Quantum Mechanics and its Emergent Macrophysics

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Preface

The quantum theory of macroscopic systems has become a vast interdisciplinary subject, which extends far beyond the traditional area of condensed matter physics to general questions of complexity, self-organisation and chaos. It is evident that the subject must be based on conceptual structures quite different from those of quantum microphysics, since the macroscopic properties of complex systems are expressible only in terms of concepts, such as entropy and various kinds of order, that have no relevance to the microscopic world. Moreover, the empirical fact that systems of different microscopic constitutions exhibit similar macroscopic behavior provides grounds for suspecting that macrophysics is governed by very general features of the quantum properties of many-particle systems. Accordingly, it appears natural to pursue an approach to the theory of its emergence from quantum mechanics that is centred on macroscopic observables and certain general features of quantum structures, independently of microscopic details.

This book is devoted to precisely such an approach. It is thus in line with such classic works as Onsager's nonequilibrium thermodynamics, Landau's fluctuating hydrodynamics and the renormalisation theory of critical phenomena. However, thanks to developments in mathematical physics over the last three decades, we now have a framework, that was not available to Onsager and Landau, for a general approach to the problem of the passage from microphysics to macrophysics.

The developments in question are in the areas of operator algebraic quantum theory, quantum stochastic processes and classical dynamical systems. The relevance of these three areas to our project may be briefly summarised as follows. Firstly, operator algebraic quantum theory is the generalisation of quantum mechanics to systems that may have infinite numbers of degrees of freedom. It therefore provides the natural framework for the generic model of macroscopic systems, idealised as infinitely extended assemblies of particles of finite mean number density. This idealisation is essential for the precise specification of different levels of macroscopicality and for the sharp mathematical characterisations of quintessentially macroscopic properties of matter, such as phase transitions and irreversible evolutions, whose description would otherwise be blurred by finite size effects. Secondly, the theory of quantum stochastic processes, which is naturally cast within the operator algebraic framework, provides structures pertinent to the dynamics of both open and closed quantum systems, whether near to or far from thermal equilibrium. Thirdly, the theory of classical dynamical systems, with its various scenarios of regular and chaotic motion, becomes essential for the treatment of the classical evolutions that generally emerge at the macroscopic level.

This book represents a further development of the approach to the theory of collective phenomena presented in my OUP monograph "Quantum theory of collective phenomena", although it is designed to be readable as a self-contained work. Its essentially new features are embodied in the central roles of macroscopic observables and quantum stochastic processes in the treatment of collective phenomena, both near to and far from thermal equilibrium.

The book is divided into four parts. Part I consists of a concise presentation of the operator algebraic framework for quantum mechanics, and of a formulation, within this framework, of the concepts of symmetry, order and disorder, together with an approach to the theory of irreversibility. Part II provides a general quantum statistical treatment of both equilibrium and nonequilibrium thermodynamics. The former contains a new characterisation of a complete set of thermodynamical variables and the latter provides a nonlinear generalisation of the Onsager theory. Parts III and IV are concerned with ordered and chaotic structures that arise in some key areas of condensed matter physics. Specifically, Part III is devoted to a derivation of macroscopic superconductive electrodynamics from the basic assumptions of off-diagonal long range order, gauge covariance and thermodynamical stability by methods that circumvent the enormously complicated quantum many-body problem. Part IV, on the other hand, presents a framework for the theory of phase transitions in dissipative systems far from thermal equilibrium, as illustrated by a quantum stochastic treatment of a laser model that supports normal, coherent and chaotic radiation.

The choice of topics here, although inevitably dependent on my personal interests, has been made with the aim of presenting a coherent approach to the vast problem of the emergence of macroscopic phenomena from quantum mechanics.

The book is addressed to research physicists, mathematicians and scientists interested in interdisciplinary studies. I have endeavoured to keep the mathematics as simple as possible, without sacrificing rigour. The book is thus designed to be readable on the basis of a knowledge of standard quantum mechanics, mathematical analysis and vector space theory. Any additional mathematics required here is expounded in self-contained form, either in the main text or in appendices.

Geoffrey L. Sewell

Notation

We employ the following standard notation throughout the book. Other symbols are defined in the text.

$:=$ signifies "is defined to be equal to".

$X \backslash Y$ denotes the complement, in a set X, of a subset Y.

$\mathbf{C}$ denotes the set of all complex numbers: the complex conjugate of a complex number c will be denoted by $\bar{c}$.

$\mathbf{R}$ denotes the set of all real numbers.

$\mathbf{R}_+$ denotes the set of nonnegative real numbers.

$\mathbf{Z}$ denotes the set of all integers.

$\mathbf{N}$ denotes the set of all nonnegative integers.

Part I

The algebraic quantum mechanical framework and the description of order, disorder and irreversiblity in macroscopic systems: prospectus

Part I is devoted to a concise operator algebraic formulation of the quantum theory of macroscopic systems and to a description, within the framework thereby provided, of symmetry, order, disorder and irreversibility.

We start, in Chapter 1, with a brief general discussion of the application of quantum theory to macroscopic specimens of matter, arguing that these may naturally be idealised as systems with infinite numbers of degrees of freedom and thus described within a framework, due originally to Segal [Seg] and to Haag and Kastler [HK], that is based on the algebraic structure of their observables rather than on any one of the infinity of possible underlying Hilbert space representations thereof. We formulate this framework in Chapter 2, and demonstrate how it serves to provide qualitative distinctions between the descriptions of matter at different levels of macroscopicality and a natural characterisation of its pure phases.

