\mathcal{A}_o := \bigcup_{\Lambda\in\mathcal{F}} i_\Lambda(\mathcal{A}_\Lambda) \quad \text{and} \quad \mathcal{A} = {}^n\overline{\mathcal{A}_o}.$$

POSTULATE 11 (Local commutativity). Whenever $\Lambda_1, \Lambda_2 \in \mathcal{F}$ satisfy $\Lambda_1 \bowtie \Lambda_2$, and $\Lambda_3 \in \mathcal{F}$ is such that both $\Lambda_1 \subseteq \Lambda_3$ and $\Lambda_2 \subseteq \Lambda_3$:

$$A_1 \in \mathcal{A}_{\Lambda_1} \text{ and } A_2 \in \mathcal{A}_{\Lambda_2} \;\Rightarrow\; i_{31}(A_1)\, i_{32}(A_2) = i_{32}(A_2)\, i_{31}(A_1) \quad .$$

The following result is then immediate.

COROLLARY 12. *If $\Lambda_1 \bowtie \Lambda_2$, then*

$$A_1 \in \mathcal{A}_{\Lambda_1} \text{ and } A_2 \in \mathcal{A}_{\Lambda_2} \;\Rightarrow\; i_{\Lambda_1}(A_1)\, i_{\Lambda_2}(A_2) = i_{\Lambda_2}(A_2)\, i_{\Lambda_1}(A_1) \quad .$$

For the aspects of QSP considered here, it will be an innocent abuse of language to refer to the above postulate as simply the *postulate of locality.*

POSTULATE 13 (Covariance). An action $\nu : (g, A) \in G \times \mathcal{A}_o \to \nu_g[A] \in \mathcal{A}_o$ is given so that for every region $\Lambda \in \mathcal{F}$, ν_g induces a $^*-$isomorphism between $\mathcal{A}_\Lambda$ and $\mathcal{A}_{g[\Lambda]}$, where $g[\Lambda]$ denotes the image of the region Λ under the point transformation g.

Upon using theorem 10, this can be lifted to $\mathcal{A}$, namely $\nu_g[i_\Lambda(\mathcal{A}_\Lambda)] = i_{g[\Lambda]}(\mathcal{A}_{g[\Lambda]})$:

COROLLARY 14. *The action of G extends by continuity to a norm-continuous group representation $\nu : g \in G \to \mathrm{Aut}(\mathcal{A})$.*

DEFINITION 15. With the above notations, $\mathcal{A}_o$ is called the algebra of local observables; and $\mathcal{A}$ is called the algebra of quasi-local observables. Moreover, if φ is a state on $\mathcal{A}$ such that $\forall\, g \in G : \varphi \circ \nu_g = \varphi$, let π_φ be the corresponding GNS representation. The von Neumann algebra $\mathcal{N}_\varphi = \pi_\varphi(\mathcal{A})''$ is called the algebra of global observables relative to the state φ.

Note that quasi-local observables involve norm limits; they are therefore general, algebraic objects that can be defined abstractly, i.e. without reference to any particular Hilbert space representation. In contrast, global observables that are not quasi-local involve weak-operator limits, and thus depend on the Hilbert space representation in which these limits are taken; for the purposes of QSP these observables depend, via the GNS construction, on the physical situation for which they are defined, i.e. on the state with respect to which they are considered. This aspect of the theory will be discussed in details in subsection 3.5 — see in particular the preliminaries to scholium 23, and remark 26(1) — and it will be essential for the treatment of phase transitions, inasmuch as these involve averages of observables, for instance the spontaneous magnetization in ferromagnets; see subsection 5.7 below.

Part II. A concrete example of a net of observable-algebras.
This example exhibits the construction of the algebra of observables for an infinite quantum spin-lattice system that obtains in the thermodynamical limit of finite systems such as the one treated in subsection 3.3 above. Consider indeed an infinite 1-dimensional lattice $\mathbb{Z}$ with a quantum $\frac{1}{2}-$spin sitting at each node (or "site"); hence a copy $\mathcal{A}_k$ of the C^*-algebra $\mathcal{M}(2,\mathbb{C})$ of 2×2 matrices with complex entries is associated to each site $k \in Z$; i.e. $\mathcal{A}_k$ is generated by the Pauli matrices (44), i.e. by the three observables corresponding to the three components of a $\frac{1}{2}-$spin sitting at site k.

Let now $\mathcal{F}$ be the net of all finite subsets $\Lambda \subset Z$. To each of these Λ is then associated the "local" C^*-algebra $\mathcal{A}_\Lambda = \otimes_{k\in\Lambda}\mathcal{A}_k$ which is thus a copy of $\mathcal{M}(2^{|\Lambda|},\mathbb{C})$, where $|\Lambda|$ denotes the number of sites in Λ.

Let now Λ_1 and Λ_2 be two finite regions, with $\Lambda_1 \subseteq \Lambda_2$. An injective $^*-$homomorphism of $\mathcal{A}_{\Lambda_1}$ into $\mathcal{A}_{\Lambda_2}$ obtains by linearity from its restriction to monomials, namely

$$i_{21}(A_1 \otimes A_2 \otimes \ldots \otimes A_{|\Lambda_1|}) \;=\; B_1 \otimes B_2 \otimes \ldots \otimes B_{|\Lambda_2|}$$

with

$$\forall\, k \in \Lambda_2 \,:\, B_k = \begin{cases} A_k & \text{if} \quad k \in \Lambda_1 \\ I_k & \text{if} \quad k \notin \Lambda_1 \end{cases} \quad .$$

These inclusions satisfy postulate 9.

Here, two finite regions are in the relation $\Lambda_1 \bowtie \Lambda_2$ whenever $\Lambda_1 \cap \Lambda_2 = \emptyset$. Since the commutators of observables attached to individual sites vanish whenever the two sites are different, any two observables attached to disjoint regions do commute. Formally, this is to say that postulate 11 is satisfied.

Finally, let $G := \mathbb{Z}$ denote the additive group of translations of the lattice. To define the action of G on the algebra of local observables it is sufficient to notice that for all $g \in G$ and all $\Lambda \in \mathcal{F}$: $|g[\Lambda]| = |\Lambda|$, so that both $\mathcal{A}_{g[\Lambda]}$ and $\mathcal{A}_\Lambda$ are copies of the same matrix algebra, namely $\mathcal{M}(2^{|\Lambda|},\mathbb{C})$: the images of a local observable and its translate are simply different copies of the same matrix; this indeed defines ν_g in such a way that postulate 13 is satisfied.

3.5 Quantum ergodic theory and macroscopic observables

While classical ergodic theory concerns itself with *measures* μ that are invariant under a group G and their *mixing* properties, quantum ergodic theory discusses the properties of $G-$invariant *states* and their *clustering* properties. Accordingly, in this subsection I will discuss also the roles of *space and/or time averages* in explaining at least part of the success of QSP; compare with [Uffink, 2006] and, in particular, with [Earman and Rédei, 1996].

Therefore, one question to be addressed in this subsection must be whether and how ergodic theory may serve as a cornerstone to build up statistical mechanics. Traditionally, under the impetus of the emphasis the Ehrenfests' placed on Boltzmann's ergodic hypothesis (or rather its measure-theoretical version, the quasi-ergodic hypothesis), the group G is taken to be the group $\mathbb{R}$ governing the *time evolution.* Nevertheless, partly in response to some swaying to and fro in Boltzmann's own writings, the jury is still out on the fundamental issue of this hypothesis' relevance for the foundations of CSP; see in particular [Uffink, 2006, section I.3, and subsections I.4.3 and I.6.1]. It is also remarkable that already Gibbs [Gibbs, 1902] chose to emphasize the role of mixing properties, i.e. properties which are stronger than metric transitivity and make more precise the presumption that the dynamics is 'erratic'; cf. e.g. [Uffink, 2006, sections I.4.1 and I.5]; other issues are touched upon in [Emch and Liu, 2002, pp. 317–330]; and, for a pertinent account that takes stock of the work done in the second half of the twentieth century, by the Lebowitz and Sinai schools, see [Szasz, 1996].

Consequently, I will concentrate here on two sub-questions: (i) the extent to which the mathematics of classical ergodic theory may be generalized to the formalism of quantum theory; and (ii) the extent to which such generalizations may help formulate better certain aspects of the foundations of QSP.

The answer to the first of these sub-questions is that much of the mathematics goes through, with some minor adjustments. The answers to the second is more

complex. On the one hand, as long as the focus remains on the time evolution the main issues persist, among which is the paucity of realistic models. On the other hand, when the group G deals with the geometry of the problem, quantum ergodic theory — especially and the roles of averages, and theorems linking extremal invariance and clustering properties — does help distinguish, within QSP, the quantum aspects of the microscopic description and the classical aspects of the macroscopic world. Thus, I divide the presentation in two parts, according to whether ergodicity is considered with respect to the time evolution or with respect to space symmetries.

A. Ergodicity with respect to time

Some insight is gained from a model first proposed in [Ford *et al.*, 1965], which comes in two versions, classical and quantum. The quantum version has been controlled mathematically in [Davies, 1972]. It is proven there that an infinite 1-dimensional chain of weakly coupled 1-dimensional quantum harmonic oscillators may serve as a thermal reservoir for a single 1-dimensional quantum oscillator in the chain and that a diffusion equation governs the evolution of the latter. This is accomplished by a rigorous treatment of the van Hove weak-coupling/long-time limit about which more will be said in subsection 6.1 below. Anticipating some mathematical definitions to be made precise later on — see paragraph 5.3.C — it is sufficient for the present discussion to register that, in this van Hove limit, a reduced evolution obtains which is a contractive semi-group of completely positive maps $\{\gamma_s \mid s \in \mathbb{R}^+\}$ acting on the von Neumann algebra $\mathcal{N}_o \simeq \mathcal{B}(\mathcal{L}^2(\mathbb{R},\mathbb{C}))$ attached to the site of the single oscillator considered. Moreover this evolution, when observed from any one-dimensional subspace $\{x\mathbf{u} \mid x \in \mathbb{R}\}$ in the 2-dimensional phase space $\{\xi P + \eta Q \mid \zeta = (\xi,\eta) \in \mathbb{R}^2\}$ of the single oscillator, is described by a classical distribution $\mu(x,s)$ that satisfies for all $s \in \mathbb{R}^+$ the *diffusion equation:*

$$(57)\quad \partial_s \mu(x,s) = D\,\left[\,\partial_x^2 + \beta(V'(x)\,\partial_x + V''(x))\,\right]\,\mu(x,s)$$

where $\beta = 1/kT$ is the natural temperature, $V = \frac{1}{2}\omega\, x^2$ is a harmonic potential, while the diffusion constant D and the frequency ω are numbers, the values of which depend only on the direction $\zeta/|\zeta| \in \mathbb{R}^2/S^1$. Note that the corresponding invariant measure is the canonical equilibrium, Gaussian measure $\mu(x) = Z^{-1}\,\exp(-\beta V(x))$ with $Z = \int_R dx \mu(x)$, i.e. $Z^{-1} = \sqrt{2\pi\beta\omega}$.

The point of the model here is that the dissipative system described by the contractive *semi-group* $\{\gamma_s \mid s \in \mathbb{R}^+\}$ governing this Markovian diffusion process admits a canonical dilation to a conservative dynamical system. Indeed, there exists a *group* $\{\alpha_s \mid s \in \mathbb{R}\}$ of automorphisms of the von Neumann algebra $\mathcal{N} = \pi_\varphi(\mathcal{A})''$ describing the full chain of oscillators in the equilibrium state φ corresponding to the temperature β when the interactions are switched off. In conformity with subsection 3.4 the algebra of quasi-local observables $\mathcal{A}$ is here the C^*-algebra $\otimes_{k\in\mathbb{Z}}\mathcal{N}_k$ where the $\mathcal{N}_k$ are copies of $\mathcal{N}_o$. The free equilibrium state has the form $\varphi = \otimes\varphi_k$ where φ_k is the von Neumann canonical equilibrium state for the oscillator at the site k. Let now i be the injection of $\mathcal{N}_o$ into $\mathcal{N}$ and φ_o

denote the restriction of φ to $\mathcal{N}_o$, i.e. $\forall\, N_o \in \mathcal{N}_o\ :\ \varphi_o(N_o) = \varphi(i[N_o])$. Let further $E : \mathcal{N} \to \mathcal{N}_o$ be the canonical conditional expectation with respect to the state φ, satisfying $\varphi_o \circ E = \varphi$. The sense in which $\{\mathcal{N}, \alpha, E\}$ is a dilation of $\{\mathcal{N}_o, \gamma\}$ is that

$$(58)\ \ \forall\,(s, N_o) \in \mathbb{R}^+ \times \mathcal{N}_o\ :\ \gamma_s[N_o] \,=\, E \circ \alpha_s \circ i\,[N_o] \quad .$$

For details, see [Emch, 1976] where, in particular, this result was noted to be very reminiscent of the classical flow of Brownian motion constructed by Hida [Hida, 1970] who also proved that this flow is a classical Kolmogorov flow, in the sense of the following definition.

DEFINITION 16. A classical dynamical system $\{\Omega, \mathcal{E}, \mu, \alpha^*\}$ consisting of a probability space $\{\Omega, \mathcal{E}\}$, a probability measure μ, and a group $\{{\alpha^*}_t \mid t \in \mathbb{R}\}$ of automorphisms of $\{\Omega, \mathcal{E}\}$ such that $\forall\, t \in \mathbb{R}\ :\ \mu \circ {\alpha^*}_t = \mu$, is said to be a classical Kolmogorov flow whenever there exists a $\sigma-$subring $\mathcal{A} \subset \mathcal{E}$ such that, with the notation $\mathcal{A}_t = {\alpha^*}_t[\mathcal{A}]$:

(1) $\forall\, t > 0\ :\ \mathcal{A} \subset \mathcal{A}_t$; (2) $\bigvee_{t\in\mathbb{R}} \mathcal{A}_t = \mathcal{E}$; and (3) $\bigwedge_{t\in\mathbb{R}} \mathcal{A}_t = \{\emptyset, \Omega\}$.

Kolmogorov flows are characterized among classical dynamical systems by their having strictly positive dynamical entropy; thus they sit pretty high in the classical ergodic hierarchy, above the Lebesgue spectrum condition, and thus above the weaker conditions of mixing and ergodicity; for didactic accounts, cf. e.g. [Arnold and Avez, 1968; Cornfeld *et al.*, 1982].

The conservative quantum dynamical system described above as the canonical dilation of a contractive semigroup, does satisfy a quantum generalization of definition 16, namely:

DEFINITION 17. A quantum dynamical system $\{\mathcal{N}, \varphi, \alpha\}$ consisting of a von Neumann algebra $\mathcal{N}$, a faithful normal state φ on $\mathcal{N}$, and a group $\alpha = \{\alpha_t \mid t \in \mathbb{R}\}$ of automorphisms of $\mathcal{N}$, with $\forall\, t \in \mathbb{R}\ :\ \varphi \circ \alpha_t = \varphi$, is said to be a generalized Kolmogorov flow whenever there exists a von Neumann subalgebra $\mathcal{A} \subset \mathcal{N}$ such that, with the notation $\mathcal{A}_t = \alpha_t[\mathcal{A}]$:

(1) $\forall\, t > 0\ :\ \mathcal{A} \subset \mathcal{A}_t$; (2) $\bigvee_{t\in\mathbb{R}} \mathcal{A}_t = \mathcal{N}$; (3) $\bigwedge_{t\in\mathbb{R}} \mathcal{A}_t = \mathbb{C}I$; and

$$(4)\ \ \forall\, t \in \mathbb{R}\ :\ \tau_t[\mathcal{A}] = \mathcal{A}\,,$$

where $\{\tau_t \mid t \in \mathbb{R}\}$ is the modular group canonically associated to φ.

REMARKS 18.

1. The $\bigvee$ in condition (2) involves a weak-operator closure, namely (2) means that $\mathcal{N}$ is the smallest von Neumann algebra that contains all the $\mathcal{A}_t$; the $\bigwedge$ in condition (3) is simply the usual intersection; thus (3) signifies that no operator belongs to all $\mathcal{A}_t$ unless it is a multiple of the identity.

2. The modular group τ will be introduced in section 4; let it suffice to say here that, if we were dealing with a finite system, τ would be the group of automorphisms of $\mathcal{N}$ associated to the Hamiltonian corresponding to von Neumann's canonical equilibrium density matrix.

3. Definition 17 encompasses definition 16 when $\mathcal{N}$ is taken to be the abelian von Neumann algebra $\mathcal{L}^\infty(\Omega, \mathcal{E})$ acting on the Hilbert space $\mathcal{H} = \mathcal{L}^2(\Omega, \mathcal{E}, \mu)$; in this case $\forall\, t \in R\,:\ \tau_t = id$, and condition (4) is then trivially satisfied.

4. In the general case, condition (4) is necessary to ensure the existence of a conditional expectation $E : \mathcal{N} \to \mathcal{A}$.

5. Except for the positivity of the dynamical entropy — which depends on a consensus that is still pending about a physically meaningful definition of quantum dynamical entropy; see nevertheless [Narnhofer and Thirring, 1994b; Tuyls, 1998] and references therein — all the ergodic properties of classical Kolmogorov systems carry over straightforwardly from the classical to quantum realm [Emch, 1976]. In the model described above these properties are exhibited in the quantum triple $\{\mathcal{N}, \varphi, \alpha\}$.

6. Definition 17 was first proposed in [Emch, 1976]. Generalizations of this definition, involving the passage from W^*- to C^*-algebras, were then explored in [Narnhofer and Thirring, 1989].

7. The material of the present remark may be found in [Arnold and Avez, 1968] and is inserted here only as a preparation for the next remark. In classical ergodic theory the next rung up the ergodic ladder, just above Kolmogorov flows, is occupied by Anosov flows. These flows formalize an observation made in 1898 by Hadamard, namely that the geodesics on manifolds of negative curvature exhibit exponential sensitivity to initial conditions, in contrast with the usual linear sensitivity characteristic of free flows on flat manifolds. If the manifold is furthermore compact, one may intuitively expect that Hadamard's observation entails some kind of mixing behaviour. This is indeed the case: the first ever Hamiltonian flow shown to be ergodic — the geodesic flow on a compact surface of constant negative curvature — is already an Anosov flow. These flows exhibit exponentially contracting and expanding directions transversal to the direction of the flow, thus prefiguring a microscopic explanation for the empirically observed Lyapunov coefficients. The discrete-time archetype is the Arnold CAT map operating of the torus $T^2 := \mathbb{R}^2/\mathbb{Z}^2$. One ought to note that up to Kolmogorov flows, classical ergodic theory may be viewed as a chapter in probability theory; Anosov flows, in addition, involve an essential appeal to differential geometry, as was recognized only in the second half of the twentieth century through the work of the Russian school.

8. In order to explore possible quantum extensions of the concept of Anosov flow, a quantum analog of the latter has been devised by the present author in collaboration with Narnhofer, Sewell and Thirring [Emch *et al.*, 1994a]; for an antecedent, see [Benatti *et al.*, 1991a]; for a discussion of dynamical entropy in this context, see [Andries *et al.*, 1995]; for reviews and some general perspectives, see [Narnhofer, 2001; Narnhofer, 2005].

One essential feature of this extension is that now the phase space of this quantum CAT map is the noncommutative torus T^2_θ, an ubiquitous staple of Connes' noncommutative geometry; cf. e.g. [Connes, 2000, section XIII] or [Garcia–Bondia *et al.*, 2003, chapter 12]; and for the place these tori occupy in the geometric quantization programme, cf. [Emch, 1998b]. As for quantum ergodic theory, it was noted already in [Emch *et al.*, 1994a] that the generators of the expanding and contracting horocycles form a basis in the 2-dimensional distinguished space of derivations that are not approximately inner — i.e. cannot be uniformly approximated by inner derivations [Garcia–Bondia *et al.*, 2003, section 12.3].

The presence of expanding and contracting directions in quantum as well as in classical Anosov flows offers a bridge from classical to quantum chaos. The problem of what is quantum chaos — or what it ought to be — has received attention from different prospectives; cf. e.g. [Gutzwiller, 1990]; for a philosophical perspective, cf. [Belot and Earman, 1997], and for a recent review, cf. in this volume [Landsman, 2006, section 5.6].

The investigations sketched in this remark, with applications to QSP in view, also have a mathematical parallel in QFT, cf. [Borchers, 1999; Wiesbrock, 1997]; see also subsection 5.5 below.

Summary and warning. It seems fair to infer that the *mathematical* generalization of classical ergodic kinematics to the quantum realm will carry through quite well. Nevertheless, the discussion of the underlying *physical* dynamics, when confronted with Hamiltonian mechanics, does not fare any more smoothly in the quantum case than it does in the classical case. Some of the conceptual problems may already be illustrated with the help of the model discussed at the beginning of this subsection. There, the dissipative dynamical system $\{\mathcal{N}_o, \gamma\}$ may be viewed as the reduced dynamics of two different conservative dynamical systems; both of these act on the same infinite assembly of harmonic oscillators. From the first system the reduced dynamics obtains only through the van Hove limit which compounds the very long-time effects — on a single subsystem — of a very weak coupling with, and within, the bath. But there is nothing in common between the time scale of the dynamics that governs the original conservative system and the time scale pertaining to the other conservative system, viz. the one obtained as the canonical dilation of the dissipative system. So there is little reason to believe that the ergodic behaviour of the latter reflects any global dynamical property of the former.

While this may be blamed on some naive modeling, it nevertheless emphasizes that the time scale of the conservative microscopic description and that of the emerging macroscopic description may differ significantly. In more sophisticated models, this will have to be taken into consideration and the complicated behaviour of the microscopic description may have to be washed away — one way or another — before a clean ergodic behaviour is manifested at the macroscopic level. It appears that van Hove's idea is a reasonable way to do this; see subsection 6.1

below.

Starting with their initial motivation in Boltzmann's works, most presentations of classical ergodic theory focus on the properties of the time-evolution, in particular on the transitivity of measures and the *time*-averages of observables. Its generalization to the quantum realm invites the consideration of other aspects of classical ergodic theory, namely the *space* averages with respect to the actions of *other* groups beside those that govern the evolution. This will be done in the second part of this subsection.

B. Ergodicity with respect to space

As was already recognized by Haag [1959b] for QFT, the "other" group of most immediate relevance to QSP is the group of space translations, introduced as a part of the postulate of covariance in the Haag–Kastler axioms; cf. postulate 13 above. With $n = 1, 2, \dots$, let $\mathbb{X}^n$ denote either the Euclidean space $\mathbb{R}^n$ or the "cubic" lattice $\mathbb{Z}^n$; and let $|x|$ denote the length of the vector $x \in \mathbb{X}^n$. Henceforth, we concentrate on the abelian group $G \simeq \mathbb{X}^n$ of all translations $x \in \mathbb{X}^n \mapsto x+a \in \mathbb{X}^n$ where $a \in \mathbb{X}^n$. Let further $\{\mathcal{A}_\Lambda \mid \Lambda \in \mathcal{F}\}$ be the corresponding Haag–Kastler net of local algebras, and $\mathcal{A}$ be their C^*- inductive limit, with $\mathcal{A}$ equipped with the group of automorphisms $\{\nu_a \mid a \in X^n\}$ defined as in corollary 14. Let again $\mathcal{A}_o \subset \mathcal{A}$ denote the algebra of local observables. For any fixed pair (Λ_1, Λ_2) of elements in $\mathcal{F}$, there exists $a_{12} \in G$ such that $a[\Lambda_1] \bowtie \Lambda_2$ for all $a \in G$ with $|a| > |a_{12}|$. Consequently, by locality (see postulate 11) whenever $a \in G$ with $|a| > |a_{12}|$, $A_1 \in \mathcal{A}_1$ and $A_2 \in \mathcal{A}_2$, we have $\nu_a[A_1]\, A_2 = A_2\, \nu_a[A_1]$. By continuity, this entails

COROLLARY 19. *For all* $A, B \in \mathcal{A}$: $\lim_{|a|\to\infty} \| \nu_a[A]\, B - B\, \nu_a[A] \| = 0$, *i.e. the group* G *of translations acts on the algebra* $\mathcal{A}$ *of quasi-local observables in a* norm-asymptotic abelian manner.

This property makes no sense in the original von Neumann framework for the quantum mechanics of finite systems. In the generalized Haag–Kastler framework devised for infinite systems, this statement which is straighforwardly correct for space translations is rarely satisfied by the time evolution in realistic models that have been controlled.

This raises three questions: the first is whether this property has useful consequences; the second is whether this property can be weakened without jeopardizing the consequences that may be derived from it; and the third is whether any of the weakened forms of this property may be satisfied by the time evolution. I will argue that the answers to the first two questions are "yes". Specifically, in regard to the first question, see in particular corollary 30 below; and in response to the second, see the forthcoming theorem 25. However, here again, I will warn against the seduction of hypotheses that may ensure a positive answer to the third question, but may be hard to satisfy in specific models; see also the last paragraph in 5.4.B and remark 63(6) below.

DEFINITION 20. A state φ on the algebra $\mathcal{A}$ of quasi-local observables is said to

be translation invariant whenever $\forall\,(a,A)\in G\times\mathcal{A}\,:\,\varphi(\nu_a[A])=\varphi(A)$, a situation denoted by $\varphi\circ\nu=\varphi$. The state φ is said to be extremal translation invariant if it is translation invariant and may not be written as a convex sum of different translation invariant states.

With G denoting the group of translations of $\mathbb{X}^n=\mathbb{R}^n$ or $\mathbb{Z}^n$, G is trivially identified with $\mathbb{X}^n$. Let $\mathcal{C}=\mathcal{C}(G)$ be the set of all complex-valued, continuous, bounded functions $f:G\to\mathbb{C}$. Henceforth, this set is equipped with the usual point-wise addition and multiplication of functions, and with the sup-norm $\|f\|=\sup_{x\in G}|f(x)|$. These operations equip $\mathcal{C}$ with the structure of an (abelian) C^*-algebra. Define then an action of G on $\mathcal{C}$ by $a[f](x)=f(x-a)$.

DEFINITION 21. With the above notations, an invariant mean on $\mathcal{C}$ is a state η on $\mathcal{C}$ such that $\forall\,(a,f)\in G\times\mathcal{C}\,:\,\eta(a[f])=\eta(f)$.

Given $\mathbb{X}^n$, there are several such means. For instance, the ergodic mean on $\mathbb{R}$ may be defined as follows. Let $\mathcal{C}_e=\{f\in\mathcal{C}\mid\lim_{a\to\infty}1/2a\int_{-a}^{a}dx\,f(x)\ \text{exists}\}$. Then $\forall\,f\in\mathcal{C}_e$, let $\eta_e(f):=\lim_{a\to\infty}1/2a\int_{-a}^{a}dx\,f(x)$; which then extends by continuity to $\mathcal{C}$, so as to give an invariant mean, which is the one I will prefer to use in the sequel. One may wish to define similarly the mean η_+ on $\mathcal{C}_+=\{f\in\mathcal{C}\mid\lim_{x\to\infty}f(x)\ \text{exists}\}$. And, similarly, another mean η_- obtains from the functions that admit a limit as $x\to-\infty$.

To define averages of states and of observables, notice that for every state φ on the algebra $\mathcal{A}$ of quasi-local observables and any $A,B\in\mathcal{A}$, the functions $\varphi(\nu_\bullet[A]B):a\in G\mapsto\varphi(\nu_a[A]B)\in\mathbb{C}$ — here the symbol $\bullet$ serves as a reminder to mark the place of the variable a — are continuous and bounded, namely by $\|A\|\,\|B\|$. Thus the functions $\varphi(\nu_\bullet[A]B)$ belong to $\mathcal{C}$. When $B=I$ we write simply $\varphi(\nu_\bullet[A])$ for $\varphi(\nu_\bullet[A]I)$. With these notations, the following definition makes sense.

DEFINITION 22. Given an invariant mean η on $\mathcal{C}$ and any state φ on the algebra $\mathcal{A}$ of quasi-local observables, the average $\eta[\varphi]$ of the state φ is defined as the translation invariant state

$$\eta[\varphi]:A\in\mathcal{A}\mapsto\eta\left(\varphi(\nu_\bullet[A])\right)\in\mathbb{C}\quad.$$

A translation invariant state φ is said to be $\eta-$clustering whenever

$$\forall\,A,B\in\mathcal{A}\,:\,\eta\left(\varphi(\nu_\bullet[A]\,B)\right)=\varphi(A)\,\varphi(B)\quad.$$

Warnings concerning terminology:

1. $\eta-$clustering is also referred to as "weak clustering".

2. $\eta-$clustering should not be confused with the stronger property called "weak mixing", namely

$$\forall\,A,B\in\mathcal{A}\,:\,\eta\,|\varphi(\nu_\bullet[A]\,B)\,-\,\varphi(A)\,\varphi(B)|=0$$

where for any complex number z, $|z|$ denotes absolute value of z. The name "weak mixing" conforms to the usage in classical ergodic theory, cf. e.g. [Arnold and Avez, 1968, p. 21].

3. The property simply called *clustering* does not involve averaging, and thus is stronger; it is:

$$\forall\, a \in \mathbb{R}^n \text{ and } \forall\, A, B \in \mathcal{A} : \lim_{\lambda\to\infty} \varphi(\nu_{\lambda a}[A]\, B) = \varphi(A)\, \varphi(B) \quad .$$

This property is called "mixing" in classical ergodic theory, cf. e.g. [Arnold and Avez, 1968, p. 20].

4. An even stronger property is introduced in definition 27 below.

5. Each of the above properties expresses how much the correlations between $\nu_a[A]$ and B decay with large distances $|a|$ when the system is in the state φ. The term "clustering" affixed to these properties, also used in QFT, seems to be inherited from scattering theory where it expresses the asymptotic independence of separate scattering products, or "clusters".

The definition of the average of an observable is a little bit more involved. For the general mathematical framework, cf. e.g. [Emch, 1972a, subsection 2.2.d]; in particular, for the general statements and proofs corresponding to scholium 23 and theorem 25 below, cf. [Emch, 1972a, lemma, pp. 174–175] and [Emch, 1972a, theorem 8, pp. 183–184]. Note that, here, the asymptotic abelianness of the action of the group of space translations — corollary 19 above — allows the simpler presentation offered below. *This is where global observables* — cf. definition 15 above — *enter the picture.*

Let φ be a translation invariant state on the algebra $\mathcal{A}$ of quasi–local observables, and $\{\pi_\varphi, \mathcal{H}, \Phi\}$ be the GNS triple associated to φ. Let further $\mathcal{N}_\varphi = \pi_\varphi(\mathcal{A})''$ and $\mathcal{Z}_\varphi = \mathcal{N}_\varphi \cap \mathcal{N}'_\varphi$.

For $a \in G$ fixed, and A running over $\mathcal{A}$, the map $\pi_\varphi(A)\Phi \in \mathcal{H} \mapsto \pi_\varphi(\nu_a[A])\Phi \in \mathcal{H}$ extends uniquely to a unitary operator $U_a \in \mathcal{U}(\mathcal{H}) := \{U \in \mathcal{B}(\mathcal{H}) \mid U^*U = UU^* = I\}$. This defines a continuous unitary representation $U : a \in G \mapsto U_a \in \mathcal{U}(\mathcal{H})$ such that $\forall\, (a, A) \in G \times \mathcal{A} : U_a \pi_\varphi(A) U_a^* = \pi_\varphi(\nu_a[A])$.

As usual, let $U(G)' := \{B \in \mathcal{B}(\mathcal{H}) \mid \forall\, a \in G : U_a B = B U_a\}$ denote the commutant of $U(G)$. Equivalently here, $U(G)' = \{B \in \mathcal{B}(\mathcal{H}) \mid \forall\, a \in G : U_a B U_a^* = B\}$.

Finally, let $\mathcal{P} := \{\Psi \in \mathcal{H} \mid \forall\, a \in G : U_a \Psi = \Psi\}$; and denote by P the orthogonal projector from $\mathcal{H}$ onto $\mathcal{P}$.

SCHOLIUM 23. For every invariant mean η on $\mathcal{C}$, the map

$$\eta_\varphi : A \in \mathcal{A} \mapsto \eta_\varphi[A] \in \mathcal{Z}_\varphi \cap U(G)'$$

defined, for all $A \in \mathcal{A}$ by

$$\forall\ \Psi_1, \Psi_2 \in \mathcal{H} : (\Psi_1, \eta_\varphi[A]\Psi_2) = \eta\,(\Psi_1, \pi_\varphi(\nu_\bullet[A])\Psi_2)$$

is a $^*-$homomorphism and satisfies $\eta_\varphi[A]\,P = P\,\eta_\varphi[A] = P\,\eta_\varphi[A]\,P$.

DEFINITION 24. Let η be an invariant mean on $\mathcal{C}$; φ be a translation invariant state on the algebra $\mathcal{A}$ of quasi-local obervables; $\mathcal{N}_\varphi = \pi_\varphi(\mathcal{A})''$ be the algebra of global observables associated to the state φ, via the GNS triple $\{\pi_\varphi, \mathcal{H}, \Phi\}$; and $\mathcal{N}_\varphi^G = \{N \in \mathcal{N}_\varphi \mid \forall\, a \in G : U_a N U_a^* = N\}$ be the algebra of translation invariant global observables. Then the average of a quasi-local observable $A \in \mathcal{A}$ is defined as the translation invariant global observable $\eta_\varphi[A] \in \mathcal{N}_\varphi^G$.

We are now ready to enunciate the central quantum ergodic theorem relative to the action of the group of space translations.

THEOREM 25. *Let $\nu : a \in G \to \mathrm{Aut}(\mathcal{A})$ denote the action of the space-translation group on the algebra $\mathcal{A}$ of quasi-local observables; and let η be any invariant mean on $\mathcal{C}$. Then the following conditions on a translation invariant state φ on $\mathcal{A}$ are equivalent:*

1. *φ is extremal translation invariant;*
2. *φ is $\eta-$clustering, i.e. $\forall\, A, B \in \mathcal{A} :\ \eta\,(\varphi(\nu_\bullet[A]\,B)) = \varphi(A)\,\varphi(B)$;*
3. *the canonical extension $\tilde{\varphi} : N \in \mathcal{N}_\varphi \mapsto (\Phi, N\,\Phi) \in \mathbb{C}$ of φ to the von Neumann algebra $\mathcal{N}_\varphi$ of global observables associated to φ is the only translation invariant normal state on this algebra;*
4. *the invariant subspace $\mathcal{P} \subset \mathcal{H}$ is one-dimensional;*
5. *the average $\eta_\varphi[A]$ of every quasi-local observable $A \in \mathcal{A}$ is a multiple of the identity, namely $\eta_\varphi[A] = \varphi(A)\,I$;*
6. *all translation invariant global observables $N \in \mathcal{N}_\varphi^G := \mathcal{N}_\varphi \cap U(G)'$ are multiples of the identity;*
7. *$\mathcal{Z}_\varphi \cap U(G)' = \mathbb{C}\,I$ where $\mathcal{Z}_\varphi := \mathcal{N}_\varphi \cap \mathcal{N}_\varphi{}'$.*

REMARKS 26.

1. Recall that in definition 15 three kinds of observables were introduced. The *local* observables relative to some finite region Λ are described in the original von Neumann formalism [von Neumann, 1932c] where, typically, $\mathcal{A}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda)$, and $\mathcal{H}_\Lambda = \mathcal{L}^2(\Lambda, dx)$. Thus one refers to local observables as self-adjoint elements of $\mathcal{A}_o = \cup_{\Lambda \in \mathcal{F}} \mathcal{A}_\Lambda$. The *quasi-local observables,* defined abstractly as observables that are norm-limits of local observables, pertain to the microscopic description of many-body systems that are infinitely extended in space; section 5 below opens with three concrete QSP examples. These 'quasi-local' observables belong to the C^*-algebra $\mathcal{A} = {}^n\overline{\mathcal{A}_o}$. Observables of the third kind, the *global observables,* appear at the macroscopic level when bulk properties of matter are investigated; they belong to the von Neumann algebra $\mathcal{N}_\varphi := \pi_\varphi(\mathcal{A})''$ obtained as the weak-closure of the

GNS representation π_φ (of $\mathcal{A}$) corresponding to a state φ (on $\mathcal{A}$) specifically obtained by a process called the thermodynamical limit, several examples of which are discussed in the following sections.

Space averages are examples of such *global observables.* A concrete example in ferromagnetism obtains with any one of the three components of the magnetization. Observables of this third kind depend on the global state of the system considered, thus reflecting the preparation of the system. For instance, when the state is extremal translation invariant, these observables are multiples of the identity operator — recall the equivalence of conditions (1) and (5) in theorem 25 — hence their value is the same in all configurations that differ only locally from the given state. Their assuming different values in configurations that differ globally from one another serves as witness for the existence of different thermodynamical phases; cf. subsection 5.7.

2. A global state φ on $\mathcal{A} = {}^n\overline{\mathcal{A}_o}$ with $\mathcal{A}_o = \bigcup_{\Lambda\in\mathcal{F}} \mathcal{A}_\Lambda$ is usually defined by continuity from

$$(59)\ \ \forall\,\Lambda \text{ and } \forall\, A_\Lambda \in \mathcal{A}_\Lambda \quad : \quad \varphi(A_\Lambda) = \lim_{\substack{|\Omega|\to\infty,\\ \Omega\in\mathcal{F},\Omega\supseteq\Lambda}} \varphi_\Omega(A_\Lambda)$$

where $\{\varphi_\Omega | \Omega \in \mathcal{F}\}$ is a consistent family of local states. The local states are themselves defined with respect to some consistent boundary conditions; e.g. periodic boundary conditions on every Λ. Hence, the global state φ and thus the von Neumann algebra $\mathcal{N}_\varphi := \pi_\varphi(\mathcal{A})''$ of global observables may depend on the boundary conditions one has chosen. This happens in particular in the presence of the long-range order that often accompanies the onset of phase transitions. This dependence on initial conditions, *even in the thermodynamical limit,* is an ubiquitous phenomenon, known already in classical statistical physics.

Indeed, in an argument that was later confirmed to be correct — for references, cf. e.g. [Emch and Liu, 2002, pp. 416–417] — Peierls [1936] pointed out the fact that the Ising model in two dimensions develops, for sufficiently low temperatures, a sensitivity to boundary conditions: one phase — say the one with strictly positive magnetization — may be selected by clamping all spins on the boundary in the "up" position.

3. Here again, in the special case where $\{\mathcal{N}, \varphi\}$ is $\{\mathcal{L}^\infty(\Omega), \mu\}$, the above theorem reduces to the known classical case. Note however that the theorem is stated here for *space translations* rather than for the *time evolution;* the reason is that the proof uses asymptotic abelianness which space translations satisfy — see corollary 19 above — or some weakened form such as (61) in remark 31 below. Yet, even such a weakened form of asymptotic abelianness is hard to come by for the time evolution of quantum dynamical models.

The clustering condition (2) in the theorem may be strengthened when the representation π_φ is primary, i.e. when the center $\mathcal{Z}_\varphi := \pi_\varphi(\mathcal{A})'' \cap \pi_\varphi(\mathcal{A})'$ satisfies $\mathcal{Z}_\varphi = \mathbb{C}I$. Specifically, for any region $\Lambda \in \mathcal{F}$, let

$$\mathcal{A}_\Lambda{}^c := {}^n\overline{\cup_{\Omega\in\mathcal{F};\Omega\bowtie\Lambda}\mathcal{A}_\Omega},$$

where, for any subset $\mathcal{B} \subset \mathcal{A}$, ${}^n\overline{\mathcal{B}}$ denotes the closure of $\mathcal{B}$ in the norm-topology of $\mathcal{A}$. As a consequence of locality $A \in \mathcal{A}_\Lambda$ and $B \in \mathcal{A}_\Lambda{}^c$ entail $AB - BA = 0$. Let now $\mathcal{N}_{\varphi,\Lambda}{}^c := \pi_\varphi(\mathcal{A}_\Lambda{}^c)''$.

DEFINITION 27. A state φ on the algebra $\mathcal{A}$ of quasi-local observables is said to be uniformly clustering whenever for any $A \in \mathcal{A}$ and every $\epsilon > 0$, there exists a region $\Lambda \in \mathcal{F}$ depending on A and ϵ, such that

(60) $\forall\, B \in \mathcal{A}_\Lambda{}^c : |\varphi(AB) - \varphi(A)\varphi(B)| \leq \epsilon\,\|B\|$.

DEFINITION 28. The elements of the von Neumann algebra $\mathcal{N}_\varphi{}^\infty := \bigcap_{\Lambda\in\mathcal{F}} \mathcal{N}_{\varphi,\Lambda}{}^c$ are called observables at infinity with respect to φ.

SCHOLIUM 29. For each state φ separately, the observables at infinity are central, i.e. $\mathcal{N}_\varphi{}^\infty \subseteq \mathcal{Z}_\varphi$. Moreover the following two conditions on a state φ are equivalent:

1. all observables at infinity are multiples of the identity operator, i.e. $\mathcal{N}_\varphi{}^\infty = \mathbb{C}\,I$;
2. φ is uniformly clustering.

Note that definitions 27, 28 and scholium 29 do not require that φ be space-translation invariant, although they involve in an essential manner the local structure of $\mathcal{A}$. For space-translation invariant states one has in addition:

COROLLARY 30. *The following two conditions:*

1. *φ is a translation invariant state on the algebra $\mathcal{A}$ of quasi-local observables;*
2. *the algebra $\mathcal{N}_\varphi$ of global observables is a factor, i.e. $\mathcal{Z}_\varphi = \mathbb{C}\,I$*

jointly entail that

a. *φ is extremal translation invariant (and so satisfies the equivalent conditions noted in theorem 25);*
b. *φ is uniformly clustering.*

REMARKS 31.

1. Condition (2) in corollary 30 is satisfied whenever φ is an extremal KMS state; cf. subsection 5.6 below.
2. The proofs of theorem 25, scholium 29, and corollary 30 are not trivial, but they were all known by the early 1970s; cf. e.g. [Emch, 1972a, theorem II.2.8 and theorem IV.1.7].

3. In particular, the proof of theorem 25 shows that the equivalence of its seven conditions may be obtained in more general contexts where the action of the group of space translations is replaced by an action with respect to which the invariant state φ satisfies the condition of $\eta-$*abelianness,* namely the condition:

   (61) $\forall\, A, B, C \in \mathcal{A} : \eta\,\{\varphi(C^*[\nu_g[A]\,B - B\nu_g[A]]C)\} = 0$.

   This condition is much weaker that the norm-asymptotic abelianness proven in corollary 19 for the action of the translation group.

4. It is therefore tempting to try and transfer the above considerations to the group $\mathbb{R}$ governing the time evolution of a quantum dynamical system. In fact *if* φ is an extremal $\mathbb{R}-$invariant state, then such a dynamical system will be $\eta-$abelian in the sense of (61), *provided* the vector Φ of the GNS representation — which, by construction, is cyclic for $\pi_\varphi(\mathcal{A})$ — is also cyclic for the von Neumann algebra $\pi_\varphi(\mathcal{A})'$, a condition equivalent to the requirement that Φ be separating for the von Neumann algebra $\mathcal{N}_\varphi := \pi_\varphi(\mathcal{A})''$, i.e. $N \in \mathcal{N}_\varphi$ and $N\Phi = 0$ entail $N = 0$. The condition that a von Neumann algebra $\mathcal{N}$ admits a vector Φ that is cyclic for both $\mathcal{N}$ and $\mathcal{N}'$ is referred to by saying that this von Neumann algebra is in standard form; for the relevance of this condition in the present context cf. definition 36 and theorem 39 below. This however only raises again the question of whether φ is extremal under the evolution responsible for the approach to equilibrium. In this respect, we may note that this is the case for the dilated evolution in the example of a chain of weakly coupled harmonic oscillators, discussed at the beginning of this subsection, and in general for the evolution α of generalized Kolmogorov flows; cf. definition 17; see nevertheless the "warning" following remark 18, or subsection 5.4(B).

5. On the mathematical side, quantum ergodic theory may be concerned with group actions more general than space or time translations. In fact, theorem 25 and the third remark just above extend without modifications to the actions of *amenable* groups, i.e. groups $\mathcal{G}$ that admit an invariant mean in the sense of definition 21 (where $G = \mathbb{R}^n$ or $\mathbb{Z}^n$ is replaced by $\mathcal{G}$). For a general presentation of the theory of amenable groups, cf. e.g. [Greenleaf, 1969] or for a brief review geared to applications in QSP [Emch, 1972a, pp. 164–172]. Restricting attention here to locally compact groups, let it suffice to note that compact groups, abelian groups, and semi-direct products thereof are amenable; in particular the rotation groups, translation groups, and Euclidean groups in finite-dimensional Euclidean spaces are amenable. However, *no* non-compact semi-simple Lie group is amenable, so that in particular the Lorentz group of 4-dimensional relativisitic QFT is *not* amenable.

6. Pushing the theory even further than amenable group actions may be done by considering "large groups of automorphisms" of a C^*-algebra $\mathcal{A}$, i.e.

actions $\alpha : \mathcal{G} \to \mathrm{Aut}(\mathcal{A})$ that satisfy for every self-adjoint $A \in \mathcal{A}$ and every $\mathcal{G}-$invariant state φ on $\mathcal{A}$:

$$(62) \quad {}^{w-op}\overline{co\{\pi_\varphi(\alpha_g[A]) \mid g \in \mathcal{G}\}} \cap \pi_\varphi(\mathcal{A})' \neq \emptyset \quad ,$$

where for any subset S of a vector space, $co\{S\}$ denotes the "convex hull" of S, i.e. the collection of all convex combinations of elements in S; and for any set $\mathcal{B} \subset \mathcal{B}(\mathcal{H})$, ${}^{w-op}\overline{\mathcal{B}}$ denotes the closure of $\mathcal{B}$ in the weak-operator topology of $\mathcal{B}(\mathcal{H})$. The notion of *large group of automorphisms* was introduced by Størmer in 1967 who used it soon afterwards to prove a quantum analogue of de Finetti's exchangeability theorem in classical probability theory [Størmer, 1969]; for a review and some applications to the semantic foundations of quantum theory, cf. e.g. [Emch, 2005] and references therein. Note that any amenable group action for which the system is $\eta-$abelian for some mean η is a large group of automorphisms for this system.

Here again, one can hardly resist the conclusion that quantum ergodic theory is now a mature mathematical theory in search of further physical applications to QSP, most notably through the understanding it provides for the various clustering (or mixing) properties described in the present section; cf. e.g. subsections 5.4 and 5.7 below.

4 THE KMS CONDITION FOR EQUILIBRIUM

The identification of the KMS condition as a canonical characterization of equilibrium states appears in the confluence of two currents of thought.

The first source is the recognition by Kubo [1957] and by Martin & Schwinger [1959] that objects which play a central role in condensed matter physics, namely the so-called thermal Green functions — cf. e.g. [Bonch-Bruevich and Tyablikov, 1962] — possess remarkable analytic properties. For a foretaste, see scholium 32 below.

The second source of inspiration is recognizable in the original texts [Murray and von Neumann, 1936] of what was to become the theory of von Neumann algebras, and is emphasized in the candid reminiscences of one of the pioneers of this theory [Murray, 1990]. A great deal of the theory could be built from the following observation: there are matrix algebras $\mathcal{N}$ which, together with their commutant $\mathcal{N}'$, satisfy the following properties:

(i) they are factors, i.e. have trivial center: $\mathcal{N} \cap \mathcal{N}' = \mathbb{C}I$; (ii) $\mathcal{N}$ and $\mathcal{N}'$ admit a common cyclic vector Φ; (iii) there exists an involutive antiunitary operator J such that $J\Phi = \Phi$ and $N \in \mathcal{N} \mapsto JNJ \in \mathcal{N}'$ is bijective. For a concrete, simple example, see equation (71) below.

Each of the two facets of the theory — analytic and algebraic — involves some mathematical intricacies; hence the division of this section into two subsections: first, a simple example; and second, the general theory.

4.1 A Wignerian Approach

In this subsection, I wish to abide by Wigner's famous dictum [Wigner, 1962]: *"Please explain it with* 2×2 *matrices."* Accordingly I proceed with the description of what happens to a quantum 1/2−spin in canonical equilibrium at natural temperature $\beta > 0$ in a magnetic field B parallel to the z-axis. The observables are the self-adjoint elements of the algebra $\mathcal{M}$ of 2×2 matrices with complex entries. The Hamiltonian is

$$(63)\quad H = -B\sigma^z = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} \quad \text{with} \quad \epsilon_1 = -B\ ,\ \epsilon_2 = +B.$$

The canonical equilibrium state is, according to von Neumann's characterization (38):

$$(64)\quad \psi_H : M \in \mathcal{M} \to \mathrm{Tr}(\rho_H M) \quad \text{with} \quad \rho_H = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

where $\lambda_n = {Z_H}^{-1} \exp(-\beta\epsilon_n)$, with $Z_H = \exp(-\beta\epsilon_1) + \exp(-\beta\epsilon_2)$ denoting the partition function of the system.

In the Heisenberg picture, conjugate to Schrödinger's picture (39), the evolution is

$$(65)\quad \left.\begin{array}{c} \alpha_t : M \in \mathcal{M} \to \alpha_t[M] = U^*(t) M U^*(-t) \in \mathcal{M} \\ \text{with} \quad U^*(t) = \begin{pmatrix} e^{i\epsilon_1 t} & 0 \\ 0 & e^{i\beta\epsilon_2 t} \end{pmatrix} . \end{array}\right\}$$

To make computations easier and, moreover, immediately generalizable to higher dimensions, consider the matrices

$$E_{mn} : \Psi \in \mathbb{C}^2 \mapsto (\Psi_n, \Psi)\Psi_m \in \mathbb{C}^2$$

where $\{\Psi_n \mid n = 1, 2\}$ are eigenvectors of H, i.e. with

$$\Psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\ ;\ \Psi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\ :$$

$$E_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix};\quad E_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix};\quad E_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix};\quad E_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

These matrices form a basis in $\mathcal{M}$ and — with ψ_H and α_t as in (64) and (65) — satisfy

$$E_{kl}E_{mn} = \delta_{lm}E_{kn}\ \ ,\ \ \psi_H(E_{mn}) = \lambda_m\delta_{mn}\ \ ,\ \ \alpha_t(E_{mn}) = e^{i(\epsilon_m - \epsilon_n)t}E_{mn}\ .$$

From these relations and the identity $\exp[-\beta(\epsilon_m - \epsilon_n)]\lambda_n = \lambda_m$, one obtains that the analytic functions

$$f_{klmn} : z \in \mathbb{C} \to \lambda_n\, e^{i(\epsilon_m - \epsilon_n)z}\delta_{lm}\delta_{kn}$$

satisfy $\forall\, t \in \mathbb{R}:\ f_{klmn}(t) = \psi_H(E_{kl}\alpha_t[E_{mn}])$ and $f_{klmn}(t+i\beta) = \psi_H(\alpha_t[E_{mn}]E_{kl})$. Moreover, on the strip

$$\Omega_\beta := \{z \in \mathbb{C} \mid 0 \leq \operatorname{Im} z \leq \beta\}\,,$$

the analytic functions f_{klmn} are bounded, namely by $\exp(|\epsilon_m - \epsilon_n|\,\beta)$.

These two properties of the canonical equilibrium state ψ_H extend by linearity to the time correlation functions

$$(66)\quad f_{MN}(t) = \psi_H(M\alpha_t[N]) \quad \text{and} \quad f_{MN}(t+i\beta) = \psi_H(\alpha_t[N]M)$$

with M and N arbitrary in $\mathcal{M}$.

Conversely, suppose that φ is a state on $\mathcal{M}$ such that for every pair M, N of elements in $\mathcal{M}$ there exists a function $f_{M,N} : z \in \Omega_\beta \mapsto f_{M,N}(z) \in \mathbb{C}$ such that

(i) $f_{M,N}$ is bounded and continuous on the strip Ω_β ;

(ii) $f_{M,N}$ is analytic inside that strip;

(iii) for all $t \in \mathbb{R}$: $f_{M,N}(t) = \varphi(M\alpha_t[N])$ and $f_{M,N}(t+i\beta) = \varphi(\alpha_t[N]M)$.

Then in particular, with $M = I$, the function $f_{I,N}$ is periodic with period $i\beta$. It may then be extended to a function that is both bounded and analytic on the whole complex plane. The classical Liouville's theorem — cf. e.g. [Churchill and Brown, 1990, theorem 43.1] — thus entails that this function must be constant, i.e. for all $(t, N) \in \mathbb{R} \times \mathcal{M}$: $\varphi(\alpha_t[N]) := \operatorname{Tr} U^*(-t)\rho U^*(t)N$ is equal to $\operatorname{Tr}\rho N = \varphi(N)$; and thus

$$\rho = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix}$$

where the values of μ_1 , μ_2 positive with $\mu_1 + \mu_2 = 1$ are computed presently. Upon comparing, for every pair of indices (m, n) the analytic continuation of

$$f_{mn}(t) = \varphi(E_{nm}\alpha_t[E_{mn}]) = e^{i(\epsilon_m - \epsilon_n)t}\mu_n$$

and

$$f_{mn}(t+i\beta) = \varphi(\alpha_t[E_{mn}]E_{nm}) = e^{i(\epsilon_m - \epsilon_n)t}\mu_m$$

one obtains $\exp[-\beta(\epsilon_m - \epsilon_n)]\mu_m = \mu_n$ and thus, upon imposing the normalization $\varphi(I) = 1$, i.e. $\mu_1 + \mu_2 = 1$:

$$\mu_n = \frac{e^{-\beta\mu_n}}{e^{-\beta\mu_1} + e^{-\beta\mu_2}} = \lambda_n \quad .$$

Thus, indeed $\varphi = \psi_H$.