We then proceed, in Chapter 3, to a general formulation of entropy, symmetry, order and disorder, within the operator algebraic framework, and to a discussion of the limitations of our present conception of these entities. In particular, we demonstrate that, on the one hand, entropy does not necessarily provide a measure of disorder, since some pure states can have spatially chaotic structures; while, on the other hand, order, or structural organisation, can carry relatively high entropy, just as coherent signals can coexist with intense background noise.

Chapter 4 is devoted to the theory of irreversibility and macroscopic causality in conservative quantum systems. Here we formulate the concepts of microscopic reversibility and macroscopic irreversibility within the operator algebraic framework, and demonstrate how the latter ensues from the former, subject to appropriate initial conditions, in rather simple concrete examples.

Chapter 1

Introductory discussion of quantum macrophysics

Quantum theory began with Planck's [Pl] derivation of the thermodynamics of black body radiation from the hypothesis that the action of his oscillator model of matter was quantised in integral multiples of a fundamental constant, h. This result provided a microscopic theory of a macroscopic phenomenon that was incompatible with the assumption of underlying classical laws. In the century following Planck's discovery, it became abundantly clear that quantum theory is essential to natural phenomena on both the microscopic and macroscopic scales. Its crucial role in determining the gross properties of matter is evident from the following considerations.

(1) The stability of matter against electromagnetic collapse is effected only by the combined action of the Heisenberg and Pauli principles [DL, LT, LLS, BFG].

(2) The third law of thermodynamics is quintessentially quantum mechanical and, arguably, so too is the second law.[1]

(3) The mechanisms governing a vast variety of cooperative phenomena, including magnetic ordering [Ma], superfluidity [La1, BCS] and optical and biological coherence [Ha1, Fr1], are of quantum origin.

As a first step towards contemplating the quantum mechanical basis of macrophysics, we note the empirical fact that macroscopic systems enjoy properties that are radically different from those of their constituent particles. Thus, unlike systems of few particles, they exhibit irreversible dynamics, phase transitions and various ordered structures, including those characteristic of life. These and other macroscopic phenomena signify that complex systems, that is, ones consisting of enormous numbers of interacting particles, are qualitatively different from the sums of their constituent parts. Correspondingly, theories of such phenomena must be based not only on quantum mechanics *per se* but also on conceptual structures that serve to represent the characteristic features of highly complex systems. Among the key general

[1] The essential point here is that the classical statistical mechanical formulation of entropy depends on an arbitrary subdivision of phase space into microcells (cf. [Fe, Chapter 8]).

concepts involved here are ones representing various types of order, or organisation, disorder, or chaos, and different levels of macroscopicality. Moreover, the particular concepts required to describe the ordered structures of superfluids and laser light are represented by macroscopic wave functions [PO, Ya, GH, Se1] that are strictly quantum mechanical, although radically different from the Schrödinger wave functions of microphysics.

To provide a mathematical framework for the conceptual structures required for quantum macrophysics, it is clear that one needs to go beyond the traditional form of quantum mechanics [Di, VN1], since that does not discriminate *qualitatively* between microscopic and macroscopic systems. This may be seen from the fact that the traditional theory serves to represent a system of N particles within the standard Hilbert space scheme, which takes the same form regardless of whether N is 'small' or 'large'. In fact, it was this very lack of a sharp characterisation of macroscopicality that forced Bohr [Bo] into a dualistic treatment of the measuring process, in which the microscopic system under observation was taken to be quantum mechanical, whereas the macroscopic measuring apparatus was treated as classical, even though it too was presumably subject to quantum laws.

However, a generalised version of quantum mechanics that provides the required qualitative distinctions between different grades of macroscopicality has been devised over the last three decades, on the basis of an *idealisation* of macroscopic systems as ones possessing infinite numbers of degrees of freedom. This kind of idealisation has, of course, long been essential to statistical thermodynamics, where, for example, the characterisation of phase transitions by singularities in thermodynamical potentials necessitates a passage to the mathematical limit in which both the volume and the number of particles of a system tend to infinity in such a way that the density remains finite [YL, LY, Ru1]. Its extension to the full description of the observables and states of macroscopic systems [AW, HHW, Ru1, Em1] has served to replace the merely quantitative difference between systems of 'few' and 'many' (typically 10^{24}) particles by the qualitative distinction between finite and infinite ones, and has thereby brought new, physically relevant structures into the theory of collective phenomena [Th, Se2].

The key element of the generalisation of quantum mechanics to infinite systems is that it is based on the algebraic structure of the observables, rather than on the underlying Hilbert space [Seg, HK]. The radical significance of this is that, whereas the algebra of observables of a finite system, as governed by the canonical commutation relations, admits only one irreducible Hilbert space representation [VN2], that of an infinite system has infinitely many inequivalent such representations [GW]. Thus, for a finite system, the algebraic and Hilbert space descriptions are equivalent, while, for an infinite one, the algebraic picture is richer than that provided by any irreducible representation of its observables.

Moreover, the algebraic quantum theory of infinite systems, as cast in a form designed for the treatment of fundamental problems in statistical mechanics and quantum field theory [Em1, BR, Th, Se2, Haa1], admits just the structures required for the treatment of macroscopic phenomena. In particular, it permits clear definitions of various kinds of order, as well as sharp distinctions between global and local variables, which may naturally be identified with macroscopic and microscopic ones. Furthermore, the wealth of inequivalent representations of the observables permits a natural classification of the states in both microscopic and macroscopic terms. To be specific, the vectors in a representation space[2] correspond to states that are macroscopically equivalent but microscopically different, while those carried by different representations are macroscopically distinct. Hence, the macrostate corresponds to a representation and the microstate to a vector in the representation space. This is of crucial significance not only for the description of the various phases of matter, but also for the quantum theory of measurement. The specification of the states of a measuring apparatus in microscopic and macroscopic terms has provided a key element of a fully quantum treatment [He, WE] of the measurement process that liberates the theory from Bohr's dualism.

Our approach to the basic problem of how macrophysics emerges from quantum mechanics will be centred on macroscopic observables, our main objective being to obtain the properties imposed on them by general demands of quantum theory and many-particle statistics. This approach has classic precedents in Onsager's [On] irreversible thermodynamics and Landau's fluctuating hydrodynamics [LL1], and is at the opposite pole from the many-body-theoretic computations of condensed matter physics [Pi, Tho]. Our motivation for pursuing this approach stems from the following two considerations. Firstly, since the observed laws of macrophysics have relatively simple structures, which do not depend on microscopic details, it is natural to seek derivations of these laws that are based on general quantum macrostatistical arguments. Secondly, by contrast, the microscopic properties of complex systems are dominated by the molecular chaos that is at the heart of statistical physics; and presumably, this chaos would render unintelligible any solutions of the microscopic equations of motion of realistic models of such systems, even if these could be obtained with the aid of supercomputers.

Thus, we base this treatise on macroscopic observables and certain general structures of complex systems, as formulated within the terms of the algebraic framework of quantum theory. The next three chapters are devoted to a concise formulation of this framework, for both conservative and open systems (Chapter 2), and of the descriptions that it admits of symmetry, order and disorder (Chapter 3), and of irreversibility (Chapter 4).

[2] To be precise (cf. Section 2.6.3), this is true for primary representations.

Chapter 2

The generalised quantum mechanical framework

The traditional form of quantum theory is based on the model in which the pure states and observables of a system correspond to the normalised vectors, ψ, and the self-adjoint operators, A, respectively, in a certain Hilbert space, $\mathcal{H}$, with the interpretation that the expectation value of an observable A for the state ψ is $(\psi, A\psi)$ (cf. [VN1]). To be precise, this model is designed for systems with finite numbers of degrees of freedom, since for any such system, the canonical commutation relations, which govern the algebraic structure of its observables, admit only one irreducible Hilbert space representation [VN2]. The picture of the system provided by this representation therefore fully captures its algebraic properties.

The situation is radically different, however, for a system with an infinite number of degrees of freedom, since the algebraic structure of its observables generally admits infinitely many inequivalent irreducible representations [Haa2, GW]. Hence, as first appreciated by Segal [Seg] and Haag and Kastler [HK], the picture based on the algebraic structure of the observables of such a system is much richer than that provided by any particular irreducible representation.

This last observation has led to a reformulation of quantum theory, in which the primary objects are the observables, endowed with algebraic structures stemming from the canonical commutation relations, rather than any particular representation thereof. This provides a natural generalisation of traditional quantum theory to systems with infinite numbers of degrees of freedom, such as those arising in both statistical mechanics and quantum field theory.

This chapter is devoted to a formulation of the algebraic framework of this generalised quantum theory. We have endeavoured to keep the mathematics as simple as possible here without sacrificing rigour. In the appendix to this chapter, we provide a rudimentary account of the theory of Hilbert spaces, which suffices for the purposes of this book. Readers who are not conversant with Hilbert spaces may find it helpful to begin the chapter by reading the appendix.

2.1 OBSERVABLES, STATES, DYNAMICS

The generic model of a physical system, Σ, as expressed in the most basic terms, consists of three essential components, $(\mathcal{O}, S, \mathcal{D})$, representing its observables, states and dynamics, respectively. Here, the observables are the variables, such as functions of positions and momenta, that can, in principle, be measured. The states, on the other hand, are the functionals on the observables that serve to specify their expectation values. Thus, if $A \in \mathcal{O}$ and $\rho \in S$, then $\rho(A)$ is the expectation value of the observable A when the state of Σ is ρ. We sometimes denote $\rho(A)$ by $\langle \rho; A \rangle$. Finally, $\mathcal{D}$ is a dynamical law that specifies the expectation value, $\langle \rho; A \rangle_t$, of the observables A at time t, given that the initial state of the system is ρ.

Evidently, the model of Σ comprises the structures of $\mathcal{O}$, S and $\mathcal{D}$. Here, we formulate these structures for nonrelativistic quantum systems of both finite and infinite numbers of degrees of freedom.

2.2 FINITE QUANTUM SYSTEMS

We start by examining both the algebraic and the Hilbert space structures of the standard model of finite quantum systems, as formulated, for example, in Von Neumann's book [VN1].