In summary, one obtained by elementary means an elementary illustration of the first facet of the theory, its analytic aspect:

SCHOLIUM 32. Let $H = -B\sigma^z$ be the Hamiltonian describing a spin $\frac{1}{2}$ in a magnetic field B . Then, for any state φ on $\mathcal{M} = \mathcal{M}(2,\mathbb{C})$, the following conditions are equivalent:

(I) φ is the canonical equilibrium state ψ_H with respect to the Hamiltonian H;

(II) for every pair (M,N) of elements of $\mathcal{M}$ there exists a function $f_{M,N} : z \in \Omega_\beta \to \mathbb{C}$ such that

$$(67)\quad \left.\begin{array}{l} f_{M,N} \text{ is bounded and continuous on } \Omega_\beta\,; \\ f_{M,N} \text{ is analytic in the interior of } \Omega_\beta\,; \\ \forall\, t \in \mathbb{R}: \left\{\begin{array}{ll} f_{M,N}(t) & = \varphi(M\,\alpha_t[N]) \\ f_{M,N}(t+i\beta) & = \varphi(\alpha_t[N]\,M) \end{array}\right. \end{array}\right\} \quad .$$

Moving now towards the algebraic aspect of the theory, one pursues with the same simple model, and let φ be a faithful state over $\mathcal{M}$, i.e. a state such that $M \in \mathcal{M}$ and $\varphi(M^*M) = 0$ entail $M = 0$. Without loss of generality one may choose a basis in which the density matrix ρ corresponding to φ is diagonal, with eigenvalues λ_n $(n = 1, 2)$ strictly positive since φ is supposed to be faithful. Consider the representation π of $\mathcal{M}$ given by:

$$(68)\quad \forall\, M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathcal{M} \quad : \quad \pi(M) = \begin{pmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix} = M \otimes I$$

acting on the Hilbert space $\mathbb{C}^4$ equipped with its standard scalar product in which Ψ_{kl} defined by

$$\Psi_{11} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad , \quad \Psi_{21} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad \Psi_{12} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad \Psi_{22} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

is an orthonormal basis. The vector

$$(69)\quad \Phi = \sum_k \lambda_k{}^{\frac{1}{2}}\, \Psi_{kk} = \begin{pmatrix} \lambda_1{}^{\frac{1}{2}} \\ 0 \\ 0 \\ \lambda_2{}^{\frac{1}{2}} \end{pmatrix}$$

satisfies $\Psi_{mn} = \lambda_n{}^{\frac{1}{2}}\, \pi(E_{mn})\Phi$, from which one reads:

$$\mathbb{C}^4 = \{\pi(M)\Phi \mid M \in \mathcal{M}\} \quad \text{and} \quad \forall\, M \in \mathcal{M} : (\Phi, \pi(M)\Phi) = \varphi(M) \quad .$$

Hence $\{\mathcal{H} = \mathbb{C}^4, \pi, \Phi\}$ is the canonical GNS triple associated to the state φ. Moreover, since φ is assumed to be faithful, $\|\pi(M)\Phi\| = 0$ entails $M = 0$, i.e. Φ is also separating for $\pi(\mathcal{M})$. The essential step now is to introduce the two operators J and Δ defined on $\mathcal{H}$ by the conditions that J is antilinear, Δ is linear, with

$$J\Psi_{mn} = \Psi_{nm} \quad \text{and} \quad \Delta\Psi_{mn} = \frac{\lambda_m}{\lambda_n}\Psi_{mn}\ .$$

Note that, since Δ is given here with its spectral resolution, the functions of this operator may be defined by linearity from $f(\Delta) : \Psi_{mn} \in \mathbb{C}^4 \mapsto f(\frac{\lambda_m}{\lambda_n})\Psi_{mn} \in \mathbb{C}^4$. In particular, $\{\Delta^{is} | s \in \mathbb{R}\}$ is a continuous group of unitary operators acting on $\mathbb{C}^4$.

One verifies immediately from their definition above that the operators J and Δ satisfy the following properties. Firstly,

(70) J is an isometry, $J^2 = I$, Δ is self−adjoint, $J\Delta J = \Delta^{-1}$, $J\Phi = \Phi = \Delta\Phi$.

Secondly,

$$(71)\quad J \begin{pmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix} J = \begin{pmatrix} a^* & 0 & b^* & 0 \\ 0 & a^* & 0 & b^* \\ c^* & 0 & d^* & 0 \\ 0 & c^* & 0 & d^* \end{pmatrix} \in I \otimes \mathcal{M}$$

i.e. upon denoting by $\mathcal{N}$ the image $\pi(\mathcal{M})$ of $\mathcal{M}$ through the representation π, we have: $J\mathcal{N}J = \mathcal{N}'$; hence (71) gives an explicit bijection from $\mathcal{N}$ onto its commutant $\mathcal{N}'$. The relation (71) is a particular case of the general Tomita–Takesaki duality (see theorem 39 below).

Thirdly, with $\beta > 0$ arbitrary, but fixed, we have $\forall t \in \mathbb{R} : \Delta^{-it/\beta}\Psi_{mn} = \exp[i(\epsilon_m - \epsilon_n)t]\,\Psi_{mn}$. Hence $\Delta^{-it/\beta}\pi(E_{mn})\Delta^{it/\beta}\Psi_{kl} = \exp[i(\epsilon_m - \epsilon_n)t]\pi(E_{mn})\Psi_{kl}$ with $\epsilon_n = c - (1/\beta)\ln\lambda_n$ where c is an arbitrary real constant. Consequently, the unitary group $\{\Delta^{it/\beta} \mid t \in \mathbb{R}\}$ implements a group of automorphisms of $\mathcal{N}$, namely

$$(72)\quad \tau_t : N \in \mathcal{N} \to \tau_t[N] = \Delta^{-it/\beta} N \Delta^{it/\beta} \in \mathcal{N}$$

with, for all $(t, M) \in \mathbb{R} \times \mathcal{M}$, $\tau_t[\pi(M)] = \pi(\alpha_t[M])$ with $\alpha_t[M] = \exp^{iHt} M \exp^{-iHt}$ and $H = \sum_n \epsilon_n E_{nn}$. Summing up, this establishes that φ is the canonical equilibrium state at natural temperature β for the Hamiltonian H just constructed.

Fourthly, the operator $S = J\Delta^{\frac{1}{2}}$ satisfies $S\,\pi(E_{mn})\Phi = \pi(E_{nm})\Phi$ and thus, since J and therefore S are antilinear:

$$(73)\quad \forall N \in \mathcal{N} : \quad S\,N\,\Phi = N^*\,\Phi \quad .$$

Finally, the generator L of the unitary group $\{\Delta^{it/\beta} \mid t \in T\}$ on $\mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$ is

$$(74)\quad L = H \otimes I - I \otimes H\,,$$

so that the spectrum of L is symmetric around 0 : $Sp(L) = \{\epsilon_2 - \epsilon_1, 0, 0, \epsilon_1 - \epsilon_2\}$.

SCHOLIUM 33. Let $\{\mathbb{C}^4, \pi, \Phi\}$ be the GNS triple canonically associated to a faithful state φ on the algebra $\mathcal{M}$ of 2×2 matrices; and let $\mathcal{N}$ be the von Neumann algebra $\pi(\mathcal{M}) = \{\pi(M) \mid M \in \mathcal{M}\}$ acting on $\mathcal{H} = \mathbb{C}^4$. Then

1. $\mathcal{N}$ is isomorphic to $\mathcal{M}$ and φ may be regarded as a faithful state on $\mathcal{N}$;

2. Φ is both cyclic and separating for $\mathcal{N}$;

3. the anti-linear operator defined by $S : N\Phi \in \mathcal{H} = N^*\Phi \in \mathcal{H}$ has polar decomposition $S = J\Delta^{\frac{1}{2}}$ where J is an involutive, anti-linear isometry from $\mathcal{H}$ onto itself, and Δ is a positive operator acting on $\mathcal{H}$;

4. J establishes a duality between $\mathcal{N}$ and its commutant; specifically: $N \in \mathcal{N} \mapsto JNJ \in \mathcal{N}'$ is an anti-linear bijection;

5. $\{\Delta^{-it/\beta} \mid t \in \mathbb{R}\}$ implements a group of automorphisms τ_t of $\mathcal{N}$ with respect to which the state φ satisfies the analyticity condition described in scholium 32;

6. $J\Phi = \Phi = \Delta\Phi \quad , \quad J^2 = J \quad \text{and} \quad \forall\, s \in \mathbb{R} : J\Delta^{is} = \Delta^{is}J \quad .$

REMARKS 34. Upon surveying the proofs of scholia 32 and 33, one verifies that they can be extended verbatim from $\mathcal{M} = \mathcal{M}(2,\mathbb{C})$ to $\mathcal{M} = \mathcal{M}(n,\mathbb{C})$ where n is any finite positive integer. These scholia extend further to $\mathcal{M} = \mathcal{B}(\mathcal{H})$ where $\mathcal{H}$ is a Hilbert space (with countable basis) provided that:

(i) the Hamiltonian H satisfies $\mathrm{Tr}(-\beta H) < \infty$;

(ii) the state φ is countably additive, retaining the condition that φ be faithful.

Indeed, under these circumstances one can read again the proofs of the scholia, now for the $^*-$algebra $\mathcal{E} = \mathrm{Span}\{\pi(E_{mn}) \mid m,n = 1,\ldots\}$ of all finite linear combinations of the operators $\pi(E_{mn})$ with $E_{mn} : \Psi \in \mathcal{H} \to (\Psi_n, \Psi)\Psi_m \in \mathcal{H}$ where again $\{\Psi_n \mid n = 1,2,\ldots\}$ is an orthonormal basis in $\mathcal{H}$. The extension from $\mathcal{E}$ to the von Neumann algebra $\mathcal{B}(\mathcal{H})$ obtains since the assumptions that φ is countably additive and faithful allow one to use standard continuity arguments, namely here, e.g. [Dixmier, 1957, theorem I.3.5, lemma I.4.4, proposition I.4.1]; or [Kadison and Ringrose, 1983/1986, volume ii, chapter 7]. In particular, $\mathcal{N} = \pi(\mathcal{B}(\mathcal{H})) = \{\pi(\mathcal{M}) \mid M \in \mathcal{B}(\mathcal{H})\}$ is already a von Neumann algebra — i.e. $\mathcal{N} = \mathcal{N}''$ — and is isomorphic to $\mathcal{B}(\mathcal{H})$. Since $\mathcal{B}(\mathcal{H})$ is a factor, so is $\mathcal{N}$, i.e. the center of this von Neumann algebra is trivial: $\mathcal{N} \cap \mathcal{N}' = \mathbb{C}I$. Moreover $\mathcal{N}$ may be identified with $\mathcal{B}(\mathcal{H}) \otimes \mathbb{C}I$ and $\mathcal{N}'$ with $\mathbb{C}I \otimes \mathcal{B}(\mathcal{H})$.

The von Neumann formalism for quantum mechanics [von Neumann, 1932c] allows one to go this far, but no further. Recall that some of the reasons why one needs to proceed further were indicated in subsection 3.3. The next subsection provides an important tool toward achieving this.

4.2 The Kubo–Martin–Schwinger condition and the Tomita–Takesaki theory

The above results suggest three definitions; the first two are just matters of mathematical terminology, but the third is at the heart of this section.

DEFINITION 35. A state φ on a von Neumann algebra $\mathcal{N}$ is said to be normal whenever it is countably additive., i.e. $\varphi(\sum_n P_n) = \sum_n \varphi(P_n)$ for each countable family $\{P_n\}$ of mutually orthogonal projections in $\mathcal{N}$.

This simply extends to general von Neumann algebras condition (35), already recognized in [von Neumann, 1932c] as the quantum analogue of the complete additivity of probability measures. The next definition formalizes in the present context some of the notions encountered in the motivating examples covered in the previous subsection.

DEFINITION 36. A von Neumann algebra $\mathcal{N}$ acting on a Hilbert space $\mathcal{H}$ is said to be in standard form whenever there exists a vector $\Phi \in \mathcal{H}$ that is both cyclic and separating for $\mathcal{N}$, i.e. $\mathcal{N}\Phi$ is norm dense in $\mathcal{H}$ and for $N \in \mathcal{N}$, $N\Phi = 0$ entails $N = 0$.

REMARKS 37. This concept has been around for a long time, but it seems fair to say that full recognition of its central importance in the general theory of von Neumann algebras had to wait for the Tomita–Takesaki modular theory [Tomita, 1967; Takesaki, 1970a]. At the most basic level, notice that if $\mathcal{N}$ is in standard form, one may assume without loss of generality that $\|\Phi\| = 1$, so that $\varphi : N \in \mathcal{N} \to (\Phi, N\Phi) \in \mathbb{C}$ is a faithful normal state on $\mathcal{N}$.

Conversely it follows, from the same continuity arguments as those used in remark 34 above, that if φ is any normal state on a von Neumann algebra $\mathcal{N}$, the GNS representation π corresponding to φ is already a von Neumann algebra; if φ is faithful, then $\mathcal{N}$ is isomorphic to $\pi(\mathcal{N})$. Thus the canonical GNS vector Φ is not only cyclic, but it is also separating. Hence whenever φ is a faithful normal state, $\mathcal{N}$ is isomorphic to $\pi(\mathcal{N})$ which is a von Neumann algebra presented in standard form

The third definition pertains to the core of this section. It is an adaptation of the work of [Kubo, 1957; Martin and Schwinger, 1959], proposed by [Haag *et al.*, 1967] as an extension of the definition of canonical equilibrium states on the global C^*-algebra to be associated to an infinite system.

DEFINITION 38. Let $\mathcal{A}$ be a C^*-algebra, and let $\alpha : t \in \mathbb{R} \to \alpha_t \in \mathrm{Aut}(\mathcal{A})$ be a group of automorphisms of $\mathcal{A}$. A state φ on $\mathcal{A}$ is said to satisfy the KMS condition with respect to α for the natural temperature β if for every pair (A, B) of elements of $\mathcal{A}$ there exists a function $f_{A,B}$ defined on the strip $\Omega_\beta = \{z \in \mathbb{C} \mid 0 \leq \mathrm{Im} z \leq \beta\}$, such that $f_{A,B}$ is bounded and continuous on Ω_β; $f_{A,B}$ is analytic in the interior of Ω_β; and $\forall\, t \in \mathbb{R} : f_{A,B}(t) = \varphi(A\,\alpha_t[B])$ and $f_{A,B}(t + i\beta) = \varphi(\alpha_t[B]\,A)$.

The main mathematical result of this section, taken from the Tomita–Takesaki modular theory [Tomita, 1967; Takesaki, 1970a], may now be stated.

THEOREM 39 (Tomita–Takesaki). *Let $\mathcal{N}$ be a von Neumann algebra acting on a Hilbert space $\mathcal{H}$ and admitting a cyclic and separating unit vector Φ. Then the closed antilinear operator S obtained as the closure of the map $N\,\Phi \to N^*\,\Phi$, defined for all $N \in \mathcal{N}$, has polar decomposition $S = J\Delta$ where $J = J^2$ is an antilinear isometry from $\mathcal{H}$ onto itself, satisfying $J\mathcal{N}J = \mathcal{N}'$; and Δ is a self-*

adjoint operator (not necessarily bounded!) that is positive, and such that $J\Delta^{it} = \Delta^{it}J$; *and for any* $\beta > 0$ $\forall(t, N) \in \mathbb{R} \times \mathcal{N} : \tau_t[N] = \Delta^{-it/\beta} N \Delta^{it/\beta}$ *defines a group* $\{\tau_t\}$ *of* $^*-$*automorphisms of* $\mathcal{N}$ *with respect to which the faithful normal state* $\varphi : N \in \mathcal{N} \to (\Phi, N\Phi) \in \mathbb{C}$ *satisfies the KMS condition for* β. *Moreover* $\{\tau_t \mid t \in \mathbb{R}\}$ *is the unique group of* $^*-$*automorphisms of* $\mathcal{N}$ *with respect to which* φ *satisfies this condition.*

REMARKS 40.

1. The theorem generalizes to any arbitrary von Neumann algebra in standard form the result we described — in remark 34 — for the GNS representation of $\mathcal{B}(\mathcal{H})$ associated to any of its faithful normal states.

2. It is essential to the purpose of the present review to emphasize that the theorem does *not* require that $\mathcal{N}$ be a factor.

3. Whereas the theorem asserts that the dynamics τ is uniquely determined by the KMS condition, the converse is *not* true: when $\mathcal{N}$ is not a factor, there exist other normal states on $\mathcal{N}$ that also satisfy the KMS condition with respect to the same dynamics. Indeed, when $\mathcal{N}$ is not a factor, one verifies that for every $Z \neq 0$ that belongs to the center $\mathcal{Z} = \mathcal{N} \cap \mathcal{N}'$, $\psi : N \in \mathcal{N} \to [\varphi(Z^*Z)]^{-1}\varphi(Z^*NZ)$ defines a normal state that again satisfies the KMS condition with respect to τ for the same β. This remark, the proof of which will be given in subsection 5.6, is essential to the arguments presented in subsection 5.7.

4. Beyond its mathematical attractiveness, the legitimacy of the conjecture that the KMS condition may be regarded as a definition of canonical equilibrium states in the QSP of macroscopic systems will also be discussed in the next section.

5. Finally, mathematical probity requires us to mention that — factor or not — a major difficulty in the proof of theorem 39 resides in showing that the map $N\Phi \to N^*\Phi$ is closable; for the resolution of this problem, cf. the original papers [Tomita, 1967; Takesaki, 1970a]; it is probably fair to warn the reader that even the didactic presentation in [Kadison and Ringrose, 1983/1986, chapter 9] would have carried us beyond the bounds of this essay. To convey nevertheless an idea of the structures involved in the theorem, I resorted therefore to presenting first the models covered in the preliminary scholia 32 and 33, as these could be treated with mathematically elementary tools. The drawback was however that these models, as well as their routine extensions from $\mathcal{M}(2,\mathbb{C})$ to $\mathcal{B}(\mathcal{H})$ described in remark 34, only involve factors, in fact faithful representations of $\mathcal{B}(\mathcal{H})$, that are not sufficient to cover the macroscopic purposes of QSP where infinitely many degrees of freedom are brought to play. As Haag, Hugenholtz, and Winnink [1967] correctly envisaged, it is the generality involved in theorem 39 that is actually needed in physical applications. The temporal coincidence of this physical intuition

and the arrival on the scene of the mathematical theory of Tomita–Takesaki [1967; 1970a] is a truly remarkable event vividly recounted in [Kadison, 1990, pp. 77–79].

5 KMS CONDITION, QSP AND THERMODYNAMICS

This section presents some of the evidences supporting the physical interpretation of the KMS condition proposed in [Haag *et al.*, 1967] as an alternative definition of equilibrium states in QSP. We already saw that for finite systems the KMS condition is satisfied by the canonical equilibrium states of von Neumann, and only by those states. Now, in subsections 5.1–5.3 models are described to show how the modular structures invented and developed by [Tomita, 1967; Takesaki, 1970a] — which we saw (cf. scholium 33) are realized in finite systems in canonical equilibrium — are also encountered in the equilibrium QSP of infinite systems, thus allowing one to go beyond von Neumann's formalism [von Neumann, 1932c]. In subsection 5.4 various stability conditions are exhibited that give a thermodynamical characterization of KMS states in QSP. A brief excursion is undertaken in subsection 5.5 to indicate some vistas toward the recognition of the role the KMS condition has later been called to play in relativistic QFT, a role dubbed "revolutionary" by the practitioners. Subsection 5.6 is a mathematical interlude devoted to the algebraic characterization of *extremal* KMS states. When we return to QSP in subsection 5.7, systems that exhibit phase transitions are considered and the unique decomposition of any canonical equilibrium state into its pure thermodynamical phases is shown to be closely modeled by a unique decomposition of KMS states into extremal KMS states. In particular, this subsection is oriented toward substantiating the overarching idea that the KMS condition provides the thermodynamics of infinite systems with a conceptual scheme in which phase transitions occur accompanied by spontaneous symmetry breakdown.

5.1 Beyond Fock space: The BCS model

The first indication that something was amiss in the use of the von Neumann formalism in QSP was the Bardeen–Cooper–Schrieffer model for superconductivity, the BCS model. Indeed, in the original treatment of this model [Bardeen *et al.*, 1957], the Hamiltonian chosen to describe a specific interaction between the electrons in a finite but large metallic solid is invariant under gauge transformations of the first kind; an approximation is then proposed, which is asserted to become exact in the infinite volume limit; in this formal process however this symmetry is lost; moreover, the spectrum of the resulting Hamiltonian presents an energy gap that is temperature–dependent. One might argue that the experimentalist may not wish to be concerned with the breaking of that symmetry, but the energy gap cannot be ignored: experimentalists do measure it in the laboratory. Thus, mathematical physicists thought that they ought to understand — how or rather

whether — the Hamiltonian itself may indeed depend on the temperature. Within five years, the culprit was found by Haag [1962] to be that the whole treatment was allegedly carried out in a fixed irreducible representation of the CCR, the then ubiquitous Fock representation, and that this constraint was doing violence to the model.

Specifically, the original Hamiltonian is

$$(75)\quad H_\Lambda = \sum_{p,s} \epsilon(p) a_s(p)^* a_s(p) \;+\; \sum_{p,q} b(p)^* \tilde{v}(p,q) b(q)$$

where Λ is the region of space in which the system is contained, typically a cubic box of finite volume $|\Lambda|$; p and q label momentum and are integer multiples of $2\pi|\Lambda|^{-\frac{1}{2}}$; $s = \pm\frac{1}{2}$; $a_s(p)^*$ and $a_s(p)$ are the creation and annihilation operators for an electron of spin s and momentum p; $\epsilon(p) = -\mu + \frac{1}{2}p^2/2m$ is the energy of a free electron of momentum p; $b(p)^* = a_\uparrow(p)^* a_\downarrow(-p)^*$ is the creation operator of a so-called Cooper pair; and $b(p)^*\tilde{v}(p,q)b(q)$ is the interaction energy between two Cooper pairs, i.e. four electrons, so that the Hamiltonian (75) is *not* quadratic in the original field operators. The form of $\tilde{v}(p,q)$ will be discussed later on.

The approximating Hamiltonian is

$$(76)\quad \tilde{H}_\Lambda = \sum_{p,s} E(p) \gamma_s(p)^* \gamma_s(p)$$

where $\gamma_s(p)^*$ and $\gamma_s(p)$ are the creation and annihilation operators for the elementary excitations given by a Bogoliubov–Valatin transformation

$$(77)\quad \left.\begin{array}{ll} \gamma_\uparrow(p) & = u(p) a_\uparrow(p) + v(p) a_\downarrow(-p)^* \\ \gamma_\downarrow(p) & = -v(-p) a_\uparrow(-p)^* + u(-p) a_\downarrow(p) \end{array}\right\}$$

where

$$(78)\quad \begin{array}{ll} E(p) & = \{\epsilon(p)^2 + [\Delta(p)\Delta(p)^*]\}^{\frac{1}{2}} \\ D(p) & = \{[E(p)-\epsilon]^2 + [\Delta(p)\Delta(p)^*]\}^{\frac{1}{2}} \end{array} \quad ; \quad \begin{array}{ll} u(p) & = \Delta(p)^*/D(p) \\ v(p) & = [E(p)-\epsilon(p)]/D(p) \end{array}$$

and Δ satisfies the all-important self-consistency equation

$$(79)\quad \Delta(p) = -\sum_q \tilde{v}(p,q) \frac{\Delta(q)}{2E(q)} \tanh\left(\frac{1}{2}\beta E(q)\right) \quad .$$

Clearly $\Delta = 0$ is always a solution, in which case the spectra of H and $\tilde{H}$ coincide; this is the normal phase in which nothing particularly interesting happens. The essence of the model is that there is a critical temperature T_c (recall $\beta = 1/kT$) below which an energetically more favorable solution $\Delta \neq 0$ develops. This corresponds to the superconducting phase. We henceforth pursue the discussion for $0 < T < T_c$.

This is the phase we are interested in, and it may be useful to recall in physical terms what the physicists first saw in (76)–(79). BCS devised a limiting procedure — involving the thermodynamical limit and a "mean-field approximation" (weak,

but very long range interaction) — by which the original Hamiltonian (75) and the new Hamiltonian (76) become interchangeable in the sense that they are claimed to lead to the same limit. While (75) is expressed in terms of the electrons' creation and annhilation operators $a_s^\flat(p)$; the new Hamiltonian (76) is free in terms of the elementary excitations $\gamma_s^\flat(p)$. The energy spectrum of these excitations is $\{E(p)\}$ and differs — see (78) — from the energy spectrum $\{\epsilon(p)\}$ of the free electrons by a temperature-dependent "gap" which is observable in the laboratory; the numerical results so obtained for this gap are in very good agreement with the prediction (79); cf. [Schrieffer, 1974, Figure 1–3].

The mathematical picture however demands some explanation. Indeed: (i) the initial Hamiltonian (75) is invariant under the gauge symmetry defined, for any $\theta \in (0, 2\pi]$ by $a_s(p) \to \exp(i\theta)a_s(p)$ whereas the Hamiltonian (76) is not; and (ii) the energy spectrum $\{E(p)\}$ of the Hamiltonian (76) is temperature dependent, whereas there is no temperature dependence in (75).

The question therefore is to account for how one could possibly claim — as was done in the prevailing folklore — that such an approximation could become exact in the thermodynamical limit. For this, one has to examine where Δ comes from, namely that $\Delta(p)$ is a scalar multiple of the identity operator, to be viewed as an approximation of the operator $\hat{\Delta}(p) = \sum_q \tilde{v}(p,q)b(q)$. The argument for this is based on the remark that, under suitable assumptions on $\tilde{v}$, one can arrange for the limit $|\Lambda| \to \infty$ of $\hat{\Delta}(p)$ to exist — in the weak-operator topology — and to commute with all the creation and annihilation operators $a_s(q)^*$ and $a_s(q)$ which generate an algebra which is tacitly assumed to be irreducible. In this limit, the operator $\Delta(p)$ would be replaced by a scalar multiple of the identity. Some "suitable" assumptions seemed to be achieved when $\tilde{v}$ is the double Fourier transform

$$\tilde{v}(p,q) = \int_\Lambda dxdy f(p,x)v(x,y)f(q,y)^* \quad \text{where} \quad f(p,x) = \begin{cases} |\Lambda|^{-\frac{1}{2}} e^{ipx} & x \in \Lambda \\ 0 & x \notin \Lambda \end{cases}$$

with a nonlocal potential v such that $v(x,y)^* = v(y,x)$, $c = \int dxdy|v(x,y)| < \infty$ and $\sum_q |\tilde{v}(p,q)| < \infty$, so that $\lim_{\Lambda\to\infty} |\tilde{v}(p,q)| = 0$ and $|\tilde{v}(p,q)| \le c/|\Lambda|$.

The practitioner will recognize here an approximation of the mean molecular field type, a heuristic tool introduced, during the first ten years of the twentieth century, by P. Weiss and L.S. Ornstein in the classical theory of phase transitions. Yet, the approximation is not acceptable here without some further discussion since it leads to the paradoxes already mentioned.

We are now in a position to recognize Haag's seminal contribution [Haag, 1962]: the *tacit* assumption of the irreducibility of the representation of the field algebra is *untenable*. Giving up this assumption allows one to resolve the paradoxes: Δ and hence the coefficients u and v in the Bogoliubov–Valatin transformation (77) — rather than being multiples of the identity — now belong to the *non-trivial* center $\mathcal{Z}$ of the representation canonically associated by the GNS construction corresponding to the equilibrium state of the system. The gauge group now acts in a non-trivial manner on $\mathcal{Z}$ and thus restores the symmetry of the theory. And in

the limit considered, the time-evolution is well defined as an automorphism group of the von Neumann algebra generated by the representation. These technical niceties have been succesively refined — and confirmed — in subsequent investigations, cf. e.g. [Emch and Guenin, 1966; Thirring and Wehrl, 1967; Thirring, 1968; Dubin and Sewell, 1970; Sewell, 1982b].

5.2 Beyond Fock space: The Bose gas

Even before the modular structures were formally recognized by mathematicians, their first instantiation appeared in QSP. One can indeed discern these structures in the pioneering re-examination Araki and Woods [1963] made of the Bose–Einstein model for an ideal quantum gas; for the original version of the model, cf. subsection 2.4. The present subsection summarizes the principal aspects of the Araki–Woods treatment.