2.2.1 Uniqueness of the Representation

Let us consider first a single particle that is confined to move along a straight line. According to quantum theory, its position and momentum correspond to self-adjoint operators $\hat{q}$ and $\hat{p}$, respectively, in a separable Hilbert space $\mathcal{H}$, that satisfy the canonical commutation relation (CCR)

$$[\hat{q}, \hat{p}] = i\hbar I, \tag{2.2.1}$$

where $\hbar = h/2\pi$ and $[A, B] = AB - BA$. This form of the CCR carries some domain problems, since it implies that $\hat{q}$ and $\hat{p}$ cannot both be bounded (cf. [Em1, Section 2b]). To avoid such problems, we adopt Weyl's scheme [We], in which the CCR are re-expressed in terms of the unitary operators

$$U(a) = \exp(ia\hat{q}), \quad V(b) = \exp(ib\hat{p}) \quad \forall a, b \in \mathbf{R}, \tag{2.2.2}$$

and the relation (2.2.1) is sharpened to the form

$$U(a)V(b) = V(b)U(a)\exp(-i\hbar ab). \tag{2.2.3}$$

Thus, in Weyl's picture, a representation of the CCR comprises a triple, $(U, V, \mathcal{H})$, such that U and V are strongly continuous unitary representations of $\mathbf{R}$ in a separable Hilbert space $\mathcal{H}$ that satisfy the algebraic relation (2.2.3). In this picture, the position and momentum observables are $-i$ times the infinitesimal generators of the unitary groups $U(\mathbf{R})$ and $V(\mathbf{R})$, respectively.

The problem of classifying the representations of the CCR was resolved by Von Neumann [VN2], who proved that all *irreducible*[1] ones are unitarily equivalent to that of Schrödinger, $(U_S, V_S, \mathcal{H}_S = L^2(\mathbf{R}))$, as defined by the equations

$$(U_S(a)f)(q) = f(q)\exp(iaq), \quad (V_S(b)f)(q) = f(q + \hbar b), \quad \forall f \in L^2(\mathbf{R}). \tag{2.2.4}$$

In other words, if $(U, V, \mathcal{H})$ is an irreducible representation of the CCR, then there is a unitary mapping, W, of $\mathcal{H}$ onto $\mathcal{H}_S$, such that $U(a) = W^{-1}U_S(a)W$ and $V(b) = W^{-1}V_S(b)W$. Note that it follows from Eqs. (2.2.4) that the position and momentum operators, $\hat{q}_S$ and $\hat{p}_S$, for the Schrödinger representation, defined as $-i$ times the infinitesimal generators of $U_S(\mathbf{R})$ and $V_S(\mathbf{R})$, respectively, are given by the standard formulae

$$(\hat{q}_S f)(q) = qf(q), \quad (\hat{p}_S f)(q) = -i\hbar\frac{df(q)}{dq}. \tag{2.2.5}$$

To summarise, the essentially unique irreducible representation of the CCR is determined by its algebraic structure. Further, no more physically relevant information can be encoded in the reducible representations, since these are merely direct sums of copies of the irreducible one.

The same situation prevails for a Pauli spin, $S = (S_x, S_y, S_z)$, whose algebraic properties are given by the angular momentum commutation relations

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y, \tag{2.2.6a}$$

together with the spin one half condition that

$$S^2 = \frac{3}{4}\hbar^2 I. \tag{2.2.6b}$$

To be specific, all irreducible representations of these relations are unitarily equivalent [Wi] to the two-dimensional one,

$$S = \frac{1}{2}\hbar\sigma, \tag{2.2.7}$$

where the components $(\sigma_x, \sigma_y, \sigma_x)$ of σ are the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.2.8}$$

This representation may be conveniently expressed in terms of the basis vectors

[1] The representation $(U, V, \mathcal{H})$ is irreducible if $\mathcal{H}$ has no proper subspaces that are stable under $U(\mathbf{R})$ and $V(\mathbf{R})$.

$$\phi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \phi_{-1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.2.9}$$

via the formula

$$\sigma\phi_s = (\phi_{-s}, is\phi_{-s}, s\phi_s), \quad \text{for } s = \pm 1. \tag{2.2.10}$$

The above results concerning the essential uniqueness of the irreducible representation of the CCR and the spin algebra may readily be generalised to systems of finite numbers of degrees of freedom. These include systems of identical particles for which the demand that the observables be invariant under particle permutations implies that the vectors of the representation space are either symmetric or antisymmetric with respect to these permutations, according to whether the particles are bosons or fermions (cf. Chapter 15 of [Ja]). Further, in the case of systems confined to bounded spatial regions, the Schrödinger representation of the position and momentum operators has to be modified according to the boundary conditions, for example, those of Dirichlet if the confinement is affected by hard walls.

To summarise, the observables of a finite system have but one irreducible representation, and this is determined by their algebraic structure and by the statistics of the constituent particles.

2.2.2 The Generic Model

This last remark leads naturally to the following standard formulation [VN1] of the model of a finite system, Σ, in terms of the essentially unique irreducible representation of the algebraic structure of its observables in a separable Hilbert space $\mathcal{H}$.

The observables are represented by the self-adjoint operators in $\mathcal{H}$. To avoid domain problems, we restrict ourselves to the bounded ones. This entails no loss of generality, since any self-adjoint operator may be expressed in terms of its spectral projectors [VN1],[2] which are, of course, bounded; and furthermore, it is justified on the physical grounds that measurements provide evaluations only of bounded quantities. Accordingly, we represent the (bounded) observables of the system by the set, $\mathcal{O}$, of bounded, self-adjoint operators in $\mathcal{H}$.

The *pure* states of Σ correspond to the normalised vectors, ψ, in $\mathcal{H}$, with the interpretation that the expectation value of an observable A, for the state represented by ψ, is

$$\rho_\psi(A) = (\psi, A\psi) \equiv \mathrm{Tr}(P(\psi)A), \tag{2.2.11}$$

where $P(\psi)$ is the projection operator for ψ. Thus, the functional ρ_ψ on $\mathcal{O}$, as

[2] See the appendix, item (20).

defined by this formula, is a state of Σ, in the sense of Section 2.1. Note that the states ρ_ψ and $\rho_{\psi'}$ are the same if and only if $\psi' = \psi\exp(i\alpha)$, where the phase α is a real constant.

The *mixed* states of the system are the weighted combinations of different pure ones, $\rho_n = \rho_{\psi_n}$, that is, they are the functionals of the form

$$\rho = \sum_n c_n \rho_n,$$

acting on $\mathcal{O}$, where $\{c_n\}$ is a denumerable set of positive numbers, whose sum is unity. Hence, by Eq. (2.2.11), ρ may be represented by the density matrix $\hat{\rho} = \sum_n c_n P(\psi_n)$, according to the formula

$$\rho(A) = \mathrm{Tr}(\hat{\rho}A), \quad \forall A \in \mathcal{O}. \tag{2.2.12}$$

In fact, since $P(\psi)$ is a density matrix, it follows from Eqs. (2.2.11) and (2.2.12) that the latter formula, when extended to *all* density matrices in $\mathcal{H}$, covers both the pure and the mixed states. Moreover, the correspondence between states and density matrices given by that formula is one-to-one, since the condition that $\mathrm{Tr}((\hat{\rho}-\hat{\rho}')A) = 0$, for all observables A, implies that $\hat{\rho} = \hat{\rho}'$.[3]

Thus, the states, S, comprise the functionals ρ of the observables, that correspond to the density matrices $\hat{\rho}$ according to Eq. (2.2.12). The pure states are the ones whose density matrices are one-dimensional projectors.

Note on Quantum Interference

Suppose that ψ is a linear combination, $c_1\psi_1 + c_2\psi_2$, of two orthogonal, normalised vectors ψ_1 and ψ_2, and that ρ is the mixed state corresponding to the density matrix $|c_1|^2\rho_{\psi_1} + |c_2|^2\rho_{\psi_2}$. Then it follows from Eqs. (2.2.11) and (2.2.12) that

$$\rho_\psi(A) = \rho(A) + 2\,\mathrm{Re}\,\bar{c}_1 c_2(\psi_1, A\psi_2).$$

Here, the last term represents a *quantum interference* effect that renders the expectation value of A for the state ψ different from the sum of its expectation values for ψ_1 and ψ_2, as weighted by the probabilities $|c_1|^2$ and $|c_2|^2$, respectively. This interference is characteristic of *quantum probability* theory, and stems from the fact that quantum expectation values are given by *probability amplitudes*, as represented by vectors in a Hilbert space, rather than by classical probabilities.

[3] This may be seen by putting $A = P(\psi)$, and thereby inferring that $(\psi, (\hat{\rho}-\hat{\rho}'), \psi) = 0$ for all vectors ψ in $\mathcal{H}$.

The dynamics of the model is governed by the Hamiltonian, H, of the system. This is a self-adjoint operator[4] in $\mathcal{H}$, which is generally given by the sum of the kinetic and potential energy operators of the system. Time-translations are represented by the one-parameter group, $\{U_t \mid t \in \mathbf{R}\}$, of unitary transformations of $\mathcal{H}$, whose infinitesimal generator is $iH/\hbar$. Thus,

$$U_t = \exp(iHt/\hbar), \quad \forall t \in \mathbf{R}. \tag{2.2.13}$$

The dynamics may be equivalently formulated in the Heisenberg and Schrödinger pictures. In the former, it is carried by the observables, according to the principle that the evolute of $A(\in \mathcal{O})$ at time t is

$$A_t = U_t A U_t^{-1}, \tag{2.2.14}$$

while the states remain fixed. Thus, the time-dependent expectation value of an observable A at time t, given that the system is prepared in the state ρ, is

$$\langle \rho; A \rangle_t = \rho(A_t) \equiv \mathrm{Tr}(\hat{\rho} U_t A U_t^{-1}). \tag{2.2.15}$$

In the Schrödinger picture, on the other hand, the dynamics is carried by the states, according to the prescription that the evolute of the density matrix $\hat{\rho}$ at time t is

$$\hat{\rho}_t = U_t^{-1} \hat{\rho} U_t, \tag{2.2.16}$$

while the observables remain fixed. Thus, the time-dependent expectation value of the observable A at time t, for evolution from an initial state ρ, is $\mathrm{Tr}(U_t^{-1}\hat{\rho}U_t A)$, which is identical to the right-hand side of Eq. (2.1.15), by the cyclicity property of the Trace.