The reader is assumed to be familiar with the definition of the Weyl form of the canonical commutation relations (CCR) for a countably infinite number of degrees of freedom, as a family $\{W(f) \mid f \in \mathcal{D}(\mathbb{R}^3)\}$ of unitary operators acting on the (boson) Fock space $\mathcal{F} := \bigoplus_{N=0}^{\infty} {}^s\mathcal{H}^N$ and satisfying $\forall\, f, g \in \mathcal{D}(\mathbb{R}^3)$: $W(f)\,W(g) = \exp\{-i\,\mathrm{Im}(f,g)/2)\}$; where $\mathcal{D}(\mathbb{R}^3)$ is the space of all infinitely differentiable functions $f : \mathbb{R}^3 \to \mathbb{C}$ which have compact support; and ${}^s\mathcal{H}^N$ is the symmetric $N-$fold tensor product of the one-particle space $\mathcal{H}^1 = \mathcal{L}^2(\mathbb{R}^3)$ with itself; cf. e.g. [Emch, 1972a], or [Halvorson, 2006].

For the Bose gas at temperatures $T > T_c$ where T_c is the critical temperature found by Bose and Einstein, the GNS representation π_g corresponding to the gaseous normal phase — in the thermodynamical limit at fixed density ρ and chemical activity z — is given as follows. The Hilbert space of the representation π_g may be identified with $\mathcal{H} = \mathcal{F} \otimes \mathcal{F}$; its cyclic vector is $\Phi = \Phi_o \otimes \Phi_o$, where Φ_o is the vacuum vector in $\mathcal{F}$. Then

$$(80)\quad \pi_g[W(f)] = W(\zeta_+ f) \otimes W(K\zeta_- f)$$

where completeness demands that we specify that $\widetilde{(\zeta_+ f)}(k) = [1+\rho(\beta,z;k)]^{\frac{1}{2}}\,\tilde{f}(k)$, and $\widetilde{(\zeta_- f)}(k) = [\rho(\beta,z;k)]^{\frac{1}{2}}\,\tilde{f}(k)$, $\widetilde{(Kf)}(k) = \tilde{f}(k)^*$; $\rho(\beta,z;k) = z[\exp(\beta\epsilon(k)) - z]^{-1}$ with $\epsilon(k) = |k|^2/2m$ and z is determined by ρ and β through $\rho = (2\pi)^{-3}\int d^3k\ \rho(\beta,z;k)$.

The von Neumann algebra $\mathcal{N}_g = \{\pi_g[W(f)] \mid f \in \mathcal{D}(\mathbb{R}^3)\}''$ is a factor, the commutant of which is $\mathcal{N}_g{}' = \{\nu_g[W(f)] \mid f \in \mathcal{D}(\mathbb{R}^3)\}'$ where

$$(81)\quad \nu_g[W(f)] = W(K\zeta_- f) \otimes W(\zeta_+ f)\,.$$

Note that ν_g also gives a representation of the Weyl CCR.

In what I believe was the first presentation of the programme proposed in [Haag *et al.*, 1967] to a wide audience of mainstream physicists, namely the huge IUPAP 1966 Copenhagen meeting on statistical mechanics, Winnink [Winnink, 1967] started indeed with a summary of the above results. As the duality between the

von Neumann algebra and its commutant is already a property of finite systems — see scholium 33 and remark 34 above — Winnink's emphasis was that this property may persist in general for systems endowed with infinitely many degrees of freedom, as is the case in this specific model — the Bose gas — where the thermodynamical limit of canonical equilibrium is controlled. The emphasis on dealing with infinite systems — also advocated in the lecture [Verboven, 1967] preceding Winnink's — raised eyebrows with many of the physicists in the Copenhagen audience, to wit: "Wouldn't one think that, so to say, the motivation of going to an infinite system would be to obtain simpler results than are obtained for a finite system?" [Uhlenbeck, 1967]; or even more pointedly: "What does this have to do with statistical mechanics?"[van Kampen, 1967]. The conjecture was already floated that the formalism could be useful for an adequate description of phase transitions, a conjecture I will examine in subsections 5.6 and 5.7.

In retrospect, it is quite remarkable that Araki and Woods [1963] had already unearthed several features that were later placed in the context of the general theory that was to be built on the subsequent work of Tomita and Takesaki [Tomita, 1967; Takesaki, 1970a] for the mathematical formalism and the work of Haag *et al.* [1967] for its application to QSP. Among the results by Araki and Woods, one may note that the von Neumann factor $\mathcal{N}_g$ they constructed for $T > T_c$ is of type III — a type of factor the existence of which was known, but for which examples were then quite elusive even in the pure mathematics literature — and this was the first occurrence of this type of factor in QSP, although their ubiquity was later recognized all over in QSP and in QFT; and also in pure mathematics, but that is another story. In addition, Araki and Woods established that the unitary operators implementing time-evolution and space-translation on the von Neumann algebra $\mathcal{N}_g$ do not belong to this algebra. They also discussed the representations relative to the superfluid phase which occurs for temperatures $0 < T < T_c$, and they found that the associated GNS representation is an integral of factor representations. Incidentally, they do mention that this points to a formal analogy with the mathematical structure Haag found in his study of the BCS model; see subsection 5.1 above.

5.3 The KMS condition and the Heisenberg model

The first proof that the KMS conditions themselves are actually satisfied in concrete infinite quantum systems was provided by Araki [1969] for a class of one-dimensional quantum spin-lattice models which includes the archetypal model — originally proposed by Heisenberg [1928] as a putative model for ferromagnetism — defined by the local, so-called "exchange" Hamiltonian:

$$(82)\quad H_\Lambda = -J \sum_{k=a}^{b-1} \sigma_k \cdot \sigma_{k+1}$$

where J is the coupling constant describing interactions of neighbouring quantum spins $\sigma_k = (\sigma_k{}^x, \sigma_k{}^y, \sigma_k{}^z)$ sitting on a regular, one-dimensional finite string $\Lambda =$

$[a,b] \subset Z^1$; and $\sigma_k \cdot \sigma_{k+1}$ denotes ${\sigma_k}^x {\sigma_{k+1}}^x + {\sigma_k}^y {\sigma_{k+1}}^y + {\sigma_k}^z {\sigma_{k+1}}^z$.

The problem of determining whether this quantum model would support ferromagnetism in its thermodynamical limit — even in this one-dimensional version — turned out to be much harder to handle than the classical Ising model where only interactions $J{\sigma_k}^z {\sigma_{k+1}}^z$ are considered.

For the classical models, a method known as the *transfer-matrix* — and actually proposed for the two-dimensional Ising model [Kramers and Wannier, 1941] — allows one to treat the one–dimensional version of this classical model in a few lines for nearest neighbour interactions, or even with strictly finite-range interactions, i.e. when the interactions are strictly zero between spins that are further apart than a finite distance (the same for all pairs). At the cost of quite some work [Ruelle, 1968b], the method can be made to work for interactions that extend to infinity, while decaying sufficently fast so as to have finite moment or so that the surface energy has a bound independent of the volume.

As emphasized in some detail in [Emch, 1972b], even the nearest neighbour quantum Heisenberg model requires an extension akin to the method used for the infinite range classical case. Araki [1969] thus managed to control the thermodynamical limit φ of the canonical equilibrium state and its time correlation functions well enough to establish that for all positive temperatures $\beta > 0$, the state φ satisfies the KMS condition; and that it is extremal with respect to this condition — i.e. cannot be decomposed into a mixture of states satisfying the KMS condition — and shows no spontaneous magnetization. Thus, while physicists — with their understanding of the onset of collective behaviour in the classical case — could anticipate that this quantum one-dimensional model would not exhibit any ferromagnetic phase transition, Araki proves it.

The class of models for which Araki established the above results is strongly dependent on the one-dimensionality of the "lattice" $\mathbb{Z}$. Nevertheless, the proof does not require that the interactions be isotropic, i.e. couplings between the different components of the spins do not need to be the same in all directions. Moreover the proof does not require that the interactions between the spins on the lattice be restricted to nearest neighbours: in the original version of the proof, it was only required that they vanish between spins that are further apart than a fixed (but arbitrary) finite distance, but even this restriction has been relaxed to cover the same range as the corresponding classical models. Finally, whereas in the Heisenberg model the individual half-spins are described by copies of the algebra $\mathcal{M}(2,\mathbb{C})$, the proof accommodates as well the cases where $\mathcal{A}_k \simeq \mathcal{M}(n,\mathbb{C})$ with $n < \infty$.

Hence Araki's results support a conjecture that pure thermodynamical phases may be described by extremal KMS states; see subsection 5.7 below for further evidences.

It may be added that if, in addition, lattice translation invariance is built into the theory through the local Hamiltonian H_Λ , e.g. as in (82), then the limiting KMS state φ is invariant under the group $\mathbb{Z}$ of the lattice translations, and — since its GNS representation leads to a factor — φ is also extremal with respect to this

condition, so that space-correlations between spins decay very fast as their distance increases. Here, technically speaking, φ is exponentially, uniformly clustering in space; i.e. for any quasi-local observable $A \in \mathcal{A}_o$, there exist positive constants γ and δ such that for all finite N and all $B \in \mathcal{A}_{\mathbb{Z}\setminus[-N,N]}$: $|\varphi(AB) - \varphi(A)\varphi(B)| \leq \delta \|B\| \exp(-\gamma N)$.

Before leaving the Heisenberg model, note that in the case $T = 0$, it also offers a very nice toy model for QFT; cf. e.g. [Streater, 1967].

5.4 The KMS condition and stability

The following five points summarize the KMS story I have told so far.

1. Von Neumann's definition of quantum canonical states at finite temperature is limited to finite systems; and this limitation renders cumbersome (at best) the formalism's application to QSP — see subsection 3.3.

2. For finite systems, the von Neumann equilibrium states are exactly those that satisfy a formal analytic condition, the so-called KMS condition — see subsection 4.1.

3. The KMS condition can be extended beyond the mathematical formalism laid down by von Neumann — see subsection 4.2.

4. The KMS condition is satisfied in some concrete models of infinite systems for states that have a reliable interpretation as temperature equilibrium states — see subsections 5.2 and 5.3.

5. The KMS condition appears as well in a purely mathematical context, the Tomita–Takesaki theory of modular algebras which turns out to be very fertile; while the latter aspect of the story would carry us beyond the bounds of this essay, some hints are briefly alluded to in see subsections 4.2 and 5.2.

Before the KMS theory could be deemed adequate as a physical theory, it ought to meet at least two more concerns: (i) the formalism should allow the mathematical description of quantum phenomena that escape the grip of von Neumann's formalism; (ii) the KMS states should be stable. Subsections 5.2 and 5.3 above indicate how the first of these two concerns is met; further examples will be presented in subsection 5.7. The present subsection addresses the second concern, as various stability criteria — labeled A to E — are discussed. The order of the presentation is to direct the reader's attention to the progressive emergence of formulations whereby KMS states are characterized in terms increasingly germane to those of variational principles.

A. Cut-and-paste stability.
We begin with a model that is sufficiently simple to provide exact results supporting the expectation that a large system in a canonical equilibrium state should be

able to serve as a *thermal reservoir* for "any" of its parts. The model is a variation on the theme of the so-called XY-model; this variation was proposed and solved in [Emch and Radin, 1971]; further references will be given at the end of this subsection.

The X-Y model itself — referred to below as the 'un-partitioned system' — is a one-dimensional quantum spin-lattice gas with finite-range interactions. Specifically, for any region $\Lambda = \{k \in \mathbb{Z} \mid a \leq k \leq b\}$ with $-\infty < a+1 < b < \infty$, the Hamiltonian is

$$(83)\quad H_{[a,b]} = -\sum_{k=a}^{b-1} (1+\zeta)\sigma_k{}^x\sigma_{k+1}{}^x + (1-\zeta)\sigma_k{}^y\sigma_{k+1}{}^y \quad .$$

From the work of Araki — see subsection 5.3 above — we learned that the thermodynamical limit (as $a \to -\infty$, $b \to \infty$) of both of the following objects exists: (i) the canonical equilibrium state $\varphi_{[a,b]}$ at any finite natural temperature $\beta > 0$ and (ii) the time-evolution $\alpha_{[a,b]}$; and that the resulting state φ and evolution α of the infinite system satisfy the KMS condition.

We now split the total system in two non-interacting parts: a finite region to which we affix the subscript S, and an infinite region to which we affix the subscript R, which is the complement of Λ_S in $\mathbb{Z}$, namely:

$$\Lambda_S = [c,d] \quad \text{and} \quad \Lambda_R = (-\infty, c-1] \cup [d+1, \infty)$$

with $-\infty < a < c-1$; $c < d-1$; $d+1 < b < \infty$.

This partitioned system can be viewed as the thermodynamical limit of a finite system with Hamiltonian:

$$(84)\quad \tilde{H}_{[a,b]} = H_{[a,c-1]} + H_{[c,d]} + H_{[d+1,b]} \quad .$$

Clearly the C^*-algebras for both the original system and the partitioned system are the same, namely the C^*-inductive limit $\mathcal{A} := \otimes_{k\in\mathbb{Z}}\mathcal{A}_k$ where the $\mathcal{A}_k$ are copies of the algebra $\mathcal{M}(2,\mathbb{C})$ of the 2×2 matrices with complex entries. Thus $\mathcal{A} = \mathcal{A}_S \otimes \mathcal{A}_R$ where $\mathcal{A}_S := \otimes_{k\in\Lambda_S}\mathcal{A}_k$ and $\mathcal{A}_R := \otimes_{k\in\Lambda_R}\mathcal{A}_k$.

Again, as for the original (un-partitioned) system, the thermodynamical limit of the canonical equilibrium state and of the evolution of the partitioned system, defined from (84), do exist and satisfy the KMS condition; they are denoted here by $\tilde{\varphi}$ and $\tilde{\alpha}$.

Note that φ and $\tilde{\varphi}$ are different. For instance, φ is invariant with respect to translations along the chain, while $\tilde{\varphi}$ is not. Nevertheless, a first stability property of this model is established in [Emch and Radin, 1971], namely:

$$(85)\quad \forall A \in \mathcal{A} : \lim_{|t|\to\infty} \tilde{\varphi}(\alpha_t[A]) = \varphi(A) \quad .$$

Hence, as the full evolution α unfolds, the correlations between S and R that were cut by the partitioning are re-established: the partition is erased.

Moreover, let $\tilde{\varphi}_S$ denote the restriction of $\tilde{\varphi}$ to $\mathcal{A}_S$; and similarly for R; one has $\tilde{\varphi} = \tilde{\varphi}_S \otimes \tilde{\varphi}_R$. The evolution $\tilde{\alpha}$ preserves the partitioning, namely $\forall A \in$

$\mathcal{A}_S$ [resp.$\mathcal{A}_R$] : $\tilde{\alpha}_t[A] \in \mathcal{A}_S$ [resp.$\mathcal{A}_R$]. Hence, we have $\tilde{\alpha} = \tilde{\alpha}_S \otimes \tilde{\alpha}_R$; i.e. the two systems evolve independently. Again the KMS conditions are satisfied for S and R separately.

After this partitioning, let us now change the temperatures of S and R so that (i) $\tilde{\varphi}_{S,\beta_S}$ is the canonical equilibrium on $\mathcal{A}_S$ at some temperature β_S with respect to the evolution $\tilde{\alpha}_S$; and similarly (ii) with β_R (possibly different from β_S) for $\tilde{\varphi}_{R,\beta_R}$ (w.r.t $\tilde{\alpha}_R$) on $\mathcal{A}_R$. Let thus $\tilde{\varphi}_{S,\beta_S} \otimes \tilde{\varphi}_{R,\beta_R}$ be the initial state of the partitioned system; and denote by φ_β the canonical equilibrium on the whole system, at temperature β with respect to the original interacting evolution α. Then, the following is proven [Emch and Radin, 1971] for all β_S, $\beta_R > 0$ and for all $A \in \mathcal{A}$:

$$(86)\quad \lim_{|t|\to\infty} \tilde{\varphi}_{S,\beta_S} \otimes \tilde{\varphi}_{R,\beta_R}(\alpha_t[A]) = \varphi_\beta(A) \text{ with } \beta = \beta_R \ .$$

Hence the name *'cut-and-paste stability'*. The system is first partitioned in two parts, a finite system S surrounded by an infinite system R that do not interact with one another: the interactions across the boundaries [i.e. between the sites $c-1$ and c; and between the sites d and $d+1$] have been 'cut'. In this configuration, the finite system S and the infinite system R are separately put at (different) temperatures β_S and β_R. When these systems are 'pasted' back together, one finds that the joint evolution drives the full system $S \cup R$ to a temperature β which has to be the temperature at which R was initially, namely $\beta = \beta_R$. In this sense, R serves as a thermal reservoir for S.

The special property of the model responsible for this result is that it satisfies a remarkable condition which I now describe.

Let γ be the automorphism of $\mathcal{A}$ uniquely determined by

$$(87)\quad \forall\, k \in Z\ :\ \begin{cases} \gamma[\sigma_k{}^z] = & \sigma_k{}^z \\ \gamma[\sigma_k{}^x] = - & \sigma_k{}^x \\ \gamma[\sigma_k{}^y] = - & \sigma_k{}^y \end{cases} \quad .$$

Note in particular that the original Hamiltonian $H_{[a,b]}$ and the cut Hamitonian $\tilde{H}_{[a,b]}$ belong to the even algebra $\mathcal{A}_e := \{A \in \mathcal{A} \mid \gamma[A] = A\}$. This entails that in the thermodynamical limit $\varphi \circ \gamma = \varphi$ and $\gamma \circ \alpha \circ \gamma = \alpha$; and similarly for all the corresponding objects obtained after the partitioning. In particular, the evolution preserves the even algebra, i.e. $\forall\,(t, A) \in \mathbb{R} \times \mathcal{A}_e : \alpha_t[A] \in \mathcal{A}_e$.

Now, the special property of the model can be explicitly stated:

$$(88)\quad \forall\, A, B \in \mathcal{A}_e\ :\ \lim_{|t|\to\infty} \|A\alpha_t[B] - \alpha_t[B]A\| = 0 \quad ;$$

i.e. the evolution, when restricted to the even observables of the model, is *strongly asymptotically abelian*.

The proof — and an immediate generalization — of (86) above is a direct consequence of quantum ergodic theory (see subsection 3.5). First, one notices that φ is uniformly clustering in space, i.e. for every $\epsilon > 0$ and every $A \in \mathcal{A}$ there exists

a finite region Λ such that for every B outside this region $|\varphi(AB) - \varphi(A)\,\varphi(B)| \leq \epsilon\|B\|$. This entails that the KMS state φ is extremal with respect to this condition, i.e. cannot be decomposed into a convex combination of other KMS states; see subsection 5.6 below, and in particular definition 57. These properties are inherited by the restriction φ_e of φ to the even algbra $\mathcal{A}_e$. The asymptotic abelianness of the evolution then implies [Araki and Miyata, 1968] that the state φ_e is not only time-invariant — as we know every KMS state must be — but it is also extremal with respect to this condition, i.e. cannot be decomposed into other time-invariant states, which is to say that φ_e cannot be written as $\varphi_e = \lambda\psi_e + (1-\lambda)\chi_e$ with $0 < \lambda < 1$ and ψ_e, χ_e time-invariant, *unless* $\psi_e = \chi_e = \varphi_e$.

Since $\varphi, \varphi_e, \tilde{\varphi}_S, \tilde{\varphi}_R$ are even, one looses no information by carrying out the proof of (85) and (86) in $\mathcal{A}_e$; in particular, (88) implies the existence of the point-wise limit of $(\varphi_S \otimes \varphi_R) \circ \alpha_t$ in the LHS of (86); then the above argument shows that it must coincide with φ.

Note further that what is proven in [Emch and Radin, 1971] is in fact a stronger result, which implies (86) and thus (85) as particular cases, namely that for all even states ψ_S of the system S :

$$(89)\ \ \forall\, A \in \mathcal{A}\ :\ \lim_{|t|\to\infty} \psi_S \otimes \tilde{\varphi}_R(\alpha_t[A]) = \varphi_\beta(A)$$

which therefore reinforces the 'cut-and-paste stability' interpretation proposed immediately after equation (86).

This result may be further generalized in two ways. First, the restriction that ψ_S in (89) be an even state can be dispensed with; cf. [Araki and Barouch, 1982]. Second, as was already noticed in [Emch and Radin, 1971], an ergodic or averaged version of (89), specifically, with η denoting an invariant mean on the group $\mathbb{R}$:

$$(90)\ \ \forall\, A \in \mathcal{A}\ :\ \eta\{\psi_S \otimes \tilde{\varphi}_R(\alpha[A])\} = \varphi_\beta(A)$$

obtains [Emch and Radin, 1971], even if only a weaker version of (88) holds, namely the condition of $\eta-$asymptotic abelianness (60), i.e.

$$(91)\ \ \forall\, A, B, C \in \mathcal{A}_e\ :\ \eta\{\varphi(C^*\,[A\,\alpha[B] - \alpha[B]\,A]\,C)\} = 0 \quad .$$

Depending on one's intellectual temperament, *either* the general argument presented earlier, *or* the specific model just reviewed, raises the question of whether the KMS condition could be derived from some general stability argument. This question is addressed from several angles in (B)–(E) below.

The model presented above was discussed again in [Robinson, 1973]; see also [Araki and Barouch, 1982] and references therein. It belongs to a long line of inquiries that started as attempts to derive Newton's cooling law from first principles; related problems are usually understood under the generic label 'return to equilibrium'. As of this writing, the latest comprehensive entry on the subject may be [Bach *et al.*, 2000] where a wealth of "novel technical devices" are brought to bear; the reader will also find there an informative sample of the large literature on

the subject. In a broad sense, several — but not all — of the criteria of stability in this subsection also address this perennial problem of return to equilibrium from small or local deviations. Its ubiquity however should not overshadow two other important and largely unsolved problems; cf. subsection .6.4 below.

B. Stability against local perturbations.
Various conditions of asymptotic abelianness were investigated by Kastler *et al.* For a summary, see [Kastler, 1976] which also offers a annotated bibliography. For their main stability theorem, they settled on the notions described in definitons 41 and 42 below.

DEFINITION 41. Let $\mathcal{A}$ be a C$^*-$algebra. An evolution $\alpha : \mathbb{R} \to \mathrm{Aut}(\mathcal{A})$ is said to be L^1- asymptotically abelian on a norm dense $^*-$subalgebra $\mathcal{A}_o \subset \mathcal{A}$ when

$$\forall\, (t, A) \in \mathbb{R} \times \mathcal{A}_o : \alpha_t[A] \in \mathcal{A}_o\,;$$

and

$$\forall\, A, B \in \mathcal{A}_o \,:\, \int_{-\infty}^{+\infty} dt\, \|B\, \alpha_t[A] - \alpha_t[A]\, B\| < \infty \quad .$$

Some preliminary notations are required for Definition 42 below. With $\mathcal{A}$ and α as in definition 41 let $\mathcal{A}_{sa} = \{A \in \mathcal{A} \mid A = A^*\}$, and let $\mathcal{S}$ be the set of all states on $\mathcal{A}$, equipped with its weak topology. For $\varphi \in \mathcal{S}$ and an element $h \in \mathcal{A}_{sa}$ with $\varphi(h^2) > 0$, define

(i) the perturbed state φ^h by $\varphi^h : A \in \mathcal{A} \to \frac{1}{\varphi(h^2)}\, \varphi(hAh) \in \mathcal{A}$;

(ii) the perturbed evolution $\{{\alpha^h}_t \mid t \in \mathbb{R}\}$ by ${\alpha^h}_t : A \in \mathcal{A} \mapsto {U^h}_t\, \alpha_t[A]\, {U^h}_t{}^*$ where $\{{U^h}_t \mid t \in \mathbb{R}\}$ satisfies the so-called 'co-cycle differential equation' (the derivative is w.r.t. the norm-topology)

$$\forall\, t \in \mathbb{R} \,:\, i\, \tfrac{d}{dt} {U^h}_t = {U^h}_t \alpha_t[h] \;\text{ with initial condition } {U^h}_o = I\,.$$

To understand the sense in which α^h may be viewed as the perturbed evolution corresponding to h, note that the above co-cycle equation admits a unique continuous solution $t \in \mathbb{R} \mapsto {U^h}_t \in \mathcal{A}$; it can be computed explicitly as the norm-convergent Dyson series:

$${U^h}_t = \sum_{n=0}^{\infty} {C^h}_{t,n} \text{ with } {C^h}_{t,n} = (-i)^n \int_o^t dt_n \int_o^{t_n} dt_{n-1} \ldots \int_o^{t_2} dt_1 \alpha_{t_1}[h] \ldots \alpha_{t_n}[h].$$

This solution satisfies: (i) ${U^h}_t$ unitary, and

$$(ii) \qquad \forall\, s, t \in \mathbb{R} \,:\, {U^h}_{s+t} = {U^h}_s\, \alpha_s[{U^h}_t]\,.$$

Consequently, the evolution defined as $\{{\alpha^h}_t \mid t \in \mathbb{R}\}$ is a group of automorphisms of $\mathcal{A}$ with, in particular:

$$\forall\, s, t \in \mathbb{R} \,:\, {\alpha^h}_{s+t} = {\alpha^h}_s \circ {\alpha^h}_t \quad .$$

The interpretation of α^h as the evolution resulting from the perturbation of α by the operator h obtains from the following relation between the generators of α^h and α :

$$i\frac{d}{dt}{\alpha^h}_t\,\big|_{t=0} = i\frac{d}{dt}\alpha_t\,\big|_{t=0} + \delta^h \quad \text{with} \quad \delta^h : A \in \mathcal{A} \mapsto [h,A] := hA - Ah \in \mathcal{A} \quad .$$

DEFINITION 42. With the above notations, an $\alpha-$invariant state φ on $\mathcal{A}$ is said to be stable against inner perturbations, whenever there is a neighbourhood $\mathcal{V}_\varphi \subset \mathcal{S}$ of φ such that $\forall\, A \in \mathcal{A}$, and $\forall\, h \in \mathcal{A}_{sa}$ with $\varphi^h \in \mathcal{V}_\varphi$:

1. $\forall\, t \in \mathbb{R}\ :\ \varphi^h({\alpha^h}_t[A]) = \varphi^h(A)$;
2. with $\lambda \in \mathbb{R}\ :\ \lim_{\lambda\to 0}\ \varphi^{\lambda h}(A) = \varphi(A)$;
3. $\lim_{t\to\infty}\ \varphi^h(\alpha_t[A]) = \varphi(A)$.

THEOREM 43. *With $\mathcal{A}$, $\mathcal{A}_o$ and α as in definition 41, assume that α is L^1- asymptotically abelian on $\mathcal{A}_o$. Let φ be an $\alpha-$invariant state on $\mathcal{A}$ and assume that φ is stable against inner perturbations in the sense of definition 42. Then — under three ancillary conditions to be discussed below — φ satisfies the KMS condition with respect to α for some natural temperature β.*

REMARKS 44. The ancillary conditions of the theorem are sketched in the three entries below.

1. The state φ is assumed *not* to be a trace, i.e. there exist $A, B \in \mathcal{A}$ such that $\varphi(AB) \neq \varphi(BA)$. This is meant to avoid the classical circumstance that would arise in the limit of infinite temperature, i.e. $\beta = 0$, i.e. $T = \infty$.

2. In the GNS representation canonically associated to φ, the generator of the unitary group $U(\mathbb{R})$ that implements $\alpha(\mathbb{R})$ is assumed *not* to be one-sided. This is meant to avoid the opposite circumstance where φ would be a zero-temperature ground state, i.e. $\beta = \infty$, i.e. $T = 0$.

3. The state φ is assumed to be hyperclustering of order 4 on the $^*-$subalgebra $\mathcal{A}_o$. This technical condition requires the following to hold: for every positive integer $p \leq 4$ and all $A_1, \ldots, A_p \in \mathcal{A}_o$, there exist positive constants C and δ such that

   (92) $\forall\, t_1, \ldots, t_p \in R\ :\ \varphi_p^T(\alpha_{t_1}[A_1] \cdots \alpha_{t_p}[A_p]) \leq C\,\{\,1 + \max\,|t_k - t_l|^{1+\delta}\,\}^{-1}$

   where the truncated correlations φ_p^T are defined recursively by $0 = \varphi_o^T$, $\varphi(A) = \varphi_1^T(A)$ and $\varphi(A_1, \ldots, A_p) = \sum_P \varphi_{n_1}^T(A_{k_1}, \ldots, A_{k_{n_1}}) \ldots \varphi_{n_j}^T(A_{q_1}, \ldots, A_{q_{n_j}})$ and the sum carries over all order-preserving partitions of $S = \{1, 2, \ldots, p\}$ in subsets $S_j \subseteq S$ satisfying the following conditions: $S = \cup_j S_j$, $j \neq k \Rightarrow S_j \cap S_k = \emptyset$, and within each $S_j = \{k_1, k_2, \ldots, k_{n_j}\}$: $k_1 < k_2 < \ldots < k_{n_j}$. The reader will verify immediately that $\varphi(A_1, A_2) =$

$\varphi_2^T(A_1, A_2) + \varphi_1^T(A_1)\,\varphi_1^T(A_2)$, and then realize that the recursion relation explains better what is going on with higher truncated correlations than writing explicitly the summations over P.

Note that the φ_p^T provide a hierarchy where all correlations of lower order already have been taken into account. In particular in the case of the CCR, a remarkable result of Robinson [Robinson, 1965] shows that either this hierachy goes up indefinitely or, if the truncated φ_n^T vanish for all $n \geq N$ with $N > 2$, then they must vanish for all $n > 2$.

The concept of truncated φ_n^T is not a stranger. It comes to us as a quantum cousin of the "cumulants" of classical probability theory and of the "Ursell functions" of classical statistical mechanics. The classical equivalent of Robinson's theorem gives a characterization of the Gaussian distribution, which translates in quantum statistics as yet another characterization of the canonical equilibrium state of an assembly of free harmonic oscillators. Robinson's theorem thus gives a foretaste of why it is so difficult to produce and/or control models of QFT and QSP that are not "quasi-free".

To sum up, the third ancillary condition of the theorem aims to convey that in the course of time all time-correlations of order $p \leq 4$ are to decay rapidly enough for long time separations.

The investigations by Kastler *et al.* reported above appear to be systematically predicated on conditions of time-asymptotic abelianness (definition 41) and time-hyperclustering (remark 44(3)). Thus compare these with any of the conditions encountered in sections 3 and 4; the latter are naturally satisfied for space translations, but in constructing specific models, even these conditions are extremely difficult to impose straight on the microscopic dynamics, i.e. on the Hamiltonian that is to describe the time evolution. Whether this is an intrinsic shortcoming of the theory behind theorem 43 above, or an indication of some lack of either imagination or technical dexterity on the part of model builders remains open at this stage. Nevertheless, it appears that one weak form of asymptotic abelianness is not only sufficient but also necessary when one wants to identify, among KMS states, those that are merely extremal with respect to this condition, from those that are, moreover, extremal with respect to time-invariance; cf. e.g. [Emch, 1972a, corollary 2, p. 206]; or remark 63(6) below. Here again, reminiscences from the perennial ergodic dreams in classical statistical *Hamiltonian mechanics* would incline some to hope that such an identification could perhaps be in the cards. As I have recognized in several other parts of this essay, my crystal ball remains clouded on this issue.

C. Thermal reservoir stability.

Consider the intuitive idea that a system R may be construed as a "thermal reservoir" at temperature β, if it drives suitably devised test systems S to equilibrium at temperature β when they are coupled to R. Kossakowski *et al.* [1977] proposed to formalize this idea in the following manner; see also [Sewell, 2002, pp. 114–116].

For a concrete motivation, compare the specific XY-model described in part **A** of this subsection.

To model situations where one expects that R ought to be very much larger than S in order to exclude feedbacks from the test system S onto the reservoir R, one assumes that R is infinite and S is finite.

The putative reservoir R is described by a triple $\{\mathcal{A}^R, \alpha^R, \varphi^R\}$ where $\mathcal{A}^R$ is a C^*-algebra; α^R is an evolution group of automorphisms of $\mathcal{A}^R$; and φ^R is a state on $\mathcal{A}^R$, invariant under the evolution α^R. Denote by $\delta^R := i\frac{d}{dt}\alpha^R{}_t\big|_{t=o}$ the generator of the evolution α^R. Some ancillary conditions on R will be specified later.

The test system S is a dynamical system in the sense of von Neumann, i.e. is described by: $\{\mathcal{A}^S, \alpha^S, \varphi^S_\beta\}$ where $\mathcal{A}^S = \mathcal{B}(\mathcal{H})$; α^S is the evolution generated by a Hamiltonian H^S such that for all temperatures $\beta > 0$, $Z := \mathrm{Tr}\,\exp(-\beta H^S) < \infty$; and φ^S is given by

$$(93)\quad \varphi^S_\beta(A^S) = \mathrm{Tr}\,\rho^S_\beta\, A^S \quad \text{with} \quad \rho^S_\beta = Z^{-1}e^{-\beta H^S} \quad .$$

$\delta^S = i\,[H^S\,,\ \cdot\ ]$ will denote the generator of α^S. Finally, $\mathfrak{S}^S$ will denote the set of all countably additive states on $\mathcal{A}^S$.

A family $\{\alpha^\lambda \mid \lambda \geq 0\}$ of dynamical couplings between R and S is described by groups of automorphisms on $\mathcal{A} = \mathcal{A}^R \otimes \mathcal{A}^S$, the generator of which is of the form:

$$(94)\quad \left.\begin{array}{c} \delta^\lambda = \delta^R \otimes I + I \otimes \delta^S + \lambda\delta_V \quad \text{where} \\ \delta_V : A \in \mathcal{A} \mapsto i\,\lambda[V\,,\,A] \in \mathcal{A}\,, \quad \text{with} \quad V \in \mathcal{A}_{sa} \end{array}\right\} \quad .$$

As the ancillary conditions on R are specified, so will be the form of V; see (97) and (98) below.

The next step in the modeling is devised to emphasize the sense in which the long-time cumulative effects on S of the evolution α^λ are accounted for when R and S are coupled. For this Kossakowski *et al.* [1977] appeal to the so-called van Hove limit, an instance of which already appeared in subsection 3.5; see also remark 45 below. For the system at hand here, the van Hove limit takes the following form. First, it considers only a reduced evolution, namely only what the system S experiences of the total evolution; mathematically this reduction is achieved by $E : \mathcal{A} \to \mathcal{A}_S$, the conditional expectation defined, for all $A_S \otimes A_R$, by $E[A_S \otimes A_R] = A_S\ \varphi_R(A_R)$, and then extended by linearity and continuity to $\mathcal{A}$. Secondly, the van Hove limit requires to focus on a long-time/weak-coupling regime defined by rescaling time with an inverse power of the interaction strength. Thus, the van Hove limiting procedure consists here in proving that the following limit exists for all positive 'rescaled' times s:

$$(95)\quad \gamma^S_s : A_S \in \mathcal{A}^S \mapsto \lim_{\substack{\lambda\to 0\ ;\ t\to\infty \\ s=\lambda^2 t}} \alpha^S_{-t} \circ E \circ \alpha^\lambda_t[A_S] \in \mathcal{A}^S \quad .$$

REMARKS 45. This type of limit has a long history. I learned it first from van Hove [van Hove, 1955] where the author had proposed it as a tool to relate

macroscopic transport phenomena to the microscopic dynamics that is expected to underlie them. It emphasizes that in such discussions time ought to be rescaled in a way determined by the strength λ of the interaction. Some justifications for taking such a limit will be discussed in subsection 6.1 below.

Finally, given two C^*- algebras $\mathcal{A}$ and $\mathcal{B}$, and n a non-negative integer, one says that a map $\gamma : \mathcal{A} \to \mathcal{B}$ is *n-positive* whenever it is linear, and the induced map $\gamma_n : \mathcal{A} \otimes \mathcal{M}(n,\mathbb{C}) \to \mathcal{B} \otimes \mathcal{M}(n,\mathbb{C})$ is positive, i.e. the image of any positive element in $\mathcal{A} \otimes \mathcal{M}(n,\mathbb{C})$ is a positive element in $\mathcal{B} \otimes \mathcal{M}(n,\mathbb{C})$. When either $\mathcal{A}$ or $\mathcal{B}$ is abelian, a positive map is necessarily $n-$positive; hence $n-$positivity is a notion new to the non-commutative context of QSP. Furthermore, a map is said to be *completely positive* whenever it is $n-$positive for all $n \in \mathbb{Z}^+$. In connection with expressions like the right-hand side of (95) above, note that the composition of completely positive maps is again completely positive; and that automorphisms, states, injections and conditional expectations are completely positive maps. A collection $\{\gamma_s \mid s \in \mathbb{R}^+\}$ of maps of $\mathcal{A}$ into itself is said to form a semi-group whenever γ_o is the identity map, and $\forall\,(s,t) \in \mathbb{R}^+ \times \mathbb{R}^+ : \gamma_{s+t} = \gamma_s \circ \gamma_t$.

This should exhaust the list of general preliminaries necessary to describe the stability criterion proposed by Kossakowski *et al.* [1977], namely:

DEFINITION 46. A system $\{\mathcal{A}^R, \alpha^R, \varphi^R\}$ is said to be a thermal reservoir at temperature β whenever there is a "large enough" collection $\mathfrak{T}_\beta$ of test systems $\{\mathcal{A}^S, \alpha^S, \varphi^S_\beta\}$ and dynamical couplings $\{\alpha^\lambda\}$ such that

1. the van Hove limit (95) exists, and defines a semi-group of completely positive transformations $\{\gamma^S_s \mid s \in \mathbb{R}^+\}$ of $\mathcal{A}_S$;

2. the canonical von Neumann equilibrium state φ^S_β on $\mathcal{A}_S$ is the only state $\varphi \in \mathfrak{S}^S$ that is invariant under both α^S and γ^S;

(96) *3.* $\quad \forall\,(\psi^S\,,\,A^S) \in \mathfrak{S}^S \otimes \mathcal{A}^S \;:\; \lim_{s\to\infty} \psi^S\,(\gamma^S_s\,[A_S]) = \varphi^S_\beta\,(A_S) \quad .$

The term "large enough" in the above definition admittedly needs to be made more precise: this is where the ancillary conditions on the interaction V and the reservoir R enter the picture and allow one to prove scholium 47 and theorem 48 below.

One condition is that the interaction V in (94) be of the form

$$(97)\quad V = \sum_{k=1}^{n} B^R_k \otimes B^S_k \quad \text{with} \quad \left\{ \begin{array}{l} n \text{ is finite} \\ B^R_k \in \mathcal{A}^R{}_{sa} \text{ and } \varphi^R(B^R_k) = 0 \\ B^S_k \in \mathcal{A}^S{}_{sa} \end{array} \right\} \quad .$$

Note that the conditional expectation $E[V]$ of V vanishes.

An additional condition is that there exists $\mathcal{A}^R_o \subseteq \mathcal{A}^R$ such that: (i) $\mathrm{Span}\{\mathcal{A}^R_o \cup I\}$ (where I is the identity in $\mathcal{A}^R$) is norm dense in $\mathcal{A}^R$; (ii) for all $B^R_k \in \mathcal{A}^R_o$, the functions $t \mapsto \varphi^R(B^R_j \alpha^R_t[B^R_k])$ are in L^1; and (iii) the multi-time truncated correlations, for the state φ^R to be tested, satisfy

(98) $t_1 < \ldots < t_l$ with $|t_j - t_k| \to \infty \Rightarrow \{\varphi^R\}^T \left(\alpha^R_{t_1}[B^R_{t_1}] \cdots \alpha^R_{t_n}[B^R_{t_n}]\right) \to 0.$

Upon taking advantage of [Davies, 1974, theorem 2.3], the following results were obtained in [Kossakowski *et al.*, 1977]:

SCHOLIUM 47. These ancillary conditions are sufficient to imply that condition (1) in definition 46 is satisfied for all finite S.

This ensures that the collection $\mathfrak{T}_\beta$ of test systems will indeed be large enough.

THEOREM 48. *When the circumstances just outlined are realized, the following conditions are equivalent:*

1. *for some temperature β, the state φ^R is a KMS state on $\mathcal{A}_R$ with respect to the evolution α_R;*
2. *the system R, in the state φ^R, is a thermal reservoir for temperature β in the sense of definition 46 with "large enough" sharpened by scholium 47.*

REMARKS 49.

1. Hence, every test system S in $\mathfrak{T}_\beta$ is driven to equilibrium at temperature β by the reservoir R exactly when φ^R satisfies the KMS condition for this temperature.

2. As mentioned before, this result is largely model-independent, and does not involve, *at least explicitly,* any assumption of time asymptotic abelianness. Moreover, instead of a single model for which one can prove that a special infinite system in equilibrium serves as thermal reservoir for each of its finite parts, the present theorem characterizes a collection $\mathfrak{T}_\beta$ of test systems S for which the infinite system R serves as a thermal reservoir. Thus, the theorem is an improvement on the particular motivating model discussed in paragraph **A** above.

3. Yet, as [Kossakowski *et al.*, 1977] noticed, the decay of multi-time correlations (98) that enables their proposal to work is reminiscent of the similar conditions imposed by Kastler *et al.* in their result on stability against local perturbations; see (92) in paragraph **B** above.

4. From an empirical point of view, the theorem may be regarded as specifying a procedure to lift the notion of temperature in equilibrium QSP from finite systems to infinite systems.

5. Nevertheless, it must be noted that the circumstances under which γ^S is known to satisfy condition (1) of definition 46 and the decay of correlations in (98) do appear to involve some clustering properties that may limit the domain of applicability of the theorem to cases where $\pi_\varphi(\mathcal{A}_R)''$ is a factor, and where φ^R is extremal under both the KMS condition and the condition

of time-invariance. Hence, asymptotic abelianness enters less conspiciously here.

D. Passivity.

In [Pusz and Woronowicz, 1978] the authors noticed a property of KMS states which they called *passivity;* and they found ways to show that this property in turn entails the KMS property under assumptions that *do not* involve asymptotic abelianness in *time.*

Specifically, let $\{\mathcal{A}, \varphi, \alpha\}$ be a dynamical system where $\mathcal{A}$ is a C^*-algebra, φ be a state on $\mathcal{A}$, and $\{\alpha_t \mid t \in R\}$ is a one-parameter group of automorphisms of $\mathcal{A}$. Let then $D(\delta)$ denote the domain of the generator δ of the evolution α, i.e. $D(\delta)$ is the linear subspace of all $A \in \mathcal{A}$ such that the derivative $\delta[A] := i\frac{d}{dt}\alpha_t[A]$ exists.

Consider now the situation obtained by letting this system interact during a finite time-interval with an outside system, so that the effect of their interaction on the system of interest may be assumed to be described as the perturbed dynamics α^h satisfying the differential equations:

$$(99)\quad \forall\, A \in D(\delta)\ :\ \begin{cases} i\frac{d}{dt}{\alpha^h}_t[A] = {\alpha^h}_t[\delta[A] + [h_t, A]] \\ {\alpha^h}_{t=0}[A] = A \end{cases}$$

where h is an element of $C^1_+(\mathbb{R}, \mathcal{A}_{sa})$, the set of all continuously differentiable functions, with compact support in $\mathbb{R}^+$ and taking their values in the self-adjoint part of $\mathcal{A}$. The system is thus an open system for all times t in the support of h, i.e. for all times when the perturbation h is actually in effect. The condition that the support of h be compact and contained in $\mathbb{R}^+$ ensures that, for all times $T > \sup\{t \in \mathbb{R} \mid h_t \neq 0\}$, the external conditons are as they were at time $t = 0$. The smoothness condition $h \in C^1$ on the time-dependence of the external pertubation is a mathematical convenience that is physically reasonable. Then

$$(100)\quad L^h_T(\varphi) := \int_o^T dt\ \ \varphi({\alpha^h}_t\,[\frac{d}{dt}h_t])$$

describes the energy transmitted to the system in the time interval [0, T] during which the system was under the influence of the external perturbation h.

DEFINITION 50. The state φ is said to be passive if for all $h \in C^1_+(R, \mathcal{A}_{sa})$ and all $T > \sup\{t \in \mathbb{R} \mid h_t \neq 0\}$: $L^h_T(\varphi) \geq 0$.

Upon having advanced this definition, Pusz and Woronowicz [1978] proved the following result:

THEOREM 51. *Let $\{\mathcal{A}, \varphi, \alpha\}$ be a C^*- dynamical system, and consider the following conditions: (I) φ is either a KMS state with respect to α for some temperature $\beta > 0$; or is a ground state; and (II) φ is passive in the sense of definition 50. Then:*

1. *Without further assumptions:* $(I) \Rightarrow (II)$.

2. *If furthermore: (i) $\mathcal{A}$ admits an action $\nu : G \to \mathrm{Aut}(\mathcal{A})$ where G is a locally compact amenable group; (ii) ν commutes with the evolution α, i.e. $\forall\,(t,g) \in R \times G : \nu_g \circ \alpha_t = \alpha_t \circ \nu_g$; and (iii) φ is $\eta-$clustering with respect to the action of G. Then these conditions, taken together, entail $(II) \Rightarrow (I)$.*

REMARKS 52. The following remarks focus on part (2) of the theorem, i.e. the operational characterization of KMS states as passive.

1. In the passivity condition (II), φ has not been assumed to be invariant under the unperturbed evolution α ; in part (2) this property obtains as φ is proven to satisfy the KMS condition.

2. The condition that ν commutes with α is natural in view of the conclusion to be obtained: if an automorphism leaves invariant a KMS state, then it must commute with the evolution with respect to which this state is KMS.

3. Invariant means and amenable groups were introduced in subsection 3.5; see in particular definition 21 and remark 31(5).

4. Among the ancillary assumptions listed in (2), it is not even necessary to impose as a precondition that φ be $G-$invariant; this follows from the explicit assumption that it is $\eta-$clustering, i.e. (see definition 22):

$$\forall\ A\,,\ B\ \in \mathcal{A}\ :\ \eta^G\left(\varphi(\nu_g[A]\,B)\right) = \varphi(A)\,\varphi(B) \quad .$$

   Actually, this condition entails furthermore that φ cannot be decomposed in a convex combination of other $G-$invariant states.

5. In QSP, the natural candidate for G is the group of translations in *space*. Hence, in contrast with the stability conditions studied earlier, the assumed clustering property does not need to be with respect to time. This allows us to consider systems for which the evolution is *not* asymptotically abelian. This opening is significant when it comes to concrete modeling for the purposes of QSP: one may not wish to have to identify the weak-clustering with respect to the group $\{\nu_g \mid g \in G\}$ *and* any putative clustering with respect to the evolution $\{\alpha_t \mid t \in \mathbb{R}\}$.

6. In addition, Pusz and Woronowicz [Pusz and Woronowicz, 1978] propose an alternative route, replacing all the ancillary conditions in part (2) of the theorem by a strengthened form of passivity. Specifically, instead of considering a single dynamical system, they consider, for every positive integer, identical non-interacting copies $\{\mathcal{A}_k, \varphi_k, \alpha_k \mid k = 1, \ldots, N\}$ from which one constructs the collective dynamical system $\{\mathcal{A}^N, \varphi^N, \alpha^N\}$ where $\{\mathcal{A}^N = \otimes_{k=1}^N \mathcal{A}_k\,,\ \varphi^N = \otimes_{k=1}^N \varphi_k\,,$ and $\alpha^N = \otimes_{k=1}^N \alpha_k\,\}$. The perturbation h however is allowed to be a general element in $C^1_+(\mathbb{R}, \mathcal{A}^N)$, so that α^h is allowed not to act independently on each of the component systems. Then φ is said to be *completely passive* whenever for every positive integer N the

state φ^N is passive. Now, without further ado — i.e. without having to impose condition (2) in theorem 51 — the complete passivity of φ can be proven to be equivalent to the condition that φ satisfy the KMS condition. For QSP, the choice between the condition of complete passivity or condition (2) in the theorem, is largely a question of taste.

E. Thermodynamical stability.
To close this subsection, I wish to indicate how the concept of thermodynamical stability gives rise to yet another characterization of KMS states, this one without restriction on whether the states considered are to be extremal with respect to the KMS condition. To avoid technicalities, I present these considerations in the simplest case, namely where the system is a quantum spin-lattice and thus is described by a C^*-algebra $\mathcal{A} = \otimes_{k\in\mathbb{Z}^d}\mathcal{A}_k$ where the $\mathcal{A}_k$ are copies of a finite matrix algebra, say $\mathcal{M}(n,C)$, with n and d finite. Throughout $\Lambda \subset \mathbb{Z}^d$ denotes a connected finite subset of the lattice $\mathbb{Z}^d$; φ denotes a state on $\mathcal{A}$; φ_Λ denotes the restriction of φ to the finite matrix algebra $\mathcal{A}_\Lambda = \otimes_{k\in\Lambda}\mathcal{A}_k$; and ρ_Λ is the density matrix corresponding to φ_Λ. Furthermore it is convenient to assume here that the dynamics obtains from short-range — or possibly suitably tempered — interactions between the sites. The reader interested in how far the considerations presented below may be pursued will find a review in [Sewell, 2002]; among the original papers, let it suffice to mention for orientation purposes [Araki, 1974; Araki and Sewell, 1977; Sewell, 1977; Sewell, 1980b; Ruelle, 1968a; Robinson, 1971; Araki and Moriya, 2002].

A version of the second law of thermodynamics — compare with the equivalent form of the variational principle defined immediately after theorem 3 — defines the local free-energy relative to Λ at natural temperature $\beta = 1/kT$ as:

$$F_{\Lambda,\beta}(\varphi) = E_\Lambda(\varphi) - T\,S_\Lambda(\varphi) \quad \text{with} \quad \begin{cases} E_\Lambda(\varphi) & = \varphi_\Lambda(H_\Lambda) \\ \\ S_\Lambda(\varphi) & = -k\,\mathrm{Tr}\,\rho_\Lambda \log\,\rho_\Lambda \end{cases} .$$

Two states ψ and φ on $\mathcal{A}$ are said to satisfy the equivalence relation $\overset{\Lambda_o}{\sim}$ whenever they coincide outside the finite region Λ_o. We then write $\psi \sim \varphi$ whenever there exists Λ_o such that $\psi \overset{\Lambda_o}{\sim} \varphi$. For the quantum lattice considered here, one can then prove that the following limit exists

$$(101)\ \ \forall\,\psi\sim\varphi\ :\ \Delta F_\beta(\psi\,|\,\varphi) := \lim_{\Lambda\uparrow\mathbb{Z}^d}\,(F_{\Lambda,\beta}(\psi) - F_{\Lambda,\beta}(\varphi))\ .$$

For the order of the arguments ψ and φ in ΔF_β recall that mathematicians (and some philosophers) read from right to left, while most physicists seem to read from left to right. Thus, $\Delta F_\beta(\psi\,|\,\varphi)$, as written above, represents the increment of free-energy when passing from the state φ to any state ψ that differs from φ only in a finite region. Araki and Sewell [Araki and Sewell, 1977; Sewell, 1977] introduced the following definition and prove the following result; see also [Sewell, 1980b; Sewell, 2002].

DEFINITION 53. With $\Delta F_\beta(\varphi\,|\,\psi)$ as in (101), a state φ on $\mathcal{A}$ is said to be locally thermodynamically stable at natural temperature β whenever

$$\forall\,\psi\sim\varphi\,:\;\Delta F_\beta(\psi\,|\,\varphi)\;\geq 0\quad .$$

Hence, to require that this stability condition be satisfied is indeed a variational principle: the free-energy of the state φ cannot be reduced by going to a state ψ that differs from φ only locally.

THEOREM 54. *For a state φ on a quantum lattice system of the type considered here, the following conditions are equivalent:*

1. *φ satisfies the KMS condition at natural temperature β;*
2. *φ is locally thermodynamically stable at natural temperature β.*

REMARKS 55.

1. This result involves *in an essential manner* the local structure of the system considered, namely that the global algebra $\mathcal{A}$ is the C^*-inductive limit of local algebras $\mathcal{A}_\Lambda$ relative to bounded regions of space, where the indexing net $\mathcal{F}:=\{\Lambda\}$ is absorbing, i.e. — recall subsection 3.4, part I — for every point x in space, there is a bounded region $\Lambda\in\mathcal{F}$ such that $x\in\Lambda$. An alternative version is requiring that for every bounded region Ω of space there exists some $\Lambda\in\mathcal{F}$ such that $\Omega\subseteq\Lambda$; both versions are acceptable in axiomatic QSP.

2. Also in contrast to reservoir stability — see theorem 48 — this result is one of *internal* consistency in the sense that it establishes the equivalence of two definitions of equilibrium for the *same* system when described from two different points of view: the microscopic KMS condition and the local aspect of thermodynamics of the system considered. In particular, the argument does not involve any coupling of the system considered with any test system.

3. Extensions of the domain of validity of the theorem are desirable. In this respect, quantum spin-lattice systems with reasonably long-range interactions have been controlled. However, some technical difficulties often stand in the way toward the expected extensions to continuous systems. Typically these difficulties originate in the infinite dimensionality of the Hilbert spaces $\mathcal{H}_\Lambda$ corresponding to finite regions, and in the fact that the corresponding Hamiltonians H_Λ are unbounded; also, precautions may have to be taken to ensure that the local particle-density remains bounded.

4. One type of extension of the above variational principle is instructive, namely the shift from local stability to global stability requirements. Specifically, consider again a quantum-lattice system defined on $\mathbb{Z}^d$. Assume further that the dynamics is invariant under the translation group $G=\mathbb{Z}^d$, and restrict attention to the set $\mathfrak{S}^G$ of states ψ each of which is $G-$invariant. Assume finally that the following limits exist

$$(102)\quad f_\beta(\psi) = \lim_{\Lambda\uparrow\mathbb{Z}^d} |\Lambda|^{-1} F_{\Lambda,\beta}(\psi) \quad ; \quad \phi_\beta = \lim_{\Lambda\uparrow\mathbb{Z}^d} |\Lambda|^{-1} \log \mathrm{Tr} \exp^{-\beta H_\Lambda} \quad .$$

A state $\varphi \in \mathfrak{S}^G$ is now said to be *globally thermodynamically stable* — or GTS for short — whenever it minimizes the free-energy density, i.e. when

$$(103)\quad f_\beta(\varphi) = \min_{\psi\in S_G} f_\beta(\psi) = \phi_\beta \quad .$$

As long as one remains with $G-$invariant states on quantum-lattices having $G-$invariant dynamics with only *short-range* interactions, one has

$$\varphi \text{ is GTS} \iff \varphi \text{ is KMS} \quad .$$

However, while $\Rightarrow$ remains valid even when interactions are allowed to extend over a reasonably long range, the "short-range" requirement is essential for $\Leftarrow$. It has been suggested [Sewell, 1980b] that KMS states that are not GTS, i.e. do not minimize the free-energy density, may model metastable states.

5.5 A brief excursion into QFT

As a remark on the role of KMS states in mathematical physics I wish to mention, however briefly, the appearance of modular structures beyond the confines of non-relativistic QSP, namely their entry into relativistic QFT. For the general framework of algebraic QFT, cf. e.g. in this volume [Halvorson, 2006]; for a presentation specifically geared to QFT on curved space-times, cf. also [Wald, 1994]; and for a discussion of some of the interpretation problems raised by the materials in this section, cf. [Clifton and Halvorson, 2001].

From the perspective developed in this essay, the natural entry into the considerations to be discussed in the present subsection is through a manifestation, in Minkowski-space QFT, of the Tomita–Takesaki duality — recall scholium 33 or theorem 39.

Bisognano and Wichmann [Bisognano and Wichmann, 1975] developed a consequence of a standard result in axiomatic QFT — the Reeh–Schlieder theorem, cf. e.g. [Streater and Wightman, 1964, p.168], or [Emch, 1972a, p. 290] and references cited therein — which ensures in particular that the vacuum state φ, when restricted to a wedge $W_R = \{(x,y,z,t) \in M^{3+1} \mid z > |t|\}$, is faithful on the corresponding algebra $\mathcal{N}_R$. Thus, this restriction φ_R of φ to $\mathcal{N}_R$ equips the latter with the structure of a Tomita–Takesaki modular algebra. Here, the canonical objects of the Tomita–Takesaki theory have a seminal geometric interpretation. The involutive antiunitary operator J — corresponding to the reflection $(x,y,z,t) \to (x,y,-z,-t)$ which maps the wedge W_R to the wedge $W_L = \{(x,y,z,t) \in M^{3+1} \mid z < |t|\}$ — implements a bijection from $\mathcal{N}_R$ to $\mathcal{N}_R{}' \simeq \mathcal{N}_L$; and the modular group $\{\Delta^{i\lambda} \mid \lambda \in R\}$ implements on $\mathcal{N}_R$ the Lorentz

boost

$$\begin{pmatrix} x \\ y \\ z \\ t \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cosh(2\pi\lambda) & -\sinh(2\pi\lambda) \\ 0 & 0 & -\sinh(2\pi\lambda) & \cosh(2\pi\lambda) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ t \end{pmatrix} .$$

Since uniformly accelerated observers moving in the interior of a wedge W_R perceive its boundaries as past and future horizons, the result of Bisognano and Wichman could be interpreted as saying that in the universe of such observers — the wedge W_R — the vacuum of the field in M^{3+1} appears to be a thermal bath, in the following sense. The state $\varphi_R : N \in \mathcal{N}_R \mapsto \varphi(N) \in \mathbb{C}$ — where $\mathcal{N}_R \subset \mathcal{N}$ is the algebra corresponding to the wedge W_R, $\mathcal{N}$ is the algebra corresponding to the full Minkowski space, and φ is the vacuum defined on $\mathcal{N}$ — is a KMS state at temperature $\beta > 0$ with respect to the evolution $\{\tau_t : N \in \mathcal{N}_R \mapsto \tau_t[N] = \Delta^{-it/\beta} N \Delta^{it/\beta} \in \mathcal{N}_R \mid t \in \mathbb{R}\}$ (where, as usual, the numerical value of the natural temperature $\beta = 1/kT$ depends on the scale with respect to which the time t is measured).

The physical interest of this interpretation is enhanced by an earlier remark by Rindler [Rindler, 1966] to the effect that the universe of uniformly accelerated observers in W_R is similar to the universe around the Schwarzschild solution of the Einstein equations, i.e. around a stationary "black hole".

With this dictionary in hand, the phenomenon discovered by Bisognano and Wichmann as a consequence of the Tomita–Takesaki theory translates into an effect found independently by Unruh [1976] in an attempt to clarify the then recently discovered Hawking effect [Hawking, 1975] (also known as the Hawking radiation). The latter describes a related but different phenomenon, the creation of thermally distributed particles around a collapsing black hole. The similarities and differences between the Unruh and the Hawking effects are discussed in [Wald, 1994, chapters 5 and 7]; for some of the thermodynamical aspects of the subject in the astrophysics literature, cf. e.g. [Davies, 1978; Hawking and Page, 1983] or [Wald, 1994, chapter 6]; for the specific questions of *what* is actually measurable, *how* and *where,* see [Unruh and Wald, 1984]; and for some of the philosophical issues, see [Clifton and Halvorson, 2001].

The impact of the Bisognano and Wichmann discovery on the axiomatic QFT literature began with the work of Sewell [Sewell, 1980a; Sewell, 1982a] who generalized their results to some curved manifolds, perceived the role that the bifurcate horizon plays in the Unruh effect, and proposed to identify the Hawking temperature and the temperature in the KMS condition associated with the Tomita–Takesaki modular theory. The introduction of KMS structures in QFT then turned out to be the harbinger of a *"revolution"* [Borchers, 2000]. A few among the many developments that ensued are: an extension of the axiomatic of algebraic QFT to curved manifolds; an interpretation of the intrinsic geometry of space-time in terms of consistency relations between the modular structures to be attached to an absorbing net of intersecting wedge-like regions of GR

space-times; and the beginnings of a relativistic QSP where local KMS conditions are formulated in terms of future-directed time-like vectors that determine local rest-frames; cf. e.g. [Summers and Verch, 1996; Buchholz *et al.*, 2002; Ojima, 2003; Wiesbrock, 1997; Buchholz, 2003; Summers and White, 2003; Buchholz and Lechner, 2004]; closer to the Hawking effect proper, [Haag *et al.*, 1994; Kay and Wald, 1991; Fredenhagen and Haag, 1990]; and for a new framework [Fredenhagen, 2003].

5.6 A mathematical interlude: extremal KMS states

The role of extremal KMS states in QSP will be studied in subsection 5.7. The purpose of this section is to review some mathematical preliminaries such as the definition of extremal KMS states, their characterization in terms of their GNS representation, and the decomposition of a KMS state into its extremal components.

REMARKS 56.

1. Let $\mathcal{A}$ be a C^*-algebra, $\beta > 0$ and τ be a group of automorphisms of $\mathcal{A}$. The set $\mathfrak{S}_\beta$ of all KMS states on $\mathcal{A}$ that satisfy the KMS condition for τ and β is convex, i.e. for any two KMS states ψ and χ on $\mathcal{A}$, with respect to the same τ and β, and any $\lambda \in (0,1)$: $\varphi = \lambda\psi + (1-\lambda)\chi$ is again a KMS state for τ and β.

2. The set $\mathfrak{S}_\beta$ is closed in the w^*- topology it inherits from $\mathcal{A}$, and it is bounded in the metric topology. Hence it is w^*-compact, and the Krein–Milman theorem entails that $\mathfrak{S}_\beta$ is the w^*-closed convex hull of the set $\mathfrak{E}_\beta$ of its extreme points [Dunford and Schwartz, 1964, theorem V.8.4]. This ensures not only the existence of extremal points, but also that there are sufficiently many of them: every element in $\mathfrak{S}_\beta$ is the limit of finite convex sums of elements in $\mathfrak{E}_\beta$; see definition 57 below.

3. Moreover $\beta_1 \neq \beta_2$ entails $\mathfrak{S}_{\beta_1} \cap \mathfrak{S}_{\beta_2} = \emptyset$. Incidentally, the GNS representations constructed from states $\varphi_1 \in \mathfrak{S}_{\beta_1}$ and $\varphi_2 \in \mathfrak{S}_{\beta_2}$ with $\beta_1 \neq \beta_2$ are disjoint in the sense that no subrepresentation of one of these is unitarily equivalent to any subrepresentation of the other; cf. [Takesaki, 1970c].

DEFINITION 57. Given a von Neumann algebra $\mathcal{N}$, a group $\{\tau_t \mid t \in \mathbb{R}\}$ of automorphisms of $\mathcal{N}$, $\beta \in \mathbb{R}^+$, and $\mathfrak{S}_\beta$ as in remark 56(1) above. A state $\varphi \in \mathfrak{S}_\beta$ is said to be extremal KMS at natural temperature β if it does not admit a convex decomposition into states in $\mathfrak{S}_\beta$ — i.e. states that satisfy the KMS condition for the same τ and β. The set of all extremal KMS states is denoted $\mathfrak{E}_\beta$.

THEOREM 58. *Let φ be a faithful normal state on a von Neumann algebra $\mathcal{N}$ and τ be the unique group of automorphisms of $\mathcal{N}$ with respect to which φ satisfies the KMS condition for some natural temperature β. Denote by $\mathcal{Z}$ the center $\mathcal{N} \cap \mathcal{N}'$ of $\mathcal{N}$. Then*

A. For every $(t, Z) \in \mathbb{R} \times \mathcal{Z}$, $\tau_t[Z] = Z$.

B. For every positive non-zero element $Z \in \mathcal{Z}$ *with* $0 < Z < I$,

$$\psi(N) := \varphi(Z)^{-1}\varphi(ZN) \quad \text{and} \quad \chi(N) := \varphi(I-Z)^{-1}\varphi((I-Z)N)$$

define two states ψ *and* χ *on* $\mathcal{N}$ *that satisfy the KMS condition for the same* τ *and* β *and provide a convex decomposition of* φ .

C. For every φ *that admits a convex decomposition* $\varphi = \lambda\psi + (1-\lambda)\chi$ *into states* ψ *and* χ *on* $\mathcal{N}$ *that satisfy the KMS condition for the same* τ *and* β , *there exists a unique positive non-zero element* $Z \in \mathcal{Z}$ *with* $\|Z\| \leq 1$ *such that for all* $N \in \mathcal{N}$

$$\psi(N) = \varphi(Z)^{-1}\varphi(ZN) \quad \text{and} \quad \chi(N) = \varphi(I-Z)^{-1}\varphi((I-Z)N) .$$

Proof. As pointed out in remark 37, we may assume without loss of generality that $\mathcal{N}$ is presented in standard form, so that there exists a cyclic and separating vector $\Phi \in \mathcal{H}$ for $\mathcal{N}$ with $\forall N \in \mathcal{N} : (\Phi, N\Phi) = \varphi(N)$.

[A.] $Z \in \mathcal{Z} \Rightarrow \forall (t, N) \in \mathbb{R} \times \mathcal{N}$, $\varphi(N^*\tau_t[Z]) = \varphi(\tau_t[z]N^*)$ and thus φ being KMS entails that $\varphi(N\tau_t[Z])$ is constant in t so that $\forall\, t \in \mathbb{R} : (N\Phi, [\tau_t[Z] - Z]\Phi) = 0$. Φ being cyclic entails $[\tau_t[Z] - Z]\Phi = 0$, and then Φ being separating entails $[\tau_t[Z] - Z] = 0$.

[B.] φ being faithful and $0 < Z < I$ positive and non-zero entail $0 < \varphi(Z) < 1$; and, upon taking into account that Z and thus $Z^{\frac{1}{2}}$ belong to $\mathcal{N}'$, one verifies that ψ and χ are states on $\mathcal{N}$ and that they inherit from φ its KMS property. Moreover, one reads immediately from their definition that $\varphi = \lambda\psi(N) + (1-\lambda)\chi(N)$, where $0 < \lambda = \varphi(Z) < 1$.

[C.] Conversely, from $\varphi = \lambda\psi(N) + (1-\lambda)\chi(N)$, with $0 < \lambda < 1$ one has $\psi \leq \lambda^{-1}\varphi$ and thus there exists an element $X \in \mathcal{N}'$ such $\forall N \in \mathcal{N} : \psi(N) = (X\Phi, NX\Phi)$, i.e. ψ is a vector state on $\mathcal{N}$ and thus is normal and majorized by the normal functional $\lambda^{-1}\varphi$. Hence the Sakai-Radon-Nikodym [Sakai, 1971, proposition 1.24.4], entails that there exists some positive $Y \in \mathcal{N}$ with $\|Y\| \leq 1$ such that

$$\forall N \in \mathcal{N} : \psi(N) = \frac{1}{2}\lambda^{-1}\varphi(NY + YN) .$$

Suppose that there exists another element $\tilde{Y} \in \mathcal{N}$ with the same properties. Let then $X = Y - \tilde{Y}$. We have then $0 = \varphi(X^*X + XX^*)$ and thus, since φ is a positive linear functional and both X^*X and XX^* are positive: $\varphi(X^*X) = 0$. Since φ is faithful, $X = 0$ i.e. $Y = \tilde{Y}$ i.e. Y is unique.

It remains to be shown that the assumptions of the theorem entail that Y also belongs to $\mathcal{N}'$. Since φ and ψ are KMS, they satisfy for all $t \in \mathbb{R}$: $\varphi \circ \tau_t = \varphi$ and $\psi \circ \tau_t = \psi$. Consequently

$$\psi(N) = \psi(\tau_t[N]) = \frac{1}{2}\lambda^{-1}\phi(\tau_t[N]Y + Y\tau_t[N]) = \frac{1}{2}\lambda^{-1}\phi(N\tau_{-t}[Y] + \tau_{-t}[Y]N) .$$

From the uniqueness of $Y \in \mathcal{N}$ which we just established, we have $\forall t \in \mathbb{R} : \tau_t[Y] = Y$. φ being KMS entails therefore $\forall N \in \mathcal{N} : \varphi(NY) = \varphi(YN)$ and thus $\psi(N) = \lambda^{-1}\varphi(YN)$. Upon applying the KMS condition to both ψ and φ, we get $\forall N \in \mathcal{N} : NY = YN$ i.e. $Y \in \mathcal{N}'$. Clearly then $\lambda = \varphi(Z)$. The same argument goes through with χ replacing ψ and $(I - Z)$ replacing Z. ■

The following characterization is an immediate consequence of the above theorem:

COROLLARY 59. *With the assumptions of theorem 58, the KMS state φ is extremal KMS iff $\mathcal{N}$ is a factor, i.e. iff $\mathcal{N}$ has trivial center: $\mathcal{N} \cap \mathcal{N}' = \mathbb{C}I$.*

SCHOLIUM 60. With the assumptions of theorem 58, assume that φ is not extremal KMS, but that the center $\mathcal{Z}$ of $\mathcal{N}$ is generated by a family $\{P_k \in \mathcal{Z} \mid k = 1, 2, ...\}$ of mutually orthogonal projectors. Then there exists a unique decomposition of φ into a convex combination $\sum_k \lambda_k \varphi_k$ of states φ_k on $\mathcal{N}$ where the φ_k are extremal KMS for the same dynamics τ and the same natural temperature β.

Proof. To say that φ is a KMS state that is not extremal KMS is to say that there exist KMS states ψ_j and scalars $\mu_j \in (0, 1)$ such that $\varphi = \sum_j \mu_j \psi_j$. From part C of the theorem, for every ψ_j there exists a positive $Z_j \in \mathcal{Z}$ such that $\forall N \in \mathcal{N} : \psi_j = \phi(Z_j)^{-1}\phi(Z_j N)$. Since $\mathcal{Z}$ is an abelian von Neumann algebra with discrete spectrum, every Z_j may be written as $\sum_k z_k P_k$ with $z_k \in \mathbb{R}^+$ and the P_k are minimal projectors in $\mathcal{Z}$. Hence the $\varphi_k : N \in \mathcal{N} \mapsto {\lambda_k}^{-1}\varphi(P_k N) \in \mathbb{C}$ with $\lambda_k = \phi(P_k)$ are states on $\mathcal{N}$. From part B of the theorem, these are still KMS states for the same τ and β. Therefore, it only remains to show that the states φ_k are extremal with respect to the KMS condition.

To see this, consider the decomposition $\mathcal{H} = \oplus_k \mathcal{H}_k$ where $\mathcal{H}_k$ are the subspaces $\{\Psi_H \in \mathcal{H} \mid P_k\Psi = \Psi\}$. Since each P_k belongs to $\mathcal{Z}$, the subspaces $\mathcal{H}_k$ are stable under $\mathcal{N}$ and under $\mathcal{N}'$, i.e. whenever $X \in \mathcal{N}$ or $X \in \mathcal{N}'$, we have $\forall \Psi \in \mathcal{H}_k : X\Psi \in \mathcal{H}_k$. Let then $\mathcal{N}_k = \{P_k N P_k \mid N \in \mathcal{N}\}$, $\mathcal{N}'_k = \{P_k N P_k \mid N \in \mathcal{N}'\}$; and note that these are von Neumann algebras acting on the space $\mathcal{H}_k$ admitting there a cyclic and separating vector, namely $P_k\Phi$, such that $\forall N \in \mathcal{N}_k : \tilde{\varphi}_k(N) := (\Phi_k, N\Phi_k)$ defines a faithful normal state on $\mathcal{N}_k$; it is thus the restriction to this algebra of the state φ. Note further that for all $t \in \mathbb{R}$, $\mathcal{N}_k$ is stable under τ_t. Since $\mathcal{N}_k \cap \mathcal{N}_k{}' = \mathbb{C}I_k$ (where I_k is the identity operator in $\mathcal{H}_k$) $\tilde{\varphi}_k$ is extremal KMS. Proceeding *ab absurdo*, suppose that φ_k itself is not extremal KMS. Then there would exist some KMS state ψ on $\mathcal{N}$ and some $\lambda \in (0, 1)$ such that $\psi \leq \lambda^{-1}\varphi_k$. Denote by $\tilde{\psi}_k$ the restriction of ψ to $\mathcal{N}_k$. We have then, in particular, $\lambda^{-1}\varphi_k(N^*N) \geq \psi([NP_k]^*[NP_k]) = \psi_k(N^*N)$; i.e. $\lambda^{-1}\tilde{\varphi} \geq \tilde{\psi}_k$. Since $\tilde{\varphi}_k$ is extremal KMS and $\tilde{\psi}_k$ is KMS, the equality must prevail, i.e. $\lambda^{-1}\tilde{\varphi} = \tilde{\psi}_k$; and since $\tilde{\varphi}_k$ and $\tilde{\psi}_k$ are states, $\lambda = 1$, i.e. on $(N)_k : \tilde{\psi}_k(N^*N) = \tilde{\varphi}_k(N^*N)$. By the Schwartz inequality, we have for every $N \in \mathcal{N}$, $\tilde{\psi}_k([P_k N P_k]^*[P_k N P_k]) \leq \psi(N^*N)$, and thus $\psi \geq \varphi_k$. Together with the initial inequality, namely $\psi \leq \varphi_k$ (since we know now that $\lambda = 1$), these two inequalities reduce to $\psi = \varphi_k$. Hence φ_k is indeed an extremal KMS state on $\mathcal{N}$. Since φ_k is extremal KMS on $\mathcal{N}_k$, the restriction

$\tilde{\psi}_k$ of ψ to this algebra must coincide with $\tilde{\varphi}_k$; and thus φ_k is maximal KMS on $\mathcal{N}$. Hence φ has been decomposed into a convex combination of extremal KMS states. Uniqueness follows by contradiction. ■

DEFINITION 61. A convex set $\mathcal{C}$ is said to be a simplex whenever every point in $\mathcal{C}$ admits a unique convex decomposition into extremal points of $\mathcal{C}$.

Recall that in two-dimensional Euclidean geometry, a triangle is a simplex; indeed any point in the triangle obtains as a unique convex combination of points situated at the vertices of the triangle. But a circle is not a simplex: the set of its extreme points is the circumference of the circle, and given any point inside the circle, all secants through this point give different convex combinations of extreme points.

REMARKS 62.

1. Scholium 60 may therefore be paraphrased by saying that under the assumption that the spectrum $Sp(\mathcal{Z})$ of the center $\mathcal{Z}$ is discrete, $\mathfrak{S}_\beta$ is a simplex; and that the decomposition is a weighed sum with respect to a discrete probability measure supported by the extreme points $\mathfrak{E}_\beta$ of the set $\mathfrak{S}_\beta$ of all normal KMS states for the given dynamics τ and the given natural temperature β. From the proof of the scholium, one checks that the latter statement extends indeed to all normal states, and not just to those that are faithful.

2. In case $Sp(\mathcal{Z})$ is not discrete, the above sum must be replaced by an integral, and some measure-theoretical trimmings are necessary to specify the sense in which φ defines a *unique* measure concentrated on the boundary of $\mathfrak{S}_\beta$. The general mathematical context in which these decompositions appear is in the study of central measures, see [Takesaki, 1970a; Kadison and Ringrose, 1983/1986]. For the purpose of this essay, the simpler version just described will suffice to anchor the conceptual structure of the theory governing the unique decomposition of KMS states into their extremal components.

3. Note that the set of states on a quantum system described by the von Neumann postulates is *not* a simplex: if a density matrix has at least one eigenvalue with multiplicity greater or equal to 2, its decomposition in pure states is not unique. Hence the set of KMS states in *quantum* statistical physics possesses a *classical* property that is otherwise not heard of in the quantum realm.

4. It remains to demonstrate that this property is relevant to QSP; and thus that QSP requires the consideration of situations for which the relevant representations do not lead to factors, in contrast with the von Neumann formalism of quantum mechanics where the canonical equilibrium states lead only to factor representations — recall the end of remark 34. This problem is the object of the next subsection.

5.7 Extremal KMS states, pure thermodynamical phases

The main argument one can advance to justify the claim that pure thermodynamical phases be described in QSP as extremal KMS states originates in the conjunction of three circumstances.

The *first* is based on subsections 5.3 and 5.4 where strong evidences were given for the identification of canonical equilibrium states as KMS states.

The *second* is the fact that extremal KMS states are the elementary objects in the KMS theory. This is reminiscent of the identification of atomic levels in *spectroscopy* with irreducible representations of the group of symmetries of the system, the famous "Gruppenpest" epitomized in [Wigner, 1931]. In mathematics, this programme was extended to a systematic presentation of the familiar so-called *special functions* where these functions now appear as bases of irreducible representations of groups; cf. e.g. [Talman, 1968; Vilenkin, 1968]. Closer to the focus of this essay, the early identification — in [Murray and von Neumann, 1936] — of *factors as the building blocks* of the theory of von Neumann algebras proceeds from the same principle: a methodological option confirmed by the central decomposition of a von Neumann algebra as a direct integral of factors; cf. e.g. [Kadison and Ringrose, 1983/1986, theorem 14.2.2, pp. 1027–1028]. All the while, the group-theoretical approach continues to contribute in sorting out qualitative clssification problems in *nuclear spectroscopy,* and *elementary particles* high energy physics.

The *third* circumstance pointing to the description of pure thermodynamical phases as extremal KMS states — i.e. KMS states the GNS representations of which are factors, cf. corollary 59 above — is the mathematical fact that the decomposition of a KMS state in extremal KMS states is *unique*; cf. scholium 60 and remark 62(2) above. In the context of QSP, this fact naturally directs attention to the situation encountered in thermodynamics where an equilibrium state decomposes uniquely into its pure thermodynamical phases.

Thus, this subsection is divided into two parts. In part **A**, the above speculations are confronted with a model for QSP where everything can be computed explicitly. In part **B**, the characterization of pure thermodynamical phases as extremal KMS states is brought to bear on a famous argument by Landau offering a fundamental microscopic distinction between solids and fluids in term of space correlation functions. This exemplifies how the unique decomposition of KMS states into their extremal components helps describe the coexistence of pure thermodynamical phases in QSP and spontaneous symmetry breaking in systems undergoing phase transitions. For further discussion of the latter, cf. [Liu and Emch, 2005].

A. Quantum Weiss–Ising models for ferromagnetism

Recall first the results of Araki reported in subsection 5.3 concerning the absence of a ferromagnetic phase transition: the unique KMS state for each of the models covered there is extremal.

To check how this coincidence fares with systems that *do* exhibit several ther-

modynamical phases, we turn now to a class of models that have a long history in the physics of phase transitions [Weiss, 1907; Brout, 1965], and are accepted by mathematicians to be amenable to a sufficiently rigorous treatment [Kac, 1968], namely the Weiss–Ising models for ferromagnetism.

Consider a one-dimensional lattice $\mathbb{Z}$ where to every site $k \in \mathbb{Z}$ a quantum spin σ_k is attached. To every finite string $\Lambda \subset \mathbb{Z}$ is associated a Hamiltonian

$$(104)\quad H = -\sum_{k\in\Lambda}[B + B_{\Lambda,k}]{\sigma_k}^z \quad \text{with} \quad B_{\Lambda,k} = \frac{1}{2}\sum_{j\in\Lambda} J_{\Lambda,jk}{\sigma_j}^z$$

where B is interpreted as a homogeneous external magnetic field parallel to a fixed direction z; and $B_{\Lambda,k}$ is an average magnetic field, the so-called "molecular" field, experienced by the spin at site k resulting from all other spins in the region Λ. The artificial assumption imposed on the models of the van der Waals or Weiss-type, which makes them exactly solvable in the thermodynamical limit, is that the strength of the interaction $J_{\Lambda,jk}$ decreases with the size $|\Lambda|$ of Λ; compare this with the property $|v(p,q)| \leq c/|\Lambda|$ of the interaction of the BCS model in subsection 5.1.

Adopting here a simplified version of [Emch and Knops, 1970], we will assume that

$$(105)\quad J_{\Lambda,jk} = \begin{cases} |\Lambda|^{-1}\, J > 0 & \text{when} \quad j \neq k \\ 0 & \text{otherwise} \end{cases} .$$

Upon controlling the thermodynamical limit $|\Lambda| \to \infty$, one finds that two extremal KMS states emerge when $T < T_c$ where $1/kT_c = \beta_c = J^{-1}$. These are recognized by the following properties of a global observable — cf. definition 15 and scholium 23 — namely, the magnetization $\mathbf{M}$, the three components of which

$$M^i = \text{ weak op. limit}_{\,|\Lambda|\to\infty}\ \frac{1}{|\Lambda|}\sum_{k\in\Lambda}{\sigma_k}^i \qquad (i = x, y, z)$$

are defined in the corresponding temperature-dependent representation. They satisfy

$$(106)\quad \begin{aligned} &\text{(i)} && M^x = M^y = 0 \\ &\text{(ii)} && M^z = \tanh[\beta(B + JM^z)] \ . \end{aligned}$$

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1. For the transverse components, M^x and M^y, (106.i) was to be expected from the symmetry of the system. The interesting part is the result for the component M^z parallel to the applied magnetic field: (106.ii) is the classical self-consistency equation: the model exhibits a phase transition as there exists a temperature T_c (with $\beta_c = J^{-1}$) below which M^z does not vanish as $B \to 0$, but tends to a finite, temperature-dependent value, the so-called spontaneous magnetization.

2. Hence in the thermodynamical limit, the problem of determining the extremal KMS states of the model admits two new solutions, absent above T_c; these extremal KMS states exhibit the two opposite spontaneous magnetizations characteristic of the two pure thermodynamical phases familiar from the treatment of the classical case in e.g. [Kac, 1968].

3. A phase transition has occurred at $T = T_c$ and it is accompanied, for $T < T_c$, by a spontaneous breakdown of the flip-flop symmetry $\sigma_k{}^z \to -\sigma_k{}^z$ of the local Hamiltonians (104).

4. One ought to note at this point that the treatment in [Kac, 1968] was in the most orthodox spirit of classical statistical mechanics: an analysis by steepest descent methods of the partition function in the limit $|\Lambda| \to \infty$. The novelty in [Emch and Knops, 1970] was to consider also the evolution of the $x-$ and $y-$ components of the quantum spins and to study the resulting quantum dynamics in order to confront the interpretation of extremal KMS states with results already known from a classical treatment.

   As with the BCS model reviewed in subsection 5.1 above, which has also the structure of a 'molecular' field model, some technicalities are involved here: in the thermodynamical limit, the convergence of the evolution is established only for the von Neumann algebras belonging to the representations considered.

5. This simplified version of the model, where (105) is assumed, already allows us to demonstrate the general features explored in this subsection. We may nevertheless mention that in [Emch and Knops, 1970] $J_{\Lambda,jk}$ is allowed to depend on the distance $|j-k|$, but only in such a way that for each $k \in \mathbb{Z}$, there exists a constant c_k such that $\sum_k |J_{\Lambda,jk}| < c_k$ for every finite Λ containing k, subject to the condition that $\forall\, j,k \in \mathbb{Z} :\ \lim_{|\Lambda|\to\infty} J_{\Lambda,jk} = 0$; the set of thermodynamical phases then becomes more complex, but its description still illustrates the adequacy of the decomposition account of spontaneous symmetry breakdown.

6. We already pointed out — first in section 4.1 — that as a consequence of the Liouville theorem of complex analysis, KMS states are necessarily time-invariant. Nevertheless, as established in [Emch and Knops, 1970], the present model admits *extremal KMS states that are not extremal time-invariant* — i.e. KMS states that are convex sums of different time-invariant, but not KMS, states — although these extremal KMS states do satisfy a very strong clustering property with respect to *space-translations.* The occurrence of extremal KMS states that are not extremal time-invariant reflects the fact that the time-evolution is *not* asymptotically abelian. This is not an unexpected peculiarity of the model since experience shows that asymptotic abelianness for the group of *time*-translations is rarely satisfied in QSP — although a few exceptions are known, among them the even part of the XY-model discussed at the beginning of subsection 5.4, despite the fact that

locality entails very strong asymptotic abelianness for the group of *space*-translations.

The coexistence of liquid and gas — say vapour and liquid water — presents formal similarities with the coexistence of magnetic phases oriented in opposite directions. The lattice-gas models of classical statistical mechanics are treated in close analogy with those of their ferromagnetic counterparts: instead of attributing to each site of a regular n-dimensional Ising model, a classical spin taking the values $+1/2$ and $-1/2$, one considers a random variable indexed by the sites of the lattice and taking the values 1 or 0 depending on whether the site is occupied by a molecule or not; double (or higher) occupancy is ruled out by *fiat* in these models. Phenomenologically, liquid-vapour coexistence curves in the phase diagram translate closely to the coexistence curves in ferromagnetic materials. In particular both present a critical point, precisely located in the phase space by the occurrence of diverging fluctuations. For temperatures higher than the critical temperature, any distinction between liquid and gas is untenable, and this state of matter is best described as a fluid.

B. QSP brought to bear on the Landau argument

The situation encountered with the coexistence of fluid and crytalline phases of the same substance — say water in its fluid phase and ice phase — is phenomenologically very different from the situation presented by a gas-liquid phase transition. Here, no critical point has been located: the fluid-solid coexistence curve extends indefinitely as pressure and density are increased. A heuristic argument for the non-existence of a critical point for the fluid-solid coexistence curve was advanced by Landau; see for instance [Landau and Lifshitz, 1958b, p. 260]. The argument was taken up by Uhlenbeck in [Uhlenbeck, 1968, p. 17]: "Because the solid and the fluid are with respect to long range order qualitatively different, there cannot be a critical point, since by going around it this would imply that long range order would appear gradually, which is impossible. This is the argument of Landau and I find it completely convincing." And yet, Uhlenbeck warns on the same page that "one cannot escape the fact (intuitively evident, although not proved!) that there is already long range order in the solid phase itself."

In an impressive sequence of papers, Kastler *et al.* [1967] rose to the challenge; the various assumptions of asymptotic abelianness, pervasive in these papers, was shown to be dispensable in the version worked out in [Emch *et al.*, 1970], which is followed here.

The programme is to classify the extremal KMS states that appear in the decomposition of a Euclidean invariant KMS state. Let $\mathcal{A}$ be the C^*-algebra obtained as the C^*-inductive limit of local algebras $\mathcal{A}(\Lambda)$ over an absorbing net $\mathcal{F}$ of finite regions $\Lambda \subset \mathbb{R}^3$ (here 'finite' means finite volume: $|\Lambda| < \infty$). Let $\alpha : t \in \mathbb{R} \mapsto \alpha_t \in \mathrm{Aut}(\mathcal{A})$ describe an evolution; let $\nu : g \in \mathbb{E}^3 \mapsto \alpha_g \in \mathrm{Aut}(\mathcal{A})$ describe the action of the Euclidean group $\mathbb{E}^3$; and let φ be a KMS state on $\mathcal{A}$ with respect to the evolution α for the temperature β; φ is assumed to be invariant under the action of the Euclidean group, i.e. $\forall g \in \mathbb{E}^3 \ : \ \varphi \circ \nu_g = \varphi$; this

condition is motivated by the phenomenological expectation that the underlying interactions are Euclidean invariant.

It is convenient to assume further that φ is strongly transitive with respect to the action of $\mathbb{E}^3$ in the sense that the following two conditions are satisfied.

1. For any two states ψ and ψ' appearing in the decomposition of φ in extremal KMS states, there exists at least one $g \in \mathbb{E}^3$ such that $\psi' = \psi \circ \nu_g$.

2. For one — and therefore all — state ψ appearing in the decomposition of φ into extremal KMS states, the isotropy subgroup $G_\psi := \{g \in \mathbb{E}^3 \mid \psi \circ \nu_g = \psi\}$ contains at least three non-coplanar translations.

Note that for any $g \in \mathbb{E}^3$ and any ψ appearing in the decomposition of φ into extremal KMS states, the state $\psi_g := \psi \circ \nu_g$ also appears there; and that $G_{\psi_g} = g^{-1} G_\psi g$. Hence, up to conjugacy, all elements appearing in the decomposition of φ have the same symmetry. This conjugacy class is denoted G^φ, and is referred to it as the *intrinsic symmetry* of φ. It is the part of the Euclidean symmetry of φ that is preserved when φ is decomposed into its extremal KMS components. Consequently, condition (1) is essentially one of convenience: if it were not satisfied, one would first have to separate the decomposed states in classes of conjugate elements, and carry out the analysis sketched below for each class separately. Condition (2) excludes pathological cases which one does not want to consider here. Mathematically, it strengthens condition (1) to ensure that the orbit of each extremal state under the translation group $\mathbb{R}^3 \subset \mathbb{E}^3$ in the space of all states on $\mathcal{A}$ is closed.

It is then proven in [Emch *et al.*, 1970] that a Euclidean-invariant KMS state φ that satisfies the above conditions must necessarily belong to one of the following four classes.

The first class obtains when φ is already extremal KMS, i.e. its intrinsic symmetry is the group $\mathbb{E}^3$ itself. This case occurs *exactly when* one — and thus all — of the following *equivalent* conditions is satisfied:

1. φ is extremal $\mathbb{R}^3$ invariant, i.e. cannot be decomposed into a convex combination of states that are invariant under all translations in $\mathbb{R}^3$.

2. The spectrum of the generator $\mathbf{P}$ of the unitary representation of $\mathbb{R}^3$ canonically associated to φ by the GNS construction consists of exactly one eigenvalue, namely $\mathbf{k} = 0$, and this eigenvalue is non-degenerate.

3. φ is uniformly clustering in space, i.e. : for every $\epsilon > 0$ and $A \in \mathcal{A}$ there exists a finite region of space $\Lambda \subset \mathbb{R}^3$ such that

   (107) $\forall\, B \in \mathcal{A}(\Lambda^c) : |\varphi(AB) - \varphi(A)\varphi(B)| \leq \epsilon \|B\|$

   where $\mathcal{A}(\Lambda^c) \subset \mathcal{A}$ is the C^*-inductive limit of the local algebras $\mathcal{A}(\Omega)$ with $\Omega \in \mathcal{F}$ and $\Omega \bowtie \Lambda$, (i.e. $\Omega \cap \Lambda = \emptyset$); see definition 27, scholium 29 and corollary 30 above.

In view of these properties, a state φ belonging to this class is intepreted as a *fluid phase*.

To describe the other three classes, namely the strongly transitive Euclidean invariant KMS states that do *not* describe fluids, let us focus now on the notion of the *intrinsic translational invariance* of φ. For any state ψ that appears in the decomposition of φ into extremal KMS states, let G_ψ denote the subgroup of Euclidean symmetries of ψ, and let $H_\psi = G_\psi \cap \mathbb{R}^3$ denote the subgroup of space-translations that preserve ψ. As one reviews the definition of the conjugacy classes one verifies that this group is indeed characteristic of the original state φ. Note also that strong transitivity entails that $\mathbb{R}^3/H_\psi$ is compact.

The second class of Euclidean, strongly transitive KMS states is now specified by the following *equivalent* conditions, where ψ is any state appearing in the decomposition of φ into its extremal KMS components.

1. G_ψ is a crystallographic group.

2. φ is not extremal $\mathbb{R}^3-$invariant, and H_ψ is generated by three non-coplanar translations.

3. With $\chi = \eta^{\mathbb{R}^3}[\psi]$ — where $\eta^{\mathbb{R}^3}$ is any invariant mean over the translation group $\mathbb{R}^3$ — χ is $\eta-$clustering (see definition 22 above), but neither weakly mixing nor even partially weakly mixing, i.e. χ satisfies

$$(108)\ \ \forall\ A\,,\ B\ \in \mathcal{A}\ :\ \eta^{\mathbb{R}^3}\left(\chi(\nu_\bullet[A]\,B) - \chi(A)\,\chi(B)\right) = 0$$

but does *not* satisfy any of the stronger conditions

$$(109)\ \ \forall\ A\,,\ B\ \in \mathcal{A}\ :\ \eta^{\mathbb{R}^3}\,|\,\chi(\nu_\bullet[A]\,B) - \chi(A)\,\chi(B)\,|\,= 0$$

$$(110)\ \ \forall\ A\,,\ B\ \in \mathcal{A}\ :\ \eta^{\mathbb{R}^1}\left|\,\eta^{\mathbb{R}^2}\left(\chi(\nu_\bullet[A]\,B)\right) - \chi(A)\,\chi(B)\right| = 0$$

$$(111)\ \ \forall\ A\,,\ B\ \in \mathcal{A}\ :\ \eta^{\mathbb{R}^2}\left|\,\eta^{\mathbb{R}^1}\left(\chi(\nu_\bullet[A]\,B)\right) - \chi(A)\,\chi(B)\right| = 0$$

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1. Taken separately, each of the conditions (1–3) excludes that φ be a fluid phase. Indeed, a fluid phase is extremal KMS, so that its intrinsic symmetry is the Euclidian group $\mathbb{E}^3$, contradicting (1); a fluid phase is extremal $\mathbb{R}^3-$invariant, contradicting (2); a fluid phase is uniformly clustering (see 5.33), which implies that each of the relations (108–111) would be satisfied, whereas (109–111) are not satisfied in the present phase.

2. The other two classes to which φ may belong are characterized as follows. (109), if satisfied, would have entailed $H_\psi = \mathbb{R}^3$, thus contradicting the second part of condition (2). This would correspond to a situation where the rotational symmetry is broken whereas the translational symmetry of the state φ would be completely preserved in its decomposition into its extremal KMS components. Although this may occur in systems exhibiting spontaneous magnetization, it is not immediately relevant to the purpose of identifying the way in which the formalism distinguishes fluids from solids in a world where fundamental interactions are invariant under the Euclidean group $\mathbb{E}^3$.

   Similarly, (110) or (111), if satisfied, would have entailed H_ψ is continuous in one or two direction(s) but discrete in the complementary direction(s). Such situations have been envisaged also — as early as the mid 1930s, cf. e.g. [Landau and Lifshitz, 1958b, p. 410] — but here again, their putative existence does not bear directly on the problem at hand.

3. The space-averaged state χ, which is $\mathbb{R}^3-$invariant by construction, nevertheless keeps a memory of the symmetry of the state ψ from which it is constructed. Indeed the *discrete* part of the spectrum of the generator $\mathbf{P}_\chi$ of the unitary group representation of $\mathbb{R}^3$, associated to the GNS construction corresponding to χ, coincides with the reciprocal group of H_ψ, namely with

   (112) $H_\psi{}^* = \{\mathbf{k} \in \mathbb{R}^3 \mid \forall\, \mathbf{a} \in H_\psi \,:\, \mathbf{k}\cdot\mathbf{a} = 0 \mod 2\pi\}$

   which, in principle, is observable in X-ray diffraction patterns.

Upon keeping from the above what is relevant to the absence of a critical point in the coexistence curve between fluid and solid, the analysis of the decomposition of Euclidean invariant canonical equilibrium states into their pure thermodynamical phase components provides a rigid relation between the clustering properties and the geometric properties of these states. Namely: fluid phases exhibit a uniform clustering property (107), while crystalline phases lead to the distinctly weaker property of weak-clustering (108), thus vindicating the Landau argument.

6 WHENCE AND WHITHER QSP?

This final section may serve as a summary, a conclusion, a collection of appendices sharpening some aspects of the theory that have not been discussed in the main text; and hopefully, as a constructive prospectus for territories beyond the scope of this essay.

Let me summarize very briefly the story so far. First, recall that sections 1 to 3 reviewed some of the salient features that are variously treated in traditional texts on QSP. Then, in sections 4 and 5, I argued that the algebraic formalism of the KMS condition provides a well-defined syntax, the semantics of which supports the following associations in equilibrium QSP.

- Canonical equilibrium states are described by KMS states, a notion that translates naturally from finite systems to systems considered in the themodynamical limit.
- Pure thermodynamical phases are described by extremal KMS states.
- Pure thermodynamical phase components that appear in the unique decomposition of a canonical equilibrium state may have a symmetry lower than that of the original state: only the manifold of the different contributing phases reflects the original symmetry; cf. [Liu and Emch, 2005] where we describe the "decompositional account" of spontaneous symmetry breakdown in the quantum theory of phase transitions.

Against this background, the material of the present section is presented in four subsections. I first review the mathematical concept of a limit and its physical interpretation as used in the main text. I then discuss again the notion of macroscopic observables, taking here a perspective that opens on the next subsection: the quantum measurement problem. Finally, I present some remarks — prospective and/or revisionist? — on the pursuit of constructive confrontations between mathematical and theoretical physicists in order that they better inform the wider arenas where philosophers of science operate.

6.1 Four limiting procedures in QSP

In dealing with the topics just reviewed, and as early as in sections 2 and 3, at least four different types of limits were encountered, alone or in concert.

1. the classical limit $h \to 0$;
2. the high temperature limit $T \to \infty$;
3. the thermodynamic limit $|\Lambda| \to \infty$;
4. the van Hove limit $\{\lambda \to 0 \text{ and } t \to \infty\}$ with $\tau := \lambda^2 t$ remaining finite.

As the philosophical legitimacy of each of these four limits (or 'limiting procedures') has been variously questioned elsewhere, I ought to specify again — in the vernacular, i.e. without an explicit mention of the traditional $(\epsilon, \delta_\epsilon)$ — that the limits were consistently understood in this essay to be *controlled limits* in the sense of mathematics: you give me a tolerance, and I tell you the price; the smaller the tolerance, the higher the price; but however small the error you are willing to tolerate, there is a price under which you are guaranteed that the article will be within what you decided you are going to tolerate. Mathematical physics adds to this the requirement that the "price" be expressed in currencies recognized by the putative laboratory technician. Let us examine successively the above four limits from this perspective.

1. The classical limit.
The Planck constant is a *fundamental physical constant:* in cgs units $h \simeq 6.62 \times 10^{-27}$ ergsec; the familiar notation $\hbar := h/2\pi$ is used here. To say that it is small is a "value judgement", reflecting the energy scale which you believe is relevant for the problem you wish to discuss. To illustrate the working of limiting processes, and their physical meaning, let us examine a specific example, the classical limit of a typically quantum phenomenon, the tunnel effect in which a particle of energy E does "slip through" a barrier of height $V_o > E$. This effect was discovered in 1928 independently by Gamow and by Gurney and Condon [Gamov, 1928; Gurney and Condon, 1928; Gurney and Condon, 1929] in their search for an explanation of alpha-particle emission from heavy nuclei. The Josephson junction — an oxide layer sandwiched between two superconductors — is a more recent manifestation of this quantum phenomenon; cf. e.g. [Josephson, 1982]. Let us consider here the simplest model, quantum tunelling through a square one-dimensional barrier.

One verifies immediately that the Schrödinger equation

$$\left[-\tfrac{1}{2m}\hbar^2 \tfrac{d^2}{dx^2} + V(x)\right] \Psi(x) = E\Psi(x) \qquad \text{with}$$

$$V(x) = \begin{cases} 0 & \text{if} \quad x < a \\ V_o & \text{if} \quad -a < x < a \\ 0 & \text{if} \quad x > a \end{cases} \quad \text{where } 0 < a < \infty \text{ and } 0 < V_o < \infty \tag{113}$$

admits, whenever $0 < E < V_o$, a solution of the form

$$\Psi(x) = \begin{cases} A_- e^{ikx} + B_- e^{-ikx} & \text{if} \quad x < a \\ Ae^{\kappa x} + Be^{-\kappa x} & \text{if} \quad -a < x < a \\ A_+ e^{ikx} & \text{if} \quad x > a \end{cases} \tag{114}$$

with

$$k = \left\{\frac{2mE}{\hbar^2}\right\}^{\frac{1}{2}} \quad \text{and} \quad \kappa = \left\{\frac{2m(V_o - E)}{\hbar^2}\right\}^{\frac{1}{2}} \tag{115}$$

where the relative ratio of the five coefficients A_-, B_-, A, B, A_+ in (114) are determined by imposing four conditions, namely that Ψ and its derivative be continuous

at the boundaries $x = \pm a$. In particular, these conditions imply

$$A_- = A_+ e^{ika} \frac{1}{4ik\kappa} \left[(\kappa + ik)^2 e^{-2\kappa a} - (\kappa - ik)^2 e^{2\kappa a} \right] .$$

Then from the reverse triangle inequality $|a - b| \geq \max\{|a| - |b|\,,\, |b| - |a|\}$:

$$\left| \frac{A_-}{A_+} \right| \geq \frac{k^2 + \kappa^2}{4k\kappa} \left(e^{2\kappa a} - e^{-2\kappa a} \right) = \left[\frac{1}{2} \frac{V_o}{\sqrt{E(V_o - E)}} \right] \sinh 2\kappa a$$

Since the term [...] is independent of $\hbar$, let us emphasize the role of $\hbar$ by rewriting the above formula as:

$$(116) \quad \frac{|A_+|^2}{|A_-|^2} \leq C \, [\sinh 2\kappa a]^{-2} \quad .$$

From the definition of $A_\pm$ in (114), the left-hand side of (116) is to be interpreted as the transmission coefficient of the barrier. In the corresponding classical model, $0 < E < V_o$ entails that this coefficient vanishes. Thus, to demand that the quantum model approximates its classical counterpart is to require that the quantum transmission coefficient be arbitrarily small, say

$$(117) \quad \frac{|A_+|^2}{|A_-|^2} \leq C \, [\sinh 2K]^{-2}$$

with K as large as one desires. To ensure that (117) is satisfied, the computation leading to (116) shows that it is sufficient to have: $\kappa a > K$, i.e.

$$(118) \quad \hbar < K^{-1} \, [2m(V_o - E)]^{\frac{1}{2}} \, a \quad .$$

Hence, the classical limit of the quantum system (113) now is controlled:

(i) mathematically, through the conjunction of (117) and (118);

(ii) physically, as (118) gives an estimate of its range of validity in terms of the physical quantities that characterize this system

In this sense the classical limit is similar to the non-relativistic limit: the classical description emerges from the quantum theory in the same way as Newton's mechanics emerges from Einstein's special relativity theory. The key to a proper understanding is the evaluation of the domain of validity of the approximations. Having done so, I have no qualm assuring my insurance agent that my car is not going to tunnel out of my garage, nor do I worry about relativistic red-shift when I drive my car in congested traffic. Such are the physical parameters that prevail in my car, my garage and the town where I live; compare with [Gamov, 1940] where Gamow pretends with didactic gusto that $h \simeq 1$ ergsec or $c \simeq 15$ km/hour.

2. The high temperature limit.

Following the Ehrenfests, I have repeatedly argued in this essay that in QSP, the

classical regime emerges when the temperature is high enough. Typically, the quantities that tell us the regime in which we operate are similar to (βh) with $\beta = 1/kT$ (where k is the Boltzmann constant $k \simeq 1.38 \times 10^{-16}$ erg degree^{-1}).

To illustrate this point, let us review the results on the black-body radiation (subsection 2.1) and the specific heat of solids (subsection 2.3).

We saw qualitatively that if $h\nu \gg kT$ Planck's formula of 1900, here (1), reproduces (5) which had been previously established by Wien in 1896 [Wien, 1896]. Quantitatively, Paschen and Wanner [Paschen and Wanner, 1899] had verified in 1899 that Wien's formula is in agreement with laboratory data in the range of visible light, i.e. for wave length $\lambda = c/\nu$ between 4000 Å and 7000 Å, for temperatures up to 4000 K; this is what we would call today the "quantum regime". As the temperature at the surface of the sun is about 6000 K, going to much higher temperatures was then not an option. Nevertheless, as the ratio $h\nu/kT$ is concerned, raising T or lowering ν have the same effect; the latter means pushing the observation into the infrared, which was possible at the time. Indeed, the following year Lummer and Pringsheim [Lummer and Pringsheim, 1900] recorded systematic deviations from Wien's formula when the wavelength reaches the range of 12 to 18 μ (recall $1\mu = 10^{-6}$m and thus $12\mu = 12 \cdot 10^4$Å, compared with $\sim 7 \cdot 10^3$Å for visible red). This is the observation that prompted the purely classical derivation of the Rayleigh–Jones formula (6), and then Planck's interpolation between $h\nu \gg kT$ (Wien) and $h\nu \ll kT$ (Rayleigh–Jones). Experimentally, the passage from Pashen and Wanner to Lummer and Pringsheim thus marks very sharply in time (less than two years) the crossing of the boundary from the quantum to the classical regimes. These two regimes are numerically characterized by their distance $|\lambda - \lambda_{max}|$ from the wavelength λ_{max} — or equivalently the frequency ν_{max} — at which the Planck distribution (1) passes through a maximum.

As for the specific heat of solids, upon revisiting equations (8) and (9) Debye already verified that conclusion (10) can be sharpened to give the exact result

$$(119) \quad \text{where} \quad \left. \begin{array}{l} C_V = 3R\{4D(\frac{\Theta}{T}) - 3(\frac{\Theta}{T})[\exp(\frac{\Theta}{T}) - 1]^{-1}\} \\ D(x) = \int_o^x dt \frac{t^3}{e^t - 1} \quad \text{and} \quad k\Theta = h\nu_o \end{array} \right\} .$$

Scholium 2 was obtained by noticing that

$$D(x) \simeq \left\{ \begin{array}{lll} 1 & \text{for} & 0 < x \ll 1 \\ \\ \frac{1}{5}\pi^4 x^{-3} & \text{for} & x \gg 1 \end{array} \right. .$$

To go further than this, and determine the onset of the classical regime $C_V = 3R$, requires one to notice two things. First, C_V in (119) is a monotonically increasing *universal* function of the variable Θ/T; while it cannot be written in terms of elementary functions, it can be computed numerically. Since Θ is known in term of the cut-off ν_o on the vibrational frequencies of the crystal, its value can be determined by mechanical means: for instance, at room temperature, Θ is about

100 K (for lead) and about 400 K (for aluminium), with silver and copper in between. For these, and many other metals, the measured values of the specific heat fall remarkably close to the theoretical prediction (119); cf. e.g. [Wannier, 1966, fig.13.9, p.276]. This curve shows a monotonic and smooth passage from the classical to the quantum regimes as the temperature decreases. Specifically, we can now discuss quantitatively the onset of the classical regime. The exact expression (119) entails that the first two terms in the expansion of C_V for $\Theta/T \ll 1$ give

$$(120)\quad C_V \simeq 3R\{1 - \frac{1}{20}(\frac{\Theta}{T})^2\}$$

so that at room temperature $T \simeq 300$ K, the correction to the classical value $C_V = 3R$ ranges from about 0.6 % (for lead) to about 9 % for aluminium; both of which are in good agreement with experimental data.

For other early recognitions of the emergence of the classical regime in high temperature QSP, see subsections 2.4 and 2.6 where the classical ideal gas is recovered as controlled high temperature limits of both the Bose and the Fermi quantum gases.

3. The thermodynamical limit.

As its name indicates, the thermodynamical limit is designed to elicit various macroscopic thermodynamical behaviours from microscopic mechanical models. I find it convenient to separate here the problems addressed in non-equilibrium and in equilibrium statistical physics.

a. *Non-equilibrium physics.* In the classical realm already, one appeals to the large size of the systems considered to avoid the spurious appearance of recurrences in the theoretical modeling of physical phenomena such as the thermodynamical approach to equilibrium. For instance, to buttress Boltzmann's kinetic theory of gases, the Ehrenfests proposed the so-called dog-flea model, a stochastic model later revisited by Mark Kac. This model is reviewed in [Emch and Liu, 2002, section 3.4] where the results of a computer experiment are reported, involving $N = 100$ "fleas" jumping "at random" between two "dogs": a tendency to approach equilibrium is manifest during a few hundred jumps, whereas the frequency of recurrences, which Kac showed to increase exponentially with N, is observed to occur — as regularly as to be expected — over a range of several tens of thousands of trials.

In the quantum realm, a model for an actual experiment, the nuclear free-relaxation, is solved in subsection 3.3 above. Here again the model shows an approach to equilibrium practically unaffected by a "recurrence time" that grows as 2^N, where N is the number of lattice sites in the system, a macroscopic CaF_2 crystal. Hence the empirical justification for the limit $N \to \infty$ is that the relevant time-parameter for the experimentalist is $\sim 2^{10^{23}}$, which is indeed exorbitant; accordingly, I could not discern from the laboratory [Lowe and Nordberg, 1957] any concern about putative recurrences. The supporting analytic evidence is the explicit size-correction given in equation (49) and discussed with some detail in remarks 6.

b. *Equilibrium Physics.* In equilibrium situations, the thermodynamical limit is called upon to focus on properties of matter in bulk, so to speak navigating the high seas, away from the shoals of boundary effects. This often requires some elaborate rigging, in CSP as well as in QSP.

Roughly speaking, up to the middle of the twentieth century, this was achieved by replacing sums by integrals, as in equations (13–14). As in other parts of mathematical physics, this mathematical procedure is usually well under control, albeit physics sometimes requires unusual precautions, as shown explicitly in the caveat of equation (50).

Later on, especially in the modeling of phase transitions, when the emergence of collective behaviour turned out to be essential for the understanding of the phenomena at hand, and when existence questions were raised, more sophistication was demanded. In particular, for the limit where the size of the system is allowed to go to infinity, dimension enters the play; and then, in particular, the shapes of the regions considered must be such that the ratio of the surface to the volume goes to zero: cubes are fine; sponges are not. As indicated in the various models presented in section 5, it is possible to carry out such limiting procedures explicitly and successfully. The simplest examples are lattice systems, say spins on a lattice $\mathbb{Z}^d$. Examples of continuous systems are also given in this section 5; yet, in general, such systems, say on $\mathbb{R}^d$, require extra technical care to ensure spatial uniformity and to avoid bundling effects; hence, in the latter cases the theory is not always as fully controlled as one may desire; see nevertheless [Sewell, 2002]. Interactions with extremely long range may pose further problems with regard to: (a) the definition of the limiting state; and (b) the control of the limiting time evolution; such situations were met in subsections 5.1 and 5.7.A.

4. The van Hove limit.

We encountered particular instances of this limiting procedure in subsections 3.5 and 5.4. But a more general discussion was postponed to the present section.

In a brillant transposition of a theme van Hove had heard played to justify the Born approximation in the discussion of long-time asymptotic behaviour in scattering theory, he proposed in [van Hove, 1955] a variation allowing him to characterize a regime where the time-scale of the irreversible *macroscopic* phenomena is emphasized over the time-scale of the underlying reversible, Hamiltonian *microscopic* dynamics. Van Hove's original presentations were conducted for specific models by means of perturbation techniques, carried to all orders, in which he selected for summation the "most divergent diagrams." At first, his virtuoso performances drew considerable scepticism; cf. e.g. [van Kampen, 1962]. The main problem was to isolate the conditions under which the essentials of what would become a theory may emerge from the contingent diagrammatics attached to the solution of particular models. Systematic mathematical treatments are now available to show how a joint long-time/weak-coupling limit may lead from a conservative unitary evolution to a contractive dynamical semi-group; cf. e.g. [Martin, 1979; Davies, 1976a].

In terms of the focus of this subsection, namely the control of limits that allow one to ensure that the system considered is operating in a desired regime, here exponential decay, one aims at proving a result of the following form; cf. e.g. [Martin and Emch, 1975, section 4].

There exist finite constants $\tau_o > 0$ and $C > 0$ such that for $0 \leq \lambda^2 t \leq \tau_o$:

$$(121) \quad \left| \lim_{|\Lambda|\to\infty} (\Phi, U^o_{-t} U_t \Psi)_\Lambda - (\Phi, \exp(-[\Gamma + i\Delta]\lambda^2 t)\Psi) \right| \leq \lambda C$$

where $U^o_{-t}U_t$ describes the evolution in the so-called interaction picture, with $U^o_t = \exp(-iH_o t)$, $U_t = \exp(-i[H_o + \lambda V]\, t)$; $H_o, H + \lambda V, \Delta$ are self-adjoint operators, and Γ is not only self-adjoint, but also positive so as to describe *decay* in the time range $0 \leq \tau := \lambda^2 t \leq \tau_o$. Hence the term "long-time/weak-coupling limit": when the coupling constant λ is small enough [i.e. the RHS of 121 is small] the evolution is approximated by the contractive semi-group $S(\tau) := \exp(-[\Gamma + i\Delta]\tau)$ with $\tau = \lambda^2 t \in [0, \tau_o]$, provided the time t is sufficiently large in the scale measured by $t \simeq \tau/\lambda^2$.

The separation of the total Hamiltonian $H = H_o + \lambda V$ into an "unperturbed" or "free" part H_o and an "interaction" λV must be justified. Van Hove proposed that it is to be traced back to the fact that the observables of interest in irreversible processes are macroscopic (see subsection 6.2 below), thus determining a joint spectral resolution; then H_o appears as the "diagonal" part of H in this spectral resolution. For instance, $A = \int dk A(k) a^*(k) a(k)$ and $H_o = \int dk \epsilon(k) a^*(k) a(k)$. This remark also helps justify the use of the interaction picture $U^o_{-t}U_t$ since it entails that the observables of interest are invariant under the "free" evolution. As the macroscopic observables are translation invariant, the notation $\int dk$ is used to suggest that the momentum representation corresponds to the spectral resolution in which the observables and the free Hamiltonian are diagonal.

The understanding of the van Hove limit gained in the 1970s has since been confirmed and extended; cf. e.g. [Bach *et al.*, 2000; Derezinski and Früboes, 2005] and references therein; for baselines [Davies, 1976a], [Emch and Liu, 2002, section 15.2] and [Alicki and Fannes, 2001].

Although I do not wish to elaborate on the following historical point, I may mention incidentally that the use of the interaction picture helped van Hove discern in his perturbation expansions some *characteristic features* of many-body physics by which he suggested non-equilibrium QSP differ from the QFT supporting quantum scattering theory. To this day, however, I am not sure whether van Hove's Delphian utterances have been properly digested into the corpus of contemporary mathematical physics.

I should also mention here that coupled limits have been considered also in CSP. An example is the Grad limit for classical gases in which the volume V is kept fixed, the number of molecules $N \to \infty$, and the cross-section of the molecules $\sigma := \pi\, d^2 \to 0$ (thus the volume of each molecule $v(\sim d^3) \to 0$ and the density of the gas $\rho := \frac{N}{V} \to \infty$), while the mean-free path $\lambda = \frac{V}{N d^2}$ is kept constant; in [Grad, 1958], Grad proposed this limit as a mean to derive the Boltzmann

equation. For further references relative to the latter problem, see [Uffink, 2006, section I.6.2] or [Emch and Liu, 2002, section 3.3]; and in particular, for the 2-dimensional Lorentz gas (with now $\sigma = 2d$), cf. [Martin, 1979] where it is pointed out that the Grad limit and the van Hove limit (in a form of it adapted to this model) are equivalent in one important sense: they both predict the same ratio between the macroscopic time-scale validated by observations, and the microscopic time-scale provided by the mean free time between two successive collisions.

The related philosophical issues about the roles that asymptotic reasoning plays in explanation, reduction, and emergence are cogently discussed in [Batterman, 2002a]. The above four limiting procedures may bring additional water to this epistemological mill; see already [Grad, 1967].

In closing this subsection, I should at least mention *coarse-graining*, yet another procedure that has been transferred from the classical to the quantum realm [van Kampen, 1954; Emch, 1964]. One of the reasons for not bringing it up in this essay is that I did not need it for the considerations I developed here. And the reason for this may be that I have come to believe that the primacy of coarse-graining has been largely superseded by the syntax of infinite systems which allows one to bypass several awkward issues about the relations between the micro- and macroscopic worlds; see for instance in subsection 6.3 below. Yet, as with the thermodynamical limit, coarse-graining helped explore those macroscopic properties one wishes to see emerging from finer descriptions; in so doing, it also emphasizes that distinguishing differences of *scales* or *tempi* enables smooth negotiations of such passages.

6.2 Macroscopic observables

Coming back to the general formalism, assuming that the thermodynamic limit has been taken, and concentrating on space-translations, subsection 3.5 emphasized one feature that is new to *quantum* ergodic theory. Space-averaged observables are *essential observables* in the sense of the theory of superselection sectors prompted by [Wick *et al.*, 1952], i.e. they commute with all quasi-local observables and among themselves. This is yet another classical aspect of quantum theory. The specific classical description that emerges in this manner depends on the global preparation of the system (but is insensitive to local perturbations) as the very definition — and values — of these space-averaged observables depends on the translation-invariant state φ of the system one considers. This aspect of quantum ergodic theory shows up as a direct consequence of the "locality" assumed in the Haag–Kastler axioms.

Hence it is proper to regard the emergence of a classical macroscopic description out of a quantum microscopic description as a consequence of translation-invariance and locality; cf. subsections 3.5.B and 5.7. As we saw, the passage to the thermodynamical limit and the attendant emergence of macroscopic observables allow one to discern the simultaneneous existence of several thermodynamical

pure phases, as for instance the non-vanishing magnetization in zero magnetic field signals the presence of a permanent magnet. Similarly, the laboratory observation of a discontinuity in the derivative of the isotherms at the ends of the Maxwell plateau is better understood if one takes the thermodynamical limit: otherwise, the isotherms are analytic all along and the theoretical description of their experiencing so extreme a bend is simply neither convenient nor useful when considering a cup of tea. And again, nobody would claim that when receiving their drinks they recognize the ice-cubes only because the size of these is infinite ... which, mercifully, it isn't. Yet, the Landau criterion for distinguishing a solid from a fluid (see subsection 5.7.b) is strictly valid only when the thermodynamical limit is considered. This is a paradox only when the definition of limits is forgotten; here as elsewhere in physics, the key to the proper understanding of limits lies in their manifesting the emergence of qualitatively different regimes.

For time-averaged observables, the situation is more complicated. Recall some basic facts. To any time-invariant state φ the GNS construction associates a representation π_φ of the C^*-algebra $\mathcal{A}$ of quasi-local observables, and a unitary representation of the time evolution under which the von Neumann algebra obtained as the weak-operator closure of $\pi_\varphi(\mathcal{A})$, namely $\mathcal{N}_\varphi := \pi_\varphi(\mathcal{A})''$, is stable. Then, while the time-average of an observable always belongs to $\mathcal{N}_\varphi$ as does its space-average, the time-average now also belongs to the commutant $\mathcal{N}_\varphi{}' = \pi_\varphi(\mathcal{A})'$ of this algebra, and thus to its center $\mathcal{Z}_\varphi := \pi_\varphi(\mathcal{A})'' \cap \pi_\varphi(\mathcal{A})'$, *if and only if* the evolution is $\eta-$abelian. The latter condition — see equation (61) — may be satisfied in some particular models, but its status is as yet too precarious to enshrine this condition as a general "axiom" on the same footing as "locality".

In spite of the limitation just described, some of the remaining ergodic properties of observables under the time-evolution, together with some of the applications of the theory, were discussed in subsection 3.5.A.

6.3 The quantum measurement process viewed from the perspective of QSP

The technical literature on quantum measurement underwent some striking developments in the 1970s — cf. e.g. [Hepp, 1972; Bell, 1975; Whitten-Wolfe and Emch, 1976]; and also [Emch, 2003; Sewell, 2005] — in part as a consequence of the advent of the algebraic approach to QSP.

Insofar as there was a consensus on what the problem was, the original doctrine is best expounded in Wigner's careful exegesis of what he called the "orthodox" theory of von Neumann [von Neumann, 1932c]; Wigner's papers are collected in [Wigner, 1997, Part II] and [Wigner, 1995, Part II]; Wigner's positions on the subject were last stated in [Wigner, 1984]. Some of the philosophical issues are outlined in [Dickson, 2006].

A renewal in the understanding and implementation of several of the basic tenets of the doctrine was largely motivated by two critiques repeatedly advanced by Wigner himself. The first critique was that "to increase the accuracy of the

measurement one has to use a very large measuring apparatus" [Wigner, 1995, p. 177] or "the large size of the apparatus appears to be essential for the possibility of a measurement" [Wigner, 1995, p. 178]. The second critique is the problem of infinite regress — the so–called Wigner's friend argument; cf. e.g. [Wigner, 1995, p. 215] — that follows from the necessity "to consider the system that has been called, so far, the apparatus, to be the object of the measurement. In other words, one will bring this apparatus into interaction with a new measuring object ... [*and so on*]"; [Wigner, 1995, pp. 208-9]. As this does not appear to be a problem with which one is usually concerned in the analysis of classical measurements, Wigner reiterated a statement he attributed to Fock, but which he said he believed to be part of the teaching of the "Copenhagen school", namely that: "Measuring instruments must be described classically"; of singular relevance to the present essay, this quote is taken from a paragraph Wigner entitled "Is the measuring apparatus macroscopic?" [Wigner, 1995, p. 205].

The reason I believe to be at the core of this awkwardness is that in Wigner's heydays, physicists were still in awe of *a perceived dichotomy* between the classical and the quantum worlds. Hence a new branch of the literature on the quantum measuring problem could develop when a solution of continuity was found that bridges these two descriptions — quantum and classical — of *the one world* in which we live. This happened when the conceptualization of the physical role of limiting proceedures came under control and, in particular, the concept of macroscopic observables was understood; see subsections 6.1 and 6.2 above, references therein, and [Landsman, 2006]. I claim that the concepts developed to deal with QSP can help construct a measuring apparatus that is described in quantum terms and yet behaves, *qua* measuring apparatus, in a classical regime. I will now indicate how at least this part of the conceptual problems associated with quantum measurement has been clarified.

Let $\mathcal{A}_S$ be the algebra of observables for the system to be measured, and let $\mathcal{B} \subset \mathcal{A}_S$ be an abelian subalgebra, the self-adjoint elements of which are the observables of interest. In the interest of formal simplicity I make here the following assumptions, parts of which are easy to dispense with.

- $\mathcal{A}_S$ contains a unit I_S and is a collection of finite-dimensional matrices.
- The spectrum of $\mathcal{B}$ is non-degenerate; hence every observable $B \in \mathcal{B}$ is of the form $B = \sum_k b_k Q_k$ with $Q_k = Q_k^*$; $Q_k Q_l = \delta_{kl} Q_k$; $\sum_k Q_k = I$; and dim $Q_k = 1$.

Initially, the system of interest is in the state $\varphi_S : A \in \mathcal{A}_S \mapsto \mathrm{Tr}\rho A \in \mathbb{C}$, and we want the measuring process to determine, for all $B \in \mathcal{B}$ the values $\varphi_S(B)$, i.e. for all k , the values $\lambda_k = \varphi_S(Q_k)$, so that we can compute $\varphi_S(B) = \sum_k b_k \lambda_k$.

For this measurement, a team of quantum engineers will be asked to build a dedicated measuring apparatus described by an algebra $\mathcal{A}_M$ with self-adjoint "pointers" M_k which are in bijective correspondence with the Q_k . They prepare

this apparatus in the state φ_M . For simplicity, they assume that their $\mathcal{A}_M$ contains a unit I_M and that they arrange for $\sum_k M_k = I_M$. And finally, they try to build an interactive *Hamiltonian* mechanism such that when the system of interest and the apparatus are brought into contact the initial state $\varphi^o = \varphi_S \otimes \varphi_M$ on $\mathcal{A}_S \otimes \mathcal{A}_M$ will evolve in such a manner that the following two conditions are satisfied:

(a) concerning the measuring apparatus:

$$(122)\ \ \forall\, M_l\ :\ \begin{cases} \varphi_M(M_l) \longrightarrow \varphi^p(M_l) = \sum_k \lambda_k \psi_k(M_l) & \text{where} \\ \\ \psi_k(M_l) = \delta_{kl} \quad \text{with no dispersion} \end{cases} ;$$

(b) concerning the system to be measured:

$$(123)\ \ \forall\, A_S \in \mathcal{A}_S\ :\ \begin{cases} \varphi_S(A_S) \longrightarrow \varphi^p(A_S) = \sum_k \lambda_k \varphi_k(A_S) & \text{where} \\ \\ \varphi_k(A_S) = \begin{cases} \varphi_S(Q_k)^{-1} \varphi_S(Q_k A_S Q_k) & \text{when } \lambda_k \neq 0 \\ \varphi_S(A_S) & \text{when } \lambda_k = 0 \end{cases} \end{cases} .$$

Let me comment on these design requirements. Note first that (122) would deliver the values $\lambda_k = \varphi_S(Q_k)$ from which one computes the expectation values $\varphi_S(B)$ of all observables for the measurement of which the apparatus was designed. I will specify later — see (125) — what is meant by the requirement that the result of the measurement be "without dispersion", i.e. formally $\varphi^p([X - \varphi^p(X)I]^2) = 0$.

To relate the requirement (123) to the familiar textbook description of the measuring process, consider briefly the particular form it takes in the von Neumann framework where φ_S is a pure state on the algebra $\mathcal{A}_S = \mathcal{B}(\mathcal{H}_S)$ and the Q_k are one-dimensional; let $\{\Phi_k\}$ be an orthonormal basis in $\mathcal{H}_S$ with $Q_k \Phi_l = \delta_{kl} \Phi_k$; in term of this basis, one can write, without loss of generality $\varphi_S(A_S) = (\Phi_S, A_S \Phi_S)$ with $\Phi_S = \sum_k c_k \Phi_k$; and $\lambda_k = |c_k|^2$. Then (123) takes the form $\varphi^p(A_S \otimes I_M) = \mathrm{Tr}(\rho^p A_S)$ with $\rho^p = \sum_k |c_k|^2 Q_k$. Hence, viewed from $\mathcal{A}_S$, the pure state-vector Φ_S evolves to the mixed density matrix ρ^p . In this sense, (123) is the general form of the so-called von Neumann (non-selective) collapse postulate for the case where the initial state of the system is not necessarily a pure state.

Note that (122) and (123) are reduced descriptions of the evolution of the state φ^o : these requirements demand only that the evolution of special observables be followed; these special observables are: (a) the pointers M_l of the apparatus; and (b) all observables A_S pertaining to the system S . In particular, the requirement (123) would not be incompatible with a measuring process (which we denote as $\longrightarrow$) driven by a unitary evolution of the composite $system \cup apparatus$.

In line with von Neumann's "relative frequencies" view of quantum probability — explicitly inspired by von Mises [von Neumann, 1932c, fn. 156] — the general form (123) applies best to a measurement performed on a beam of particles rather than separately on individual particles. Hence — in line with the interpretation of 'states of physical systems' stated in subsection 3.1 — this description of the measuring process understands that the initial state of the system S is viewed

as a summary of its preparation. For instance, in the historical Stern–Gerlach experiment, an incident *beam* of silver atoms was produced by evaporation from a heated oven; cf. [Jammer, 1966, p. 133]. Thus, what the experimentalists knew was the direction of the beam and the temperature of the oven: the latter surely a macroscopic notion! Similarly, the initial state of the measuring apparatus is viewed here as the result of its preparation; adhering to this pragmatic interpretation, one ought not to impose on the initial state of a (large!) measuring apparatus that it be pure: plainly this would require an exhorbitant amount of information to be entered in its preparation — information that ought not to be actually necessary for the adequate performance of measurements aiming to collect the simple microscopic information described by the distribution $\{\lambda_k\}$.

Due to all sorts of pesky circumstances — e.g. the recurrences present in finite systems or the intrusion of the "Wigner's friend" (introduced earlier in this subsection) — our apparatus builders would be exposed to dire frustrations, unless they be granted enough time and space so that the following idelaization is a close enough approximation — to a degree chosen in advance — of their implementation of the measuring process $\varphi^o \longrightarrow \varphi^p$, namely:

$$(124)\quad \varphi^p(X) := \lim_{t\to\infty} \lim_{|\Lambda|\to\infty} \varphi^o(\alpha_t^\Lambda[X]) \quad \text{with} \quad X = \begin{cases} A_S \otimes I_M \\ \text{or} \\ I_S \otimes M_k^\Lambda \end{cases} ,$$

choosing the pointers so that in the thermodynamical limit, $\lim_{|\Lambda|\to\infty} M_k$ exist and define 'essential' observables — in the sense of subsection 6.2 above; in particular, the reader may want to review the connection with superselection rules — i.e. observables that the orthodox theory would construe to be classical. The requirement "without dispersion" in (122) may now be specified, namely one demands that

$$(125)\quad \lim_{t\to\infty} \lim_{|\Lambda|\to\infty} \left[\varphi^o(\alpha_t[(M^k]^2)_\Lambda - \{\varphi^o(\alpha_t[(M^k])_\Lambda\}^2\right] = 0 \quad .$$

There is even an additional benefit in allowing the thermodynamical limit in (124), namely that one may demand that the experimental set-up be such that the result (124) of the measurement be empirically insensitive to local perturbations in the preparation of the initial state φ_M of the apparatus. This requirement means that $\varphi^p(X)$ in (124) do not change when the initial state φ_M of the apparatus is replaced by any state $\psi_M : A \in \mathcal{A}_M \mapsto \varphi_M(D^*AD) \in \mathbb{C}$ where D is any (quasi-)local element of $\mathcal{A}_M$ satisfying the normalization $\varphi(D^*D) = 1$; or, even more generally, by any state ψ_M normal on the von Neumann algebra $\pi_{\varphi_M}(\mathcal{A}_M)''$. Such robustness pertains to the pragmatic demand that the preparation of a large(!) measuring apparatus be reasonably simple.

Here ends — at least for the main purpose of this subsection — the list of specifications demanded from our quantum engineers when constructing a measuring device.

The contribution of algebraic QSP to the solution of the quantum measurement problem is this: the above programme can be completely implemented in the

sense that specific and rigorously controllable models have been built satisfying *all* of the above specifications. These models therefore establish the applicability of the algebraic approach to the foundations of physics beyond the limitations of what Wigner called the orthodox theory. In sum, this approach encompasses the description of classical regimes unknown within the confines of the orthodox theory; cf. e.g. [Hepp, 1972; Whitten-Wolfe and Emch, 1976; Emch, 2003; Sewell, 2005] and other references listed in [Landsman, 2006, subsection 6.6].

An objection to (124), namely that real-world laboratories are finitely extended in space and in time is seductive. But it neglects the main understanding that presides over taking a limit: recall subsection 6.1 above. Here also the limit defines an asymptotic regime; thus, the control of the limiting procedures allows to take into account that good experiments do require expenses in room and allotments of time, each to be evaluated in terms of the precision to which one aims. The measuring process involves a particular instance of a general macroscopic phenomenon, the "approach to equilibrium". In subsection 6.1(3) above, I commented again on the role of the thermodynamical limit $|\Lambda| \to \infty$ in the emergence of this regime.

The role of the subsequent limit $t \to \infty$ deserves a further comment in the context of the measurement process: it does *not* say that an infinite time is required to register the result of the measurement, but rather, in accordance with our general understanding of the role of limits, the existence of the limit $t \to \infty$ asserts that for every $\epsilon > 0$, there exists a time T_ϵ that can be evaluated, and is such that the measurement has been completed *for ever, within the required precision* ϵ, when $t > T_\epsilon$. Thus in contrast with the constraint of the orthodox theory requiring that the unitary evolution be sharply interrupted at the 'end' of the measurement process, our quantum engineers do not need to make provisions for switching off the measuring device. Now, not taking first the limit $|\Lambda| \to \infty$, only requires them to review their estimate of the effects of the finite size of the apparatus; from this estimate, they evaluate how large the apparatus must be so as to allow a generous time T_Λ before which they have to switch off the measurement and avoid some nasty kickback. The *controlled* limit $|\Lambda| \to \infty$ is thus not a pragmatic limitation to the validity of the theory any more than is the theoretical implementation of the thermodynamical limit ($N \to \infty$, $|\Lambda| \to \infty$ with $D := N/|\Lambda|$ fixed) to remove astronomically long recurrences from the description of the cooloing down of your everyday cup of coffee. The description obtained in the thermodynamical limit is closer to the pragmatic account of the observed cooling down than would be its description as occuring in a finite system: the latter description would indeed be hampered by superfluous, irrelevant details. To sum up, in the actual construction of models for the measuring process, the problems that our quantum engineers encountered were not with satisfying the ancillary condition $T_\epsilon \ll \tau \ll T_\Lambda$ where τ denoted the laboratory time-scale on their wristwatch. See nevertheless [Bell, 1975].

While the models *do prove* that all the demands of the above programme are compatible, it is in the very nature of models that they *cannot* prove that

(i) the conditions of the programme are necessary to an understanding of the measuring process; nor

(ii) the conditions of the programme are sufficient, as other demands may be made, and other conditions may need to be required.

Concerning remark (i), the programme presented above emphasizes possible contributions that QSP can bring to an understanding of the quantum measurement process. One specific aim was to avoid having the theories of the measurement process beached on a conceptual sandbar between the quantum and classical worlds: the programme exploits circumstances where QSP shows how the quantum description of the one world encompasses conceptually important classical aspects. Thus the irreducible quantum/classical dichotomy has now faded into more comprehensive views, QSP being one of them. The emergence of classical behaviour in quantum theory is also one of the significant aspects of the *decoherence* programme, although the likely confluence of these two approaches has not yet gained universal acceptance. For a fair description of the latter issues, and their bearing on the measurement problem, I would recommend [Landsman, 2006]; and for a vivid and somewhat confrontational exchange on the relevance of decoherence in this context, [Anderson, 1994; Adler, 2003].

Remark (ii) above has at least two aspects. One of these aspects is that while the models that establish the internal consistency of the programme discussed in this subsection are treated with mathematical rigour, they can hardly be viewed as sufficiently realistic to satisfy our colleagues on the laboratory floor. Another aspect of the above remark (ii) on sufficiency, is that I do not know how the algebraic QSP would be helpful for formulating some of the remaining challenging questions still open in the theory of quantum measurement. If I had to single out one among these, I would direct attention first to measurements now "routinely" performed on an individual quantum system; cf. e.g. [Rauch and Werner, 2000] or [Rauch, 2005]. Whether the so-called "many worlds" and "consistent histories" approaches are really called for here is too wide a question to be addressed in this essay on QSP; cf. [Dickson, 2006; Landsman, 2006].

6.4 Mathematical physics vs. theoretical physics

Several largely unsolved problems may have been overshadowed by the abundant literature on the "return to equilibrium" of small or local deviations that are driven back to equilibrium by a thermal bath; for models of such coupled systems, see paragraphs A and C in subsection 6.4.

Most of the problems discussed below occur also in classical statistical physics; QSP offers little to alleviate them, but a little it does do, and here is how.

The first of these problems is to avoid an infinite regress: if a (small) system of interest is driven to equilibrium by a (large) thermal reservoir, whence is the reservoir getting its own canonical equilibrium and temperature? Rather than a

conceptual answer to this question, the KMS condition was originally conceived as a clever, but formal, transcription — from theoretical to mathematical physics — that turned out to be a wonderfully useful organizing tool.

This very success demanded that the KMS condition be given a deeper physical justification. Substantial answers were found later, diversely expressed as several stability conditions. The latter were presented in subsection 5.4 in an order in which their formulations increasingly sound more like *bona fide* variational principles. This development is thus in line with the widely held opinion that "a variational principle is considered to be the supreme form of a law of physics" [Itô, 1987, Art. 441]. This is good, but as in other fields, a philosophical question persists as to whether any science ought to be solely, or ultimately, founded on variational principles as mechanics and so many sciences have since the eighteenth century. Theoretical physics may have offered some other considerations in this regard, such as the "big-bang" and "decoherence," but their explanatory value, consistency and adequacy remain to be proven. In the meantime, it is not unreasonable to prefer the updated variational principles with which algebraic QSP has proven able to refine their more traditional versions.

A second problem raised by the physics literature on the return to equilibrium concerns the description of global transport phenomena such as heat conduction and electric resistivity due to the interactions between electrons and phonons or random impurities in metals. Van Hove proposed a programme — of which the van Hove limiting procedure is a part, see subsection 6.1(4) above — to approach this type of question. One of the remaining problems is to produce mathematically clean arguments for the claims that are made. An even larger problem still to be fully mastered is to go beyond the contingencies of particular *ad hoc* models. This will require one to explain in physical terms amenable to a mathematical description the general microscopic properties actually responsible for a realistic delineation of the time-scales and/or regimes in which one observes such macroscopic phenomena; the first examples that come to mind are Newton's "cooling law" and Fourier's "heat" theory, i.e. the exponential temperature equilibration of temperatures and the flow of heat that governs the steady temperature distribution in materials placed between sources at different temperatures. The materials presented in this essay, particularly in subsections 3.5 [e.g. eqn. (57)] or 5.4 [e.g. eqn. (86)], exemplify some of the first steps that have been taken profitably along this road. Further, and promising but still formal, results have been obtained in [Eckman *et al.*, 1999; Bonetto *et al.*, 2000; Bach *et al.*, 2000], yet much remains to be done to bridge these with earthly concerns for an understanding that would allow one to compute realistic estimates of the value of specific material transport coefficients.

A third and perhaps more troubling problem. Time-reversal or not [Earman, 2002; Fredenhagen, 2003], even in my dreams I have not yet seen any "cosmological arrow of time" flying convincingly through the landscape of the C^*-algebraic approach developed for QSP ... but neither may such a flight be ruled out as a

heretical foray into this formalism [Buchholz, 2003].

A fourth direction in which to look for extensions of the programme of QSP is concerned with situations arising far away from equilibrium.

Yet a fifth arena for investigations has opened, where a connection with the algebraic approach to QSP is emerging. It will indeed be interesting to observe whether and how the maturing mathematical theory of quantum stochastic processes [Parthasarathy, 1995; Hudson, 1998] will or may throw new light on the reduction process of statistical mechanics.

Finally, QSP has of course found most of its pragmatic confirmation in the praxis of condensed matter physics and the extension of the latter into the study of complex phenomena. However, getting enmeshed here into the technical concrete details indispensable to the full mastery of this praxis would have carried us much beyond the confines of this essay. A richly documented overview of the scope of this field of enquiry may be found in [Anderson, 1994]. Yet, as with [Feynman, 1998], such matters need to be taken up again to weave in more threads and knots as well as to incite new philosophical reflections:

Vingt fois sur le métier remettez votre ouvrage ...

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