We note here that it follows from equations (2.2.13), (2.2.14) and (2.2.16) that the equations of motion for the Heisenberg and Schrödinger pictures are

$$\frac{dA_t}{dt} = \frac{i}{\hbar}[H, A_t] \tag{2.2.17}$$

and

$$\frac{d\hat{\rho}_t}{dt} = -\frac{i}{\hbar}[H, \hat{\rho}_t], \tag{2.2.18}$$

these being the equations of Heisenberg and Von Neumann, respectively.[5]

[4] It is generally unbounded, and therefore not an element of $\mathcal{O}$, although it is affiliated to this set, in that its spectral projectors belong to $\mathcal{O}$ [Se3].

[5] Since H is generally unbounded, these equations should be interpreted as pertaining to their matrix elements between vectors in the domain of H. Thus, Eq. (2.2.17) should be taken to signify that $d(f, A_t g)/dt = i/\hbar((Hf, A_t g) - (A_t^{\star} f, Hg))$ for f, g in this domain.

This completes our specification of the model, within the terms of Section 2.1. We now discuss its algebraic structure in a form that can be generalised to infinite systems.

2.2.3 THE ALGEBRAIC PICTURE

The above-defined set, $\mathcal{O}$, of observables possesses the following simple algebraic properties. If $A, B \in \mathcal{O}$ and $k \in \mathbf{R}$, then kA, $(A+B)$, $(AB+BA)$ and $i(AB-BA)$ all belong to $\mathcal{O}$. In other words, $\mathcal{O}$ is closed with respect to (a) multiplication by real numbers, (b) binary addition, (c) the binary symmetrised and antisymmetrised multiplications that send the pair of elements (A, B) to $(AB+BA)$ and $i(AB-BA)$, respectively. However, it is *not* closed with respect to binary multiplication, since, if A, B are noncommuting elements of $\mathcal{O}$, then $(AB)^\star = BA \neq AB$, and so AB is not self-adjoint. In view of this situation, it is simpler to express the algebraic properties of the observables in terms of those of the set, $\mathcal{A}$, of all bounded operators in $\mathcal{H}$, than to work directly with $\mathcal{O}$.

Thus, we note that $\mathcal{O}$ comprises the self-adjoint elements of $\mathcal{A}$, and that the latter set is closed with respect to binary addition, binary multiplication, multiplication by complex numbers and the adjoint mapping $A \rightarrow A^\star$. Accordingly, $\mathcal{A}$ is termed the *algebra of observables* of the system.

The states, S, may now be formulated as the functionals ρ on this algebra that correspond to the density matrices according to the Eq. (2.2.12), as extended to $\mathcal{A}$. Thus,

$$\rho(A) = \mathrm{Tr}(\hat{\rho}A) \quad \forall A \in \mathcal{A}. \tag{2.2.19}$$

It follows easily from this formula that the functional ρ possesses the following properties.

$$\rho(A^\star A) \geq 0 \quad \forall A \in \mathcal{A} \text{ (positivity)}, \tag{2.2.20}$$

$$\rho(\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 \rho(A_1) + \lambda_2 \rho(A_2) \quad \forall A_1, A_2 \in \mathcal{A},$$

$$\lambda_1, \lambda_2 \in \mathbf{C} \text{ (linearity)} \tag{2.2.21}$$

and

$$\rho(I) = 1 \text{ (normalisation)}. \tag{2.2.22}$$

The states are therefore the *positive linear normalised* functionals on the algebra of observables that correspond to the density matrices according to the formula (2.2.19). This latter condition, which is indeed restrictive, is equivalent to the following intrinsic condition [Em2]. For any sequence $\{E_n\}$ of orthogonal projectors in $\mathcal{A}$, whose sum is the identity,

$$\sum_n \rho(E_n) = 1. \tag{2.2.23}$$

Note that this condition is nontrivial when the sequence $\{E_n\}$ is an infinite one, since it then implies a continuity condition, to the effect that the sum of a limit is equal to the limit of the sum. The functionals ρ that satisfy this condition are termed *normal.*

We now note that it follows from Eq. (2.2.19), or equivalently from Eqs. (2.2.20–2.2.23), that S is a *convex set*, that is, if $\rho_1, \rho_2 \in S$ and λ is a real number between 0 and 1, then $\lambda\rho_1 + (1-\lambda)\rho_2 \in S$. Furthermore, the *extremal* elements of S, that is, those that cannot be expressed as weighted sums of other elements, are precisely the pure states, as defined by Eq. (2.2.11).

As regards the dynamics, we see from Eq. (2.2.14) that it corresponds to transformations α_t of $\mathcal{A}$, defined by the formula

$$\alpha_t A = U_t A U_t^{-1} \quad \forall A \in \mathcal{A}, t \in \mathbf{R}. \tag{2.2.24}$$

These transformations possess the group property that $\alpha_t\alpha_s = \alpha_{t+s}$, Furthermore, they preserve the algebraic structure of $\mathcal{A}$, that is,

$$\alpha_t(\lambda A + \mu B) = \lambda\alpha_t A + \mu\alpha_t B,$$

$$\alpha_t(AB) = (\alpha_t A)(\alpha_t B) \quad \text{and} \quad \alpha_t(A^\star) = (\alpha_t A)^\star,$$

and so are termed *automorphisms* of this algebra. Thus, in the Heisenberg picture, the dynamics corresponds to a one-parameter group, $\alpha = \{\alpha_t \mid t \in R\}$, of automorphisms of $\mathcal{A}$.

To summarise, the model of Σ comprises the triple $(\mathcal{A}, S, \alpha)$, where $\mathcal{A}$ is its algebra of observables; S, its state space, is the set of positive, linear, normalised functionals on $\mathcal{A}$ that satisfy the normality condition (2.2.23); and α is the one-parameter group of automorphisms of $\mathcal{A}$, implemented by the unitaries U_t according to Eq. (2.2.24).

Finally, we note that the thermal equilibrium state, ρ_β, of the system at inverse temperature β is given by the Gibbs density matrix $\exp(-\beta H))/\mathrm{Tr}(idem)$; and, by Eq. (2.2.12) and the cyclicity of the Trace, this state is completely characterised [HHW] by the Kubo–Martin–Schwinger (KMS) conditions [Ku, MS], namely,

$$\rho(A(t)B) = \rho(BA(t + i\hbar\beta)) \quad \forall A, B \in \mathcal{A}, \tag{2.2.25}$$

where $A(t) \equiv \alpha_t A$. More precisely [HHW],[6] these conditions may be expressed in the following form.

[6] The point here is that Eq. (2.2.25) is formal, since α does not neccessarily have an analytic continuation to complex values of its argument t.

(KMS) For each pair of elements A, B of $\mathcal{A}$, there is a function, F_{AB}, on the strip $S_\beta = \{z \in \mathbf{C} \mid \mathrm{Im}(z) \in [0, \hbar\beta]\}$, such that

(i) F_{AB} is analytic in the interior of S_β and continuous on its boundaries;

(ii) $F_{AB}(t) = \rho(B\alpha(t)A) \quad \forall t \in \mathbf{R}$, and

(iii) $F_{AB}(t + i\hbar\beta) = \rho([\alpha(t)A]B) \quad \forall t \in \mathbf{R}$.

2.3 INFINITE SYSTEMS: INEQUIVALENT REPRESENTATIONS

As we have already mentioned at the beginning of this chapter, systems of infinite numbers of degree of freedom differ from finite ones in the crucial respect that the algebraic relations governing their observables generally admit inequivalent irreducible representations. We now present a simple example which illustrates the basic reasons for this.

The model that we consider is that of a chain, Σ, of Pauli spins, located on the sites of the one-dimensional lattice $\mathbf{Z}$. We represent these spins, in units of $\hbar/2$, by operators $\{\sigma_n = (\sigma_{n,x}, \sigma_{n,y}, \sigma_{n,z}) \mid n \in \mathbf{Z}\}$ in a Hilbert space $\mathcal{H}$, which satisfy the algebraic relations corresponding to Eqs. (2.2.6) and (2.2.7), namely

$$[\sigma_{n,x}, \sigma_{n,y}] = 2i\sigma_{n,z}, \text{ etc.} \tag{2.3.1a}$$

and

$$\sigma_n^2 = 3I, \tag{2.3.1b}$$

together with the condition that spins on different sites intercommute, that is,

$$[\sigma_{m,u}, \sigma_{n,v}] = 0 \quad \text{for } m \neq n, \; u, v = x, y, z. \tag{2.3.1c}$$

In order to construct explicit representations of these relations, we introduce the set, S, of doubly infinite sequences, $s = \{s_n \mid n \in \mathbf{Z}\}$, each s_n taking the value ± 1. Thus, by Eq. (2.2.8), S is the set of all configurations of the eigenvalues, ± 1, of σ_z, on the lattice $\mathbf{Z}$, that is, it is the set of mappings $n \to s_n$ of $\mathbf{Z}$ into $\{-1, 1\}$. For each $n \in \mathbf{Z}$, we define θ_n to be the transformation of S, whose action on a configuration s reverses its nth component and leaves the rest unchanged, that is,

$$(\theta_n s)_m = s_m(1 - \delta_{mn}) - s_n\delta_{mn}. \tag{2.3.4}$$

2.3.1 The Representation $\sigma^{(+)}$

We define $S^{(+)}$ to be the subset of S, consisting of those configurations, s, for which all but a finite number of components s_n take the value $+1$. Thus, $S^{(+)}$ is denumerable,[7] and consists of local modifications of the configuration, $s^{(+)}$,

[7] By contrast, S is a Cantor set.

whose components are all equal to $+1$. We define $\mathcal{H}^{(+)}$ to be the Hilbert space of square-summable functions on $S^{(+)}$, that is,

$$\left\{ f : S^{(+)} \to \mathbf{C} \mid \sum_{s \in S^{(+)}} |f(s)|^2 < \infty \right\},$$

with inner product

$$(f, g)^{(+)} = \sum_{s \in S^{(+)}} \bar{f}(s) g(s). \tag{2.3.5}$$

A complete orthonormal basis for this space is provided by the vectors $\{\phi_s^{(+)} \mid s \in S^{(+)}\}$, as defined by the formula

$$\phi_s^{(+)}(s') = \delta_{ss'} \quad \forall s, s' \in S^{(+)}. \tag{2.3.6}$$

Evidently, the correspondence between the vectors, $\phi_s^{(+)}$, and the configurations, s, is one-to-one.

We define the operators $\{\sigma_{n,u}^{(+)} \mid n \in \mathbf{Z}; u = x, y, z\}$ in $\mathcal{H}^{(+)}$ in such a way that the action of $\sigma_{n,u}^{(+)}$ on $\phi_s^{(+)}$ is the canonical analogue of that given by Eq. (2.2.10) for an isolated Pauli spin. Thus, defining $\sigma_n^{(+)} = (\sigma_{n,x}^{(+)}, \sigma_{n,y}^{(+)}, \sigma_{n,z}^{(+)})$,

$$\sigma_n^{(+)} \phi_s = \left(s_n \phi_{\theta_n s}^{(+)}, i s_n \phi_{\theta_n s}^{(+)}, s_n \phi_s^{(+)} \right) \quad \forall n \in \mathbf{Z},\ s \in S^{(+)}. \tag{2.3.7}$$

It now follows easily from this formula and Eq. (2.3.4) that the algebraic relations (2.3.1) are valid on the basis vectors $\phi_s^{(+)}$, and that therefore the operators $\sigma_{n,u}^{(+)}$ provide a representation of these relations in $\mathcal{H}^{(+)}$. Its irreducibility follows from the fact that the passage between any two of the basis vectors, ϕ_s and $\phi_{s'}$, can be effected by a finite number of spin reversals, implemented by the action of a monomial in the operators $\sigma_{n,x}^{(+)}$.

We now obtain a simple global property of this representation in terms of the polarisation observable

$$m_N^{(+)} = \frac{1}{2N+1} \sum_{n=-N}^{N} \sigma_n^{(+)}. \tag{2.3.8}$$

We see from Eqs. (2.3.7) and (2.3.8) that

$$\left(\phi_s^{(+)}, m_N^{(+)} \phi_s^{(+)} \right) = \left(0, 0, \frac{1}{2N+1} \sum_{n=-N}^{N} s_n \right)$$

and therefore, since all but a fixed finite number of the s_n are $+1$, the rest being -1,

$$\lim_{N \to \infty} \left(\phi_s^{(+)}, m_N^{(+)} \phi_s^{(+)} \right) = k \quad \forall s \in S^{(+)}, \tag{2.3.9}$$

where k is the unit vector along Oz. Similarly, it also follows from Eqs. (2.3.7) and (2.3.8) that

$$\lim_{N\to\infty}\left(\phi_s^{(+)}, m_N^{(+)}\phi_{s'}^{(+)}\right) = 0 \quad \text{for } s \neq s'. \tag{2.3.10}$$

In order to extend these results to arbitrary vectors in $\mathcal{H}^{(+)}$, we note that, by Eq. (2.3.7), the norms of the operators $\sigma_{n,u}$ are all equal to unity and therefore, by Eq. (2.3.8), $m_N^{(+)}$ is uniformly bounded. Hence, as $\{\phi_s^{(+)}\}$ is a basis in $\mathcal{H}^{(+)}$, it follows from Eqs. (2.3.9) and (2.3.10) that, for all unit vectors $f^{(+)}$ in $\mathcal{H}^{(+)}$,

$$\lim_{N\to\infty}\left(f^{(+)}, m_N^{(+)}f^{(+)}\right) = k. \tag{2.3.11}$$

This result represents a global property of the representations $\sigma^{(+)}$, which stems from the fact that the states that it carries are local modifications of the one where all the spins are aligned parallel to Oz.

2.3.2 The Representation $\sigma^{(-)}$

We may similarly construct another representation of the relations (2.3.1), based this time on the subset $S^{(-)}$ of S, consisting of configurations s, which take the value -1 except at a finite set of sites of $\mathbf{Z}$. Thus, we define the Hilbert space $\mathcal{H}^{(-)}$, the basis vectors $\phi_s^{(-)}$, and the operators $\sigma^{(-)}$ and $m_N^{(-)}$ by the condition that they have the same relationship to $S^{(-)}$ as $\mathcal{H}^{(+)}$, $\phi_s^{(+)}$, $\sigma^{(+)}$ and $m_N^{(+)}$, respectively, have to $S^{(+)}$. In this way, we obtain an irreducible representation, $\sigma^{(-)}$, of the relations (2.3.1); and since it is based on the $S^{(-)}$ configurations, it carries the global property obtained by replacing the superscripts $(+)$ by $(-)$ and k by $-k$ in Eq. (2.3.11). Thus,

$$\lim_{N\to\infty}\left(f^{(-)}, m_N^{(-)}f^{(-)}\right) = -k \tag{2.3.12}$$

for any unit vector $f^{(-)}$ in $\mathcal{H}^{(-)}$.

2.3.3 Inequivalence of $\sigma^{(\pm)}$

We see immediately from Eqs. (2.3.11) and (2.3.12) that the representations $\sigma^{(\pm)}$ of the spin algebra are globally different, in that the states that they carry have polarisations $\pm k$, respectively. This implies that they cannot be unitarily equivalent, as the following argument shows.

If the representations $\sigma^{(\pm)}$ were unitarily equivalent, there would be a unitary mapping, W, of $\mathcal{H}^{(+)}$ onto $\mathcal{H}^{(-)}$ such that $W\sigma_n^{(+)}W^{-1} = \sigma_n^{(-)}$ for all n, which would imply, by Eq. (2.3.8), that

$$Wm_N^{(+)}W^{-1} = m_N^{(-)}.$$

This, in turn, would imply that, if $f^{(\pm)}$ were unit vectors in $\mathcal{H}^{(\pm)}$ such that $f^{(+)} = W^{-1}f^{(-)}$, then the following equation would hold: