Lecture Notes on Spontaneous Symmetry Breaking and the Higgs mechanism

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N.P. Landsman

Institute for Mathematics, Astrophysics, and Particle Physics
Radboud University Nijmegen
Heyendaalseweg 135
6525 AJ NIJMEGEN
THE NETHERLANDS

email: landsman@math.ru.nl
website: http://www.math.ru.nl/∼landsman/SSB.html
tel.: 024-3652874
office: HG03.740

C'est la dissymétrie qui creé le phénomène (Pierre Curie, 1894)

1 Introduction

Spontaneous Symmetry Breaking or *SSB* is the phenomenon in which an equation (or system of equations) possesses a symmetry that is not shared by some 'preferred' solution. For example, $x^2 = 1$ has a symmetry $x \mapsto -x$, but both solutions $x = \pm 1$ 'break' this symmetry. However, the symmetry acts on the solution *space* $\{1, -1\}$ in the obvious way, mapping one asymmetric solution into another.

In physics, the equations in question are typically derived from a Lagrangian L or Hamiltonian H, and instead of looking at the symmetries of the equations of motion one may look at the symmetries of L or H. Furthermore, rather than looking at the solutions, one focuses on the initial conditions, especially in the Hamiltonian formalism. These initial conditions are *states*. Finally, in the context of SSB one is typically interested in two kinds of 'preferred' solutions: ground states and thermal equilibrium states (both of which are time-independent by definition). Thus we may (initially) say that SSB occurs when some Hamiltonian has a symmetry that is not shared by its ground state(s) and/or thermal equilibrium states.[1]

The archetypical example of SSB in *classical* mechanics is the potential

$$V(q) = -\tfrac{1}{2}\omega^2 q^2 + \tfrac{1}{4}\lambda^2 q^4, \tag{1.1}$$

often called the *double-well potential* (we assume that ω ad λ are real). It occurs in the usual single-particle Hamiltonian $h(p, q) = p^2/2m + V(q)$ in $d = 1$. It has two independent $\mathbb{Z}_2$-symmetries, namely $p \mapsto -p$ and $q \mapsto -q$. The latter is broken by, since the ground states are $\omega_0^+ = (p = 0, q = q_0)$ and $\omega_0^-(p = 0, q = -q_0)$, with $q_0 = \omega/\lambda$. These have energy $E_0 = h(0, \pm q_0) = -\omega^4/4\lambda^2$.

The same system in *quantum* mechanics, however, turns out to have unique ground state! The Hamiltonian is

$$h = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(q), \tag{1.2}$$

defined on an appropriate domain in $H = L^2(\mathbb{R})$, and its lowest energy state Ψ_0 is real, strictly positive, and symmetric under reflection in q. According to the WKB-approximation (which in cases like this has been rigorously justified), Ψ_0 has peaks above $\pm q_0$, and exponential decay in the classically forbidden regions; e.g. for $-q_0 < x < 0$ one has

$$|\Psi_0(x)| \sim e^{-\frac{\sqrt{2m}}{\hbar}\int_{-q_0}^{x} dy\, \sqrt{V(y)-E_0}}. \tag{1.3}$$

In particular, *there is no symmetry breaking*, spontaneous or otherwise.[2]

[1] In a more advanced stage of our discussion, we shall see that for infinite systems the definition of the Hamiltonian is itself at stake, whereas a good notion of time-evolution survives. In that case, symmetry of the Hamiltonian has to be replaced by symmetry of the time-evolution.

[2] For $\hbar \to 0$ this ground state converges to the convex sum $\frac{1}{2}(\omega_0^+ + \omega_0^-)$ in a suitable sense, whose explanation requires an algebraic formalism of states and observables to be developed in these notes. In any, case, the point is that in *finite* systems featuring classical SSB, a *pure* quantum ground state converges to a *mixed* classical ground state. Thus the classical limit preserves the symmetric nature of the ground state: although neither ω_0^+ nor ω_0^- is symmetric, $\frac{1}{2}(\omega_0^+ + \omega_0^-)$ is.

More generally, ground states of quantum-mechanical Hamiltonians of finite systems tend to be unique, and hence symmetric: for if the ground state were asymmetric, the symmetry would map it into another ground state, which therefore would be degenerate. Technically, the argument reads like this: suppose that $h\Psi_0 = E_0\Psi_0$ for the lowest energy E_0 of h, and assume that $[h, u] = 0$ for some unitary operator (implementing the symmetry in question). Then $hu\Psi_0 = uh\Psi_0 = E_0 u\Psi_0$. So if Ψ_0 is unique, then $u\Psi_0 = \Psi_0$ (up to a phase). A similar argument applies to equilibrium states ρ : for a finite system at temperature $T = \beta^{-1}$, one has $\rho = Z^{-1}\exp(-\beta h)$, with $Z = \mathrm{Tr}\,(\exp(-\beta h))$, so if $[h, u] = 0$, then $u\rho u^* = \rho$ (i.e., ρ is symmetric).

We see that as far as SSB is concerned, there is a fundamental difference between classical and quantum mechanics: if SSB occus classically, it tends not to occur in the corresponding quantum theory. Nonetheless, SSB is an accepted phenomenon in quantum field theory, where the Standard Model of elementary particle physics would collapse without the Higgs mechanism (in which a gauge symmetry is spontaneously broken). Moreover, the idea that SSB occurs is almost entirely based on the picture suggested by the underlying classical field theory (check any presentation of SSB in high-energy physics). Similarly, SSB lies at the basis of many theories of condensed matter physics, such as the Heisenberg theory of ferromagnetism, the Landau theory of superfluidity, the BCS theory of superconductivity, etc.[3]

To resolve this, it is usually claimed that SSB, like a genuine phase transition, can only occur in infinite systems. This is indeed the case, and one purpose of these notes is to explain this. However, since infinite systems are idealizations of finite ones, it is quite unsatisfactory to base so much of modern physics on an idealized phenomenon that seems absent in the real-world case of a finite system.

[3]It seems to have been Pierre Curie who in 1894 introduced the idea of SSB into physics (although Newton was clearly aware that the rotational symmetry of the solar system is broken by the actual state in which all planets approximately move into the same plane). More explicitly, Heisenberg's quantum-mechanical description of ferromagnetism in 1928 features a rotational symmetry of the Hamiltonian that is broken by the ground states. as he noted. In 1937 Landau introduced the notion of an *order parameter* as an essential feature of SSB, which (partly in collaboration with Ginzburg) he applied to superfluidity and superconductivity. From the 1950s onwards, SSB was implicit (and sometimes explicit) in many areas of condensed matter physics, with important contributions by Landau, Bogoliubov, and others. In high-energy physics, once again it was Heisenberg who stressed the importance of SSB, though in the unfortunate context of his flawed unified field theory of 1958 (in which chiral symmetry is spontaneously broken).

A few years later this idea was picked up by Nambu and Jona-Lasinio, who applied SSB to pion physics, and also systematically rewrote the BCS theory of superconductivity emphasizing SSB. This work led Goldstone to a general study of SSB in quantum field theory, including the theorem named after him, which was actually proved by Goldstone, Salam, and Weinberg in 1962. A year later Anderson applied the Goldstone Theorem to condensed matter physics, explaining that phonons in crystals, spin waves in ferromagnets and Cooper pairs in superconductivity were examples of Goldstone bosons. In 1964 the so-called Higgs mechanism was discovered by many people, including Higgs himself, Englert and Brout, and Guralnik, Hagen, and Kibble. In 1967 Weinberg included the Higgs mechanism in his unified model of the electroweak interaction, which is based on a $SU(2) \times U(1)$ gauge symmetry of which a mixture of some part of $SU(2)$ and $U(1)$ is spontaneously broken. The proof of renormalizibility of this model, as well as of the related theory of the strong interactions (i.e. quantum chromodynamics, which is an $SU(3)$ gauge theory without SSB) by 't Hooft in 1971 (further developed by him and Veltman in 1972) launched the Standard Model, on which all of (empirically relevant) present-day particle physics is still based.

Thus it is also of interest to see how SSB comes into existence if one passes from a finite system to an infinite one.[4] We will do this in some detail for spin systems on a lattice, where methods based on the so-called *Bethe Ansatz* (dating back to the 1930s but mainly developed by Elliott Lieb and collaborators from the 1960s onward) allow an exact determination of the ground state of a finite system.

To see what happens in the idealized case of an infinite spin system on a lattice, consider the example of the one-dimensional Heisenberg ferromagnet. The simplest approach is as follows (leaving details to the main text and the exercises). With $M_2(\mathbb{C})$ denoting the 2×2 complex matrices), let A be the (involutive) associative algebra generated by all elements of the form $a(n)$, where $a \in M_2(\mathbb{C})$ and $n \in \mathbb{Z}$, with relations of the type $\lambda a(n) + \mu b(n) = (\lambda a + \mu b)(n)$, $a(n)b(n) = (ab)(n)$,

$$[a(n), b(m)] = 0 \ \ (m \neq n), \tag{1.4}$$

etc; the idea is that $a(n)$ is the algebra of observables of a spin $\frac{1}{2}$ particle at lattice site n. Thus we may form *finite* linear combinations of *finite* products of the $a(n)$; physically, this means that only a *finite* number of sites of the lattice is observed.

We then look at some interesting representations of A. Let $S = \underline{2}^{\mathbb{Z}}$ be the set of sequences $(s_n)_{n\in\mathbb{Z}}$ with $s_n = \pm$ (so that we identify the two-element set $\underline{2}$ with $\{+,-\}$ or with $\{+1,-1\}$). This set S is uncountable, but it has many countable subsets. Two interesting examples are S^+ and S^-, where $S^\pm$ is defined as the set of all sequences in S for which $s_n \neq \pm$ for only finitely many n. Thus we can form the two *separable* Hilbert spaces $H^+ = \ell^2(S^+)$ and $H^- = \ell^2(S^-)$ in the usual way as

$$H^\pm = \left\{ \varphi : S^\pm \to \mathbb{C} \mid \sum_{s\in S^\pm} |\varphi(s)|^2 < \infty \right\}; \tag{1.5}$$

$$(\varphi, \psi) = \sum_{s\in S^\pm} \overline{\varphi(s)}\psi(s). \tag{1.6}$$

Each classical configuration $s \in S^\pm$ defines a basis vector e_s in $H^\pm$ by $e_s(t) = \delta_{st}$; the collection of all e_s, $s \in S^\pm$, forms an orthonormal basis of $H^\pm$.

We down define an action $\pi^\pm$ of A on $H^\pm$ by extension of

$$\pi^\pm(\sigma_x(n))\psi(s) = \psi(\theta_n(s)); \tag{1.7}$$

$$\pi^\pm(\sigma_y(n))\psi(s) = is_n\psi(\theta_n(s)); \tag{1.8}$$

$$\pi^\pm(\sigma_z(n))\psi(s) = s_n\psi(s); \tag{1.9}$$

$$\pi^\pm(1_2(n))\psi(s) = \psi(s). \tag{1.10}$$

[4] As we shall see, there is a formal analogy between the classical limit in a finite quantum system and the thermodynamic limit in a quantum system. Roughly speaking, it turns out that quantum ground states of large systems tend to be concentrated on all classical configurations that correspond to minima of the classical Hamiltonian. The many-body wavefunction of the ground state is nonzero also in between these peaks, but there it decays exponentially in N, the number of particles. Hence for $N \to \infty$ the peaks decouple, and the pure and symmetric quantum ground state of the finite system converges to a mixed and symmetric ground state of the infinite system. The latter, then, can be decomposed into pure ground states, each of which is asymmetric.

This means the following. First, we extend $\pi^\pm$ to arbitrary $a(n)$ for $a \in M_2(\mathbb{C})$ (of which 1_2 and the Pauli matrices $(\sigma_x, \sigma_y, \sigma_z)$ form a basis). Second, we extend $\pi^\pm$ to finite products by putting

$$\pi^\pm(a_1(n_1) \cdots a_k(n_N)) = \prod_{k=1}^{N} \pi^\pm(a_k(n_k)), \tag{1.11}$$

where all the n_l are different; in that case, the order of the terms in the product on the right-hand side does not matter because of the local commutativity condition (1.4). Thirdly, we extend $\pi^\pm$ to arbitrary elements of A by linearity. More or less by construction, $\pi^\pm$ is a *representation* of A, in the sense that it is linear and satisfies $\pi^\pm(xy) = \pi^\pm(x)\pi^\pm(y)$ for all $x, y \in A$ and $\pi^\pm(x^*) = \pi^\pm(x)^*$ for all $x \in A$. Moreover, $\pi^\pm(A)$ is *irreducible*, according to either one of the following equivalent criteria:

1. If some $x \in B(H^\pm)$ satisfies $[x, \pi^\pm(y)] = 0$ for each $y \in A$, then x is a multiple of the unit operator (*Schur's lemma*).

2. Any vector $\psi \in H^\pm$ is *cyclic* in that any other $\varphi \in H^\pm$ can be approximated by sequences of the form $(\pi^\pm(x_k))$, for some sequence (x_k) in A.

The point, then, is that π^+ and π^- are (unitarily) *inequivalent* representations of A in the sense familiar from group theory, where we say that two representation $\pi_1(A)$ and $\pi_2(A)$ on Hilbert spaces H_1 and H_2, respectively, are (unitarily) *equivalent* if there is a unitary map $u : H_1 \to H_2$ intertwining π_1 and π_2 in the sense that $u\pi_1(a) = \pi_2(a)u$ for all $a \in A$. The proof of this claim is based on the use of *macroscopic observables*. For $N < \infty$, consider the local *magnetization*, defined by

$$m_N^\pm = \frac{1}{2N+1} \sum_{n=-N}^{N} \pi^\pm(\sigma_z(n)), \tag{1.12}$$

which defines an operator on $H^\pm$. For each $\varphi \in H^\pm$, the limit $\lim_{N\to\infty} m_N^\pm \varphi$ exists,[5] and indeed it is easily shown to be $\pm$ the unit operator. Now suppose there would be a unitary operator $u : H^+ \to H^-$ such that $u\pi^+(a) = \pi^-(a)u$ for all $a \in A$. It follows that $um_N^+ = m_N^- u$, and hence $um_N^+\varphi = m_N^- u\varphi$ for each $\varphi \in H^+$. Taking $N \to \infty$ then yields $u\varphi = -u\varphi$, a contradiction. Hence such a u cannot exist.

The existence of inequivalent representations of the algebra of observables turns out to be the key to SSB. As we saw, the impossibility of SSB in a finite system was a consequence of the uniqueness of the ground state (or thermal equilibrium state) *and* the realization of the symmetry in question by a unitary operator on the Hilbert space containing this ground state. What happens in an infinite system is that the algebra of observables has a family of inequivalent irreducible (or 'thermal') representations, each containing a ground state but not a unitary realization of the symmetry, Instead, the symmetry maps some Hilbert space carrying such a representation into another one, carrying an inequivalent one. This begs the question of what is actually *meant* by a symmetry in quantum theory. We will answer this question, and others, in these notes, but only after having introduced an appropriate mathematical framework, which unifies classical and quantum mechanics. Enjoy!

[5]For experts: the limit does not exist in the operator norm.

2 Hilbert spaces

For this course it is necessary to know Hilbert space theory at the strictly mathematical level of von Neumann's book [29] (instead of the heuristic level of Dirac's book [8]).[6] For details (especially proofs) see also [12, 16, 22], [32]—[35], [49, 50, 51].

The concept of a Hilbert space is seemingly technical and special. It may therefore come as a surprise that Hilbert spaces play a central role in many areas of mathematics, notably in analysis, but also including geometry, group theory, stochastics, and even number theory. But first and foremost (at least for us), Hilbert spaces provide the mathematical formalism of quantum mechanics, as first suggested by John von Neumann almost immediately after the discovery of the basic physical principles of quantum mechanics by Heisenberg, Schrödinger, Born, Dirac, and others.[7] Indeed, the definition of a Hilbert space was first given by von Neumann in 1927 precisely for the latter purpose, but he would not have been able to do so without the preparatory work by Hilbert and his school, which produced numerous constructions now regarded as examples of the abstract notion of a Hilbert space.[8]

It is quite remarkable how a particular development within pure mathematics crossed one in theoretical physics in this way; this crossing is reminiscent to the one leading to Newton's development of the Calculus in 1666. Today, the most spectacular new application of Hilbert space theory is given by Noncommutative Geometry [7], where the motivation from pure mathematics is merged with the physical input from quantum mechanics. Consequently, this is an important field of research in pure mathematics as well as in mathematical physics.

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[6] Dirac never talked about Hilbert space and did not define what his linear spaces precisely were. As to his notation, his vectors $|\psi\rangle$ are simply called ψ here. Dirac's inner product $\langle\varphi|\psi\rangle$ is our (φ,ψ), with the same properties of being linear in the second variable and antilinear in the first. If a is an operator, Dirac wrote $\langle\varphi|a|\psi\rangle$ for our $(\varphi,a\psi)$. Dirac denoted complex conjugation by a $*$, so that his $\langle\varphi|\psi\rangle^*$ is the same as our $\overline{(\varphi,\psi)}$, and adjoints by a dagger, so that his $a^\dagger$ is our a^*. If $H=L^2(\mathbb{R})$ (see below) and $\psi\in H$, Dirac wrote $\langle x|\psi\rangle$ for $\psi(x)$, and, confusingly, $\langle p|\psi\rangle$ for $\hat{\psi}(p)$ (i.e., the Fourier transform of ψ). Dirac's expressions $|x\rangle$ and $|p\rangle$ are not vectors in some Hilbert space, but so-called *distributions*, i.e. continuous linear functionals defined on some dense subspace of $L^2(\mathbb{R})$ equipped with a topology different from the topology defined by the inner product.

[7] In 1925 Heisenberg discovered a form of quantum mechanics that at the time was called'matrix mechanics': when Heisenberg showed his work to his boss Born, a physicist who as a former assistant to Hilbert was well versed in mathematics, Born saw, after a sleepless night, that Heisenberg's multiplication rule was the same as the one known for matrices, but now of infinite size. Independently, in 1926 Schrödinger was led to a formulation of quantum theory called 'wave mechanics'. Whereas Heisenberg attempted to eliminate electronic orbits from atomic theory, Schrödinger based his work on de Broglie's idea that in quantum theory a wave should be associated to each particle. Thus in 1926 one had two alternative formulations of quantum mechanics, which looked completely different, but each of which could explain certain atomic phenomena. With hindsight, Heisenberg had a theory of quantum-mechanical observables, whereas Schrödinger had a model of quantum-mechanical states. Following heuristic ideas of Dirac, Pauli, and Schrödinger, it was von Neumann who, at the age of 23, recognized the mathematical structure of quantum mechanics.

[8] Hilbert's work formed part of the emergence of functional analysis, an area of mathematics that arose between approximately 1880–1930. Functional analysis is almost indistinguishable from what is sometimes called 'abstract analysis' or 'modern analysis,' which marked a break with classical analysis. The latter involves, roughly speaking, the study of properties of a single function, whereas the former deals with sets of functions, organized into a vector space.

2.1 Inner product, norm, and metric

The following definitions are basic to all of functional analysis. Note that the concept of a metric applies to any set (i.e., not necessarily to a vector space).

Definition 2.1 *Let V be a vector space over $\mathbb{C}$.*

1. *An* **inner product** *on V is a map $V \times V \to \mathbb{C}$, written as $\langle f, g\rangle \mapsto (f, g)$, satisfying, for all $f, g, h \in V$, $t \in \mathbb{C}$:*
   (a) $(f, f) \in \mathbb{R}^+ := [0, \infty)$ *(positivity);*
   (b) $(g, f) = \overline{(f, g)}$ *(symmetry);*
   (c) $(f, tg) = t(f, g)$ *(linearity 1);*
   (d) $(f, g + h) = (f, g) + (f, h)$ *(linearity 2);*
   (e) $(f, f) = 0 \Rightarrow f = 0$ *(positive definiteness).*
2. *A* **norm** *on V is a function $\|\cdot\| : V \to \mathbb{R}^+$ such that for all $f, g, h \in V$, $t \in \mathbb{C}$:*
   (a) $\|f + g\| \le \|f\| + \|g\|$ *(triangle inequality);*
   (b) $\|tf\| = |t|\|f\|$ *(homogeneity);*
   (c) $\|f\| = 0 \Rightarrow f = 0$ *(positive definiteness).*
3. *A* **metric** *on V is a function $d : V \times V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$:*
   (a) $d(f, g) \le d(f, h) + d(h, g)$ *(triangle inequality);*
   (b) $d(f, g) = d(g, f)$ *for all $f, g \in V$ (symmetry);*
   (c) $d(f, g) = 0 \Leftrightarrow f = g$ *(definiteness).*

These structures are related in the following way:

Proposition 2.2 1. *An inner product on V defines a norm on V by*

$$\|f\| = \sqrt{(f, f)}. \tag{2.1}$$

2. *This norm satisfies the* **Cauchy–Schwarz inequality**

$$|(f, g)| \le \|f\|\|g\|. \tag{2.2}$$

3. *A norm $\|\cdot\|$ on a complex vector space comes from an inner product iff*

$$\|f + g\|^2 + \|f - g\|^2 = 2(\|f\|^2 + \|g\|^2), \tag{2.3}$$

in which case

$$(f, g) = \tfrac{1}{4}(\|f + g\|^2 - \|f - g\|^2 + i\|f - ig\|^2 - i\|f + ig\|^2). \tag{2.4}$$

4. *A norm on V defines a metric on V through $d(f, g) := \|f - g\|$.*

2.2 Completeness

Many concepts of importance for Hilbert spaces are associated with the metric rather than with the underlying inner product or norm. The main example is *convergence*:

Definition 2.3 *1. Let $(x_n) := \{x_n\}_{n\in\mathbb{N}}$ be a sequence in a metric space (V, d). We say that $x_n \to x$ for some $x \in V$ when $\lim_{n\to\infty} d(x_n, x) = 0$, or, more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon$ for all $n > N$.*

In a normed space, hence in particular in a space with inner product, this therefore means that $x_n \to x$ if $\lim_{n\to\infty} \|x_n - x\| = 0$.

2. A sequence (x_n) in (V, d) is called a **Cauchy sequence** *when $d(x_n, x_m) \to 0$ when $n, m \to \infty$; more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x_m) < \varepsilon$ for all $n, m > N$.*

In a normed space, this means that (x_n) is Cauchy when $\|x_n - x_m\| \to 0$ for $n, m \to \infty$, in other words, if $\lim_{n,m\to\infty} \|x_n - x_m\| = 0$.

Clearly, a convergent sequence is Cauchy: from the triangle inequality and symmetry one has $d(x_n, x_m) \leq d(x_n, x) + d(x_m, x)$, so for given $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon/2$, etcetera. However, the converse statement does not hold in general, as is clear from the example of the metric space $(0, 1)$ with metric $d(x, y) = |x - y|$: the sequence $x_n = 1/n$ does not converge in $(0, 1)$. In this case one can simply extend the given space to $[0, 1]$, in which every Cauchy sequence does converge.

Definition 2.4 *A metric space (V, d) is called* **complete** *when every Cauchy sequence in V converges (i.e., to an element of V).*

- *A vector space with norm that is complete in the associated metric is called a* **Banach space**. *In other words: a vector space B with norm $\|\cdot\|$ is a Banach space when every sequence (x_n) such that $\lim_{n,m\to\infty} \|x_n - x_m\| = 0$ has a limit $x \in B$ in the sense that $\lim_{n\to\infty} \|x_n - x\| = 0$.*
- *A vector space with inner product that is complete in the associated metric is called a* **Hilbert space**. *In other words: a vector space H with inner product $(\ ,\ )$ is a Hilbert space when it is a Banach space in the norm $\|x\| = \sqrt{(x, x)}$.*

A subspace of a Hilbert space may or may not be closed. A **closed subspace** $K \subset H$ of a Hilbert space H is by definition complete in the given norm on H (i.e. any Cauchy sequence in K converges to an element of K).[9] This implies that a closed subspace K of a Hilbert space H is itself a Hilbert space if one restricts the inner product from H to K. If K is not closed already, we define its **closure** $\overline{K}$ as the smallest closed subspace of H containing K; once again, this is a Hilbert space.

[9] Since H is a Hilbert space we know that the sequence has a limit in H, but this may not lie in K even when all elements of the sequence do. This is possible precisely when K fails to be closed.

2.3 Geometry of Hilbert space

The vector spaces $\mathbb{C}^n$ from linear algebra are Hilbert spaces in the usual inner product $(z, w) = \sum_{k=1}^n \overline{z_k} w_k$. Indeed, a finite-dimensional vector space is automatically complete in any possible norm. More generally, Hilbert spaces are the vector spaces whose geometry is closest to that of $\mathbb{C}^n$, because the inner product yields a notion of orthogonality: we say that two vectors $f, g \in H$ are **orthogonal**, written $f \perp g$, when $(f, g) = 0$.[10] Similary, two subspaces[11] $K \subset H$ and $L \subset H$ are said to be orthogonal ($K \perp L$) when $(f, g) = 0$ for all $f \in K$ and all $g \in L$. A vector f is called orthogonal to a subspace K, written $f \perp K$, when $(f, g) = 0$ for all $g \in K$, etc. We define the **orthogonal complement** $K^\perp$ of a subspace $K \subset H$ as

$$K^\perp := \{f \in H \mid f \perp K\}. \tag{2.5}$$

This set is linear, so that the map $K \mapsto K^\perp$, called **orthocomplementation**, is an operation from subspaces of H to subspaces of H. Clearly, $H^\perp = 0$ and $0^\perp = H$.

Closure is an analytic concept, related to convergence of sequences. Orthogonality is a geometric concept. However, both are derived from the inner product. Hence one may expect connections relating analysis and geometry on Hilbert space.

Proposition 2.5 *Let $K \subset H$ be a subspace of a Hilbert space.*

1. *The subspace $K^\perp$ is closed, with*

$$K^\perp = \overline{K}^\perp = \overline{K^\perp}. \tag{2.6}$$

2. *One has*

$$K^{\perp\perp} := (K^\perp)^\perp = \overline{K}. \tag{2.7}$$

3. *Hence for closed subspaces K one has $K^{\perp\perp} = K$.*

Definition 2.6 *An* **orthonormal basis** *(o.n.b.) in a Hilbert space is a set (e_k) of vectors satisfying $(e_k, e_l) = \delta_{kl}$ and being such that any $v \in H$ can be written as $v = \sum_k v_k e_k$ for some $v_k \in \mathbb{C}$, in that $\lim_{N\to\infty} \|v - \sum_{k=1}^N v_k e_k\| = 0$.*

If $v = \sum_k v_k e_k$, then, as in linear algebra, $v_k = (e_k, v)$, and $\sum_k |v_k|^2 = \|v\|^2$. This is called **Parseval's equality**; it is a generalization of Pythagoras's Theorem.

Once more like in linear algebra, all o.n.b. have the same cardinality, which defines the **dimension** of H. We call an infinite-dimensional Hilbert space **separable** when it has a *countable* o.n.b. Dimension is a very strong invariant: running ahead of the appropriate definition of isomorphism of Hilbert spaces in §2.4, we have

Theorem 2.7 *Two Hilbert spaces are isomorphic iff they have the same dimension.*

[10] By definition of the norm, if $f \perp g$ one has Pythagoras' theorem $\|f + g\|^2 = \|f\|^2 + \|g\|^2$.

[11] A subspace of a vector space is by definition a *linear* subspace.

2.4 The Hilbert spaces ℓ^2

We say that H_1 and H_2 are **isomorphic** as Hilbert space when there exists an invertible linear map $u : H_1 \to H_2$ that preserves the inner product, in that $(uf, ug)_{H_2} = (f, g)_{H_1}$ for all $f, g \in H_1$; this clearly implies that also the inverse of u preserves the inner product. Such a map is called **unitary**.

To prove Theorem 2.7, we first introduce a Hilbert spaces $\ell^2(S)$ for any set S (in the proof, S will be a set labeling some o.n.b., like $S = \mathbb{N}$ in the countable case).

- If S is finite, then $\ell^2(S) = \{f : S \to \mathbb{C}\}$ with inner product
$$(f, g) = \sum_{s \in S} \overline{f(s)} g(s). \tag{2.8}$$

The functions $(\delta_s)_{s \in S}$, defined by $\delta_s(t) = \delta_{st}$, $t \in S$, clearly form an o.n.b. of $\ell^2(S)$.

Now let H be an n-dimensional Hilbert space; a case in point is $H = \mathbb{C}^n$. By definition, H has an o.n.b. $(e_i)_{i=1}^n$. Take $S = \underline{n} = \{1, 2, \ldots, n\}$. The map $u : H \to \ell^2(\underline{n})$, given by linear extension of $ue_i = \delta_i$ is unitary and provides an isomorphism $H \cong \ell^2(\underline{n})$. Hence *all* n-dimensional Hilbert space are isomorphic.

- If S is countable, then $\ell^2(S) = \{f : S \to \mathbb{C} \mid \|f\|_2 < \infty\}$, with
$$\|f\|_2 := \left(\sum_{s \in S} |f(s)|^2 \right)^{1/2}, \tag{2.9}$$

with inner product given by (2.8); this is finite for $f, g \in \ell^2(S)$ by the Cauchy–Schwarz inequality. Once again, the functions $(\delta_s)_{s \in S}$ form an o.n.b. of $\ell^2(S)$, and the same argument shows that all separable Hilbert space are isomorphic to $\ell^2(\mathbb{N})$ and hence to each other. A typical example is $\ell^2(\mathbb{Z})$.

- If S is uncountable, then $\ell^2(S)$ is defined as in the countable case, where the sum in (2.9) is now defined as the supremum of the same expression evaluated on each finite subset of S. Similarly, the sum in (2.8) is defined by first decomposing $f = f_1 - f_2 + i(f_3 - f_4)$ with $f_i \geq 0$, and g likewise; this decomposes (f, g) as a linear combination of 16 non-negative terms (f_i, g_j), each of which is defined as the supremum over finite subsets of S, as for $\|f\|_2$.

The previous construction of an o.n.b. of $\ell^2(S)$ still applies *verbatim*, as does the proof that any Hilbert space of given cardinality is isomorphic to $\ell^2(S)$ for some S of the same cardinality. In sum, we have proved (von Neumann's) Theorem 2.7.

Let us note that for infinite sets S we may regard $\ell^2(S)$ as the closure in the norm (2.9) of the (incomplete) space $\ell_c(S)$ of functions that are nonzero at finitely many $s \in S$; this means that for any $f \in \ell^2(S)$ there is a sequence (f_n) in $\ell_c(S)$ such that $\lim_{n \to \infty} \|f_n - f\|_2 = 0$. In what follows, we also encounter the Banach space

$$\ell^\infty(S) = \{f : S \to \mathbb{C} \mid \|f\|_\infty < \infty\}; \tag{2.10}$$
$$\|f\|_\infty := \sup_{s \in S} \{|f(s)|\}, \tag{2.11}$$

which is evidently the closure of $\ell_c(S)$ in the **supremum-norm** $\|\cdot\|_\infty$, in that for any $f \in \ell^\infty(S)$ there is a sequence (f_n) in $\ell_c(S)$ such that $\lim_{n \to \infty} \|f_n - f\|_\infty = 0$.

2.5 The Hilbert spaces L^2

A more complicated example of a Hilbert space is $L^2(\mathbb{R}^n)$, familiar from quantum mechanics. which can be defined either directly through measure theory (see §2.6), or indirectly, as a completion of $C_c(\mathbb{R}^n)$, the vector space of complex-valued continuous functions on $\mathbb{R}^n$ with compact support.[12] Two natural norms on $C_c(\mathbb{R}^n)$ are:

$$\|f\|_\infty := \sup\{|f(x)|, x \in \mathbb{R}^n\}, \tag{2.12}$$

$$\|f\|_2 := \left(\int_{\mathbb{R}^n} d^n x\, |f(x)|^2\right)^{1/2}. \tag{2.13}$$

The first norm is called the **supremum-norm** or **sup-norm**; see §2.7. The second norm is called the $\mathbf{L^2}$**-norm**. It is, of course, derived from the inner product

$$(f, g) := \int_{\mathbb{R}^n} d^n x\, \overline{f(x)} g(x). \tag{2.14}$$

Now, $C_c(\mathbb{R}^n)$ fails to be complete in either norm $\|\cdot\|_\infty$ or $\|\cdot\|_2$.

- The completion of $C_c(\mathbb{R}^n)$ in the norm $\|\cdot\|_\infty$ turns out to be $C_0(\mathbb{R}^n)$.[13]
- The completion of $C_c(\mathbb{R}^n)$ in the norm $\|\cdot\|_2$ is $L^2(\mathbb{R}^n)$, defined in two steps.

Definition 2.8 *The space $\mathcal{L}^2(\mathbb{R}^n)$ consists of all functions $f : \mathbb{R}^n \to \mathbb{C}$ for which there exists a Cauchy sequence (f_n) in $C_c(\mathbb{R}^n)$ with respect to $\|\cdot\|_2$ such that $f_n(x) \to f(x)$ for all $x \in \mathbb{R}^n \backslash N$, where $N \subset \mathbb{R}^n$ is a set of (Lebesgue) measure zero.*[14]

We can extend the inner product on $C_c(\mathbb{R}^n)$ to $\mathcal{L}^2(\mathbb{R}^n)$ by $(f, g) = \lim_{n\to\infty}(f_n, g_n)$, where (f_n) and (g_n) are Cauchy sequences in $\mathcal{L}^2(\mathbb{R}^n)$ w.r.t. the L^2-norm. However, this sesquilinear form fails to be positive definite (take a function f on $\mathbb{R}^n$ that is nonzero in finitely—or even countably—many points). To resolve this, introduce

$$L^2(\mathbb{R}^n) := \mathcal{L}^2(\mathbb{R}^n)/\mathcal{N}, \tag{2.15}$$

where

$$\mathcal{N} := \{f \in \mathcal{L}^2(\mathbb{R}^n) \mid \|f\|_2 = 0\}. \tag{2.16}$$

Using measure theory, it can be shown that $f \in \mathcal{N}$ iff $f(x) = 0$ for all $x \in \mathbb{R}^n \backslash N$, where $N \subset \mathbb{R}^n$ is some set of measure zero. If f is continuous, this implies that $f(x) = 0$ for all $x \in \mathbb{R}^n$. It is clear that $\|\cdot\|_2$ descends to a norm on $L^2(\mathbb{R}^n)$ by

$$\|[f]\|_2 := \|f\|_2, \tag{2.17}$$

where $[f]$ is the equivalence class of $f \in \mathcal{L}^2(\mathbb{R}^n)$ in the quotient space. However, we normally work with $\mathcal{L}^2(\mathbb{R}^n)$ and regard elements of $L^2(\mathbb{R}^n)$ as functions instead of equivalence classes thereof. So in what follows we should often write $[f] \in L^2(\mathbb{R}^n)$ instead of $f \in L^2(\mathbb{R}^n)$, which really means $f \in \mathcal{L}^2(\mathbb{R}^n)$, but who cares ...

[12] The **support** of a function is defined as the smallest closed set outside which it vanishes.

[13] This is the space of all continuous functions $f : \mathbb{R}^n \to \mathbb{C}$ that *vanish at infinity* in the sense that for each $\epsilon > 0$ there is a compact subset $K \subset \mathbb{R}^n$ such that $|f(x)| < \epsilon$ for all x outside K.

[14] A subset $N \subset \mathbb{R}^n$ has **measure zero** if for any $\epsilon > 0$ there exists a covering of N by an at most countable set (I_n) of intervals for which $\sum_n |I_n| < \epsilon$, where $\sum_n |I_n|$ is the sum of the volumes of the I_n. (Here an interval in $\mathbb{R}^n$ is a set of the form $\prod_{k=1}^n [a_k, b_k]$). For example, any countable subset of $\mathbb{R}^n$ has measure zero, but there are many, many others.

2.6 Measure theory and Hilbert space

The construction of $L^2(\mathbb{R}^n)$ may be generalized to Hilbert spaces $L^2(X,\mu)$ defined for arbitrary *locally compact Hausdorff* spaces X; the concept of a measure μ underlying this generalization is very important also for (commutative) C^*-algebras.

Let $P(X)$ be the power set of X, i.e., the set of all subsets of X, and denote the topology of X (i.e., the set of open subsets of X) by $O(X)$. A **σ-algebra** on X is a subset Σ of $P(X)$ such that $\cup_n A_n \in \Sigma$ and $\cap_n A_n \in \Sigma$ whenever $A_n \in \Sigma$, $n \in \mathbb{N}$. Note that $\mathcal{O}(X)$ is generally *not* a σ-algebra on X; it is closed under taking *arbitrary* unions (fine), but under *finite* intersections only. Let $B(X)$ be the smallest σ-algebra on X containing $O(X)$; elements of $B(X)$ are called **Borel sets** in X.

Definition 2.9 *A (Radon)* **measure** *on X is a map $\mu : B(X) \to [0,\infty]$ satisfying:*

1. *$\mu(\cup_n A_n) = \sum_n \mu(A_n)$ whenever $A_n \in B(X)$, $n \in \mathbb{N}$, $A_i \cap A_j = \emptyset$ for all $i \neq j$;*
2. *$\mu(K) < \infty$ for each compact subset K of X;*
3. *$\mu(A) = \sup\{\mu(K), K \subset A, K \text{ compact}\}$ for each $A \in B(X)$.*

An **integral** *on $C_c(X)$ is a (complex) linear map $\int_X : C_c(X) \to \mathbb{C}$ such that $\int_X f$ is in $\mathbb{R}^+$ whenever $f(x) \in \mathbb{R}^+$ for all $x \in X$ (in which case we say $f \geq 0$).*

The **Riesz–Markov Theorem** states that these concepts are equivalent:

Theorem 2.10 *There is a bijective correspondence between integrals and measures:*

- *A measure μ on X defines an integral $\int_X d\mu$ on $C_c(X)$, given on $f \geq 0$ by*

$$\int_X d\mu\, f := \sup\left\{ \int_X d\mu\, g \mid 0 \leq g \leq f, g \text{ simple} \right\}, \tag{2.18}$$

  where a **simple** *function is a finite linear combination of characteristic functions χ_K, $K \subset X$ compact, and if $g = \sum_i \lambda_i \chi_{K_i}$, then $\int_X d\mu\, g := \sum_i \lambda_i \mu(K_i)$.*

- *An integral $\int_X$ on $C_c(X)$ defines a measure μ on X, given on compact K by*

$$\mu(K) = \inf\left\{ \int_X f \mid f \in C_c(X), \chi_K \leq f \leq 1 \right\}. \tag{2.19}$$

For any $p > 0$, we define $\mathcal{L}^p(X,\mu)$ as the space of Borel functions[15] on X for which

$$\|f\|_p := \left(\int_X d\mu\, |f|^p \right)^{1/p} < \infty, \tag{2.20}$$

where the integral is defined à la (2.18). The map $\|\cdot\|_p : \mathcal{L}^p(X,\mu) \to \mathbb{R}^+$ has a p-independent null space $\mathcal{N}$, with associated Banach space $L^p(X,\mu) := \mathcal{L}^p(X,\mu)/\mathcal{N}$. For $p = 2$, the Banach space $L^2(X,\mu)$ is actually a Hilbert space with inner product

$$(f,g) := \int_X d\mu\, \overline{f} g \equiv \int_X d\mu(x)\, \overline{f(x)} g(x), \tag{2.21}$$

where similarly ambiguous notation has been used as for $L^2(\mathbb{R}^n)$ (cf. the end of §2.5).

[15] Here $f : X \to \mathbb{C}$ is **Borel** when $f_i^{-1}((s,t)) \in B(X)$ for each $0 \leq s < t$, $i = 1,2,3,4$, where $f = f_1 - f_2 + i(f_3 - f_4)$ is the unique decomposition with $f_i \geq 0$ (e.g., $f_1(x) = \max\{\mathrm{Re}((f(x)), 0\}$).

2.7 Operators on Hilbert space

An **operator** $a : H_1 \to H_2$ between two Hilbert space is simply a linear map (i.e., $a(\lambda v + \mu w) = \lambda a(v) + \mu a(w)$ for all $\lambda, \mu \in \mathbb{C}$ and $v, w \in H_1$). We write av for $a(v)$. Taking $H_1 = H_1 = H$, an operator $a : H \to H$ is just called an *operator on* H. Taking $H_1 = H$ and $H_2 = \mathbb{C}$, we obtain a *functional* on H. For example, any $f \in H$ yields a functional $\varphi : H \to \mathbb{C}$ by $\varphi(g) = (f, g)$. By Cauchy–Schwarz, $|\varphi(g)| \leq C\|g\|$ with $C = \|f\|$. Conversely, the **Riesz–Fischer Theorem** states that if some φ satisfies this bound, then it is of the above form, for a unique $f \in H$.

As in real analysis, where one deals with functions $f : \mathbb{R} \to \mathbb{R}$, it turns out to be useful to single out functions with good properties, notably continuity. So what does one mean by a 'continuous' operator $a : H_1 \to H_2$? One answer come from topology: the inner product on a Hilbert space defines a norm, the norm defines a metric, and finally the metric defines a topology, so one may use the usual definition of a continuous function $f : X \to Y$ between two topological spaces. We use an equivalent definition, in which continuity is replaced by *boundedness*:

Definition 2.11 *$a : H_1 \to H_2$ be an operator. Define $\|a\| \in \mathbb{R}^+ \cup \{\infty\}$ by*

$$\|a\| := \sup \{\|av\|_{H_2},\, v \in H_1,\, \|v\|_{H_1} = 1\}, \tag{2.22}$$

where $\|v\|_{H_1} = \sqrt{(v, v)_{H_1}}$, etc. We say that a is **bounded** *when $\|a\| < \infty$, in which case the number $\|a\|$ is called the* **norm** *of a.*

If a is bounded, then it is immediate that

$$\|av\|_{H_2} \;\leq\; \|a\|\, \|v\|_{H_1} \tag{2.23}$$

for all $v \in H_1$. This inequality is very important. For example, it implies that

$$\|ab\| \leq \|a\|\|b\|, \tag{2.24}$$

where $a : H \to H$ and $b : H \to H$ are any two bounded operators, and $ab := a \circ b$, so that $(ab)(v) := a(bv)$. Eq. (2.23) also implies the easy half of:

Proposition 2.12 *An operator on a Hilbert space H is bounded iff it is continuous in the sense that $f_n \to f$ implies $af_n \to af$ for all convergent sequences (f_n) in H.*

When H is finite-dimensional, any operator on H is bounded (and may be represented by a matrix). For an infinite-dimensional example, take $H = \ell^2(S)$ and $a \in \ell^\infty(S)$, for some set S. It is an exercise to show that if $f \in \ell^2(S)$, then $af \in \ell^2(S)$. Hence we may define a **multiplication operator** $\hat{a} : \ell^2(S) \to \ell^2(S)$ by

$$\hat{a}(f) := af, \tag{2.25}$$

that is, $(\hat{a}f)(x) = a(x)f(x)$. This operator is bounded, with

$$\|\hat{a}\| = \|a\|_\infty. \tag{2.26}$$

Similarly, take $H = L^2(\mathbb{R}^n)$ and $a \in C_0(\mathbb{R}^n)$. Once again, (2.25) defines a bounded multiplication operator $\hat{a} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, satisfying (2.26).

More generally, for locally compact X, a function $a \in C_0(X)$ defines a multiplication operator $\hat{a}$ on $H = L^2(X, \mu)$ satisfying $\|\hat{a}\| \leq \|a\|_\infty$, with equality iff the **support** of the measure μ is X (i.e., every open subset of X has positive measure).

2.8 The adjoint

Let $a : H \to H$ be a *bounded* operator. The inner product on H gives rise to a map $a \mapsto a^*$, which is familiar from linear algebra: if a is a matrix (a_{ij}) w.r.t. some o.n.b., then $a^* = (\overline{a_{ji}})$. In general, the adjoint a^* is uniquely defined by the property[16]

$$(a^* f, g) = (f, ag) \text{ for all } f, g \in H. \tag{2.27}$$

Note that $a \mapsto a^*$ is anti-linear: one has $(\lambda a)^* = \overline{\lambda} a$ for $\lambda \in \mathbb{C}$. Also, one has

$$\|a^*\| = \|a\|; \tag{2.28}$$
$$\|a^* a\| = \|a\|^2. \tag{2.29}$$

The adjoint allows one to define the following basic classes of bounded operators:

1. $n : H \to H$ is **normal** when $n^* n = n n^*$.
2. $a : H \to H$ is **self-adjoint** when $a^* = a$ (hence a is normal).
3. $a : H \to H$ is **positive**, written $a \geq 0$, when $(f, af) \geq 0$ for all $f \in H$.
4. $p : H \to H$ is a **projection** when $p^2 = p^* = p$ (hence p is positive).
5. $u : H \to H$ is **unitary** when $u^* u = u u^* = 1$ (hence u is normal).
6. $v : H \to H$ is an **isometry** when $v^* v = 1$, and a **partial isometry** when $v^* v$ is a projection (in which case $v v^*$ is automatically a projection, too).

Proposition 2.13 *1. An operator a is self-adjoint a iff $(f, af) \in \mathbb{R}$ for all $f \in H$ (and hence positive operators are automatically self-adjoint).*

2. There is a bijective correspondence $p \leftrightarrow K$ between projections p on H and closed subspaces K of H: given p, put $K := pH$, and given $K \subset H$, define p on $f \in H$ by $pf = \sum_i (e_i, f) e_i$, where (e_i) is an arbitrary o.n.b. of K.

3. An operator u is unitary iff it is invertible (with $u^{-1} = u^*$) and preserves the inner product, i.e., $(uf, ug) = (f, g)$ for all $f, g \in H$.

4. An operator v is a partial isometry iff v is unitary from $(\ker v)^\perp$ to $\mathrm{ran}(v)$.

5. An operator v is an isometry iff $(vf, vg) = (f, g)$ for all $f, g \in H$.

Similar definitions apply to (bounded) operators between different Hilbert spaces: e.g., the adjoint $a^* : H_2 \to H_1$ of $a : H_1 \to H_2$ satisfies $(a^* f, g)_{H_1} = (f, ag)_{H_2}$ for all $f \in H_2, g \in H_1$, and unitarity of $u : H_1 \to H_2$ means $u^* u = 1_{H_1}$ and $u u^* = 1_{H_2}$; equivalently, u is invertible and $(uf, ug)_{H_2} = (f, g)_{H_1}$ for all $f, g \in H_1$ (cf. §2.4).

[16] To prove existence of a^*, the Riesz–Fischer Theorem is needed. For fixed $a : H \to H$ and $f \in H$, one defines a functional $\varphi_f^a : H \to \mathbb{C}$ by $\varphi_f^a(g) := (f, ag)$. By Cauchy–Schwarz and (2.23), one has $|\varphi_f^a(g)| = |(f, ag)| \leq \|f\| \|ag\| \leq \|f\| \|a\| \|g\|$, so $\|\varphi_f^a\| \leq \|f\| \|a\|$. Hence there exists a unique $h \in H$ such that $\varphi_f^a(g) = (h, g)$ for all $g \in H$. Now, for given a the association $f \mapsto h$ is clearly linear, so that we may define $a^* : H \to H$ by $a^* f := h$; eq. (2.27) then trivially follows.

2.9 Spectral theory

The spectrum of an operator a generalizes the range of a (complex-valued) function, and is its only invariant under unitary transformations $a \mapsto u^* a u$. To get started, we first restate the spectral theorem of linear algebra. In preparation, we call a family (p_i) of projections on a Hilbert space H **mutually orthogonal** if $p_i H \perp p_j H$ for $i \neq j$; this is the case iff $p_i p_j = \delta_{ij} p_i$. Such a family is called **complete** if $\sum_i p_i f = f$ for all $f \in H$; of course, if $\dim(H) < \infty$, this simply means $\sum_i p_i = 1$.

Proposition 2.14 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a self-adjoint operator on $\mathbb{C}^n$ (i.e., an hermitian matrix). There exists a complete family (p_i) of mutually orthogonal projections so that $a = \sum_i \lambda_i p_i$, where λ_i are the eigenvalues of a. Consequently, p_i is the projection onto the eigenspace of a in H with eigenvalue λ_i, and the dimension of the subspace $p_i H$ is equal to the multiplicity of the eigenvalue λ_i.*

This is no longer true for self-adjoint operators on infinite-dimensional Hilbert spaces. For example, if $a \in C_0(\mathbb{R}, \mathbb{R})$, then the associated multiplication operator $\hat{a}$ on $L^2(\mathbb{R})$ has no eigenvectors at all! However, is has *approximate* eigenvectors, in the following sense: for fixed $x_0 \in \mathbb{R}$, take $f_n(x) := (n/\pi)^{1/4} e^{-n(x-x_0)^2/2}$, so that $f_n \in L^2(\mathbb{R})$ with $\|f_n\| = 1$. The sequence f_n has no limit in $L^2(\mathbb{R})$.[17] Nonetheless, an elementary computation shows that $\lim_{n\to\infty} \|(\hat{a} - \lambda) f_n\| = 0$ for $\lambda = a(x_0)$, so that the f_n form approximate eigenvectors of $\hat{a}$ with 'eigenvalue' $a(x_0)$.

Definition 2.15 *Let $a : H \to H$ be a* normal *operator. The* **spectrum** *$\sigma(a)$ consists of all $\lambda \in \mathbb{C}$ for which there exists a sequence (f_n) in H with $\|f_n\| = 1$ and*

$$\lim_{n\to\infty} \|(a - \lambda) f_n\| = 0. \tag{2.30}$$

1. *If λ is an eigenvalue of a, in that $af = \lambda f$ for some $f \in H$ with $\|f\| = 1$, then we say that $\lambda \in \sigma(a)$ lies in the* **discrete spectrum** *$\sigma_d(a)$ of a.*
2. *If $\lambda \in \sigma(a)$ but $\lambda \notin \sigma_d(a)$, it lies in the* **continuous spectrum** *$\sigma_c(a)$ of a.*
3. *Thus $\sigma(a) = \sigma_d(a) \cup \sigma_c(a)$ is the union of the discrete and the continuous part.*

Indeed, in the first case (2.30) clearly holds for the constant sequence $f_n = f$ (for all n), whereas in the second case λ by definition has no associated eigenvector.

If a acts on a finite-dimensional Hilbert space, then $\sigma(a) = \sigma_d(a)$ consists of the eigenvalues of a. On the other hand, in the above example of a multiplication operator $\hat{a}$ on $L^2(\mathbb{R})$ we have $\sigma(\hat{a}) = \sigma_c(\hat{a})$. Our little computation shows that $\sigma_c(\hat{a})$ contains the range $\mathrm{ran}(a)$ of the function $a \in C_0(\mathbb{R})$, and it can be shown that $\sigma(\hat{a}) = \mathrm{ran}(a)^-$ (i.e., the topological closure of the range of $a : \mathbb{R} \to \mathbb{R}$ as a subset of $\mathbb{R}$). In general, the spectrum may have both a discrete and a continuous part.[18]

[17] It converges to Dirac's delta function $\delta(x - x_0)$ in a 'weak' sense, viz. $\lim_{n\to\infty}(f_n, g) = g(x_0)$ for each fixed $g \in C_c^\infty(\mathbb{R})$, but the δ 'function' is not an element of $L^2(\mathbb{R})$ (it is a distribution).

[18] If a is the Hamiltonian of a quantum-mechanical system, the eigenvectors corresponding to the discrete spectrum are *bound states*, whereas those related to the continuous spectrum form wavepackets defining *scattering states*. Just think of the hydrogen atom. It should be mentioned that such Hamiltonians are typically *unbounded* operators; see §2.12 below.

2.10 Compact operators

Even if H is infinite-dimensional, there is a class of operators whose spectrum is discrete. First, a **finite-rank operator** is an operator with finite-dimensional range. Using Dirac's notation, for $f, g \in H$ we write $|f\rangle\langle g|$ for the operator $h \mapsto (g,h)f$. An important special case is $g = f$ with $\|f\| = 1$, so that $|f\rangle\langle f|$ is the one-dimensional projection onto the subspace spanned by f. More generally, if (e_i) is an o.n.b. of some finite-dimensional subspace K, then $\sum_i |e_i\rangle\langle e_i|$ is the projection onto K. Clearly, any *finite* linear combination $\sum_i |f_i\rangle\langle g_i|$ is finite-rank, and *vice versa*.

Definition 2.16 *A bounded operator Hilbert space is called* **compact** *iff it is the norm-limit of a sequence of finite-rank operators.*

Note that multiplication operators of the type $\hat{a}$ on $L^2(\mathbb{R}^n)$ for $0 \neq a \in C_0(\mathbb{R}^n)$ are *never* compact. On the other hand, typical examples of compact operators on $L^2(\mathbb{R}^n)$ are integral operators of the kind $af(x) = \int d^n y\, K(x,y) f(y)$ with $K \in L^2(\mathbb{R}^{2n})$.

Theorem 2.17 *Let a be a self-adjoint compact operator on a Hilbert space H. Then the spectrum $\sigma(a)$ is discrete. All nonzero eigenvalues have finite multiplicity, so that only $\lambda = 0$ may have infinite multiplicity (if it occurs), and in addition 0 is the only possible accumulation point of $\sigma(a) = \sigma_d(a)$. If p_i is the projection onto the eigenspace corresponding to eigenvalue λ_i, then $a = \sum_i \lambda_i p_i$, where the sum converges strongly, i.e., in the sense that $af = \sum_i \lambda_i p_i f$ for each fixed $f \in H$.*

The compact operators are closed under multiplication and taking adjoints, so that, in particular, a^*a is compact whenever a is. Hence Theorem 2.17 applies to a^*a. Note that a^*a is self-adjoint and that its eigenvalues are automatically non-negative.

Definition 2.18 *We say that a compact operator $a : H \to H$ is* **trace-class** *if the* **trace-norm** $\|a\|_1 := \sum_k \sqrt{\mu_k}$ *is finite, where the μ_k are the eigenvalues of a^*a.*

Theorem 2.19 *Suppose a is trace-class. Then the* **trace** *of a, defined by*

$$\mathrm{Tr}\,(a) := \sum_i (e_i, ae_i), \tag{2.31}$$

is absolutely convergent and independent of the orthonormal basis (e_i). In particular, if $a = a^*$ with eigenvalues (λ_i), then $\mathrm{Tr}\, a = \sum_i \lambda_i$. Furthermore:

1. *If b is bounded and a is trace-class, then ab and ba are trace-class, with*

$$\mathrm{Tr}\,(ab) = \mathrm{Tr}\,(ba). \tag{2.32}$$

2. *If u is unitary and a is trace-class, then uau^{-1} is trace-class, with*

$$\mathrm{Tr}\,(uau^{-1}) = \mathrm{Tr}\,(a). \tag{2.33}$$

The following notion plays a fundamental role in quantum mechanics; cf. §2.11.

Definition 2.20 *A trace-class operator $\rho : H \to H$ is called a* **density matrix** *if ρ is* positive *and* $\mathrm{Tr}\,(\rho) = 1$ *(and hence $\|\rho\|_1 = 1$). Equivalently, ρ is a density matrix if $\rho = \sum_i \lambda_i p_i$ (strongly) with $\dim(p_i) < \infty$ for all i, $0 < \lambda_i \leq 1$, and $\sum_i \lambda_i = 1$.*

2.11 Quantum mechanics and Hilbert space

We are now ready to state the mathematical model of quantum mechanics introduced by von Neumann in 1932 [29], and used at least in *mathematical* physics ever since. It is based on the general idea that physical theories are given in terms of **observables** and **states**, along with a pairing that maps a given observable a and a given state ρ into a real number $< \rho, a >$. This number may be interpreted as the *expectation value* of a given ρ (what *that* means should be discussed in a course on foundations!).

1. The *states* of a given quantum system are represented by the density matrices ρ on some Hilbert space H associated to the system.
2. The *observables* of this system are given as self-adjoint operators $a : H \to H$.
3. The *pairing* map is given by $< \rho, a > = \mathrm{Tr}\,(\rho a)$.

To see that $< \rho, a >$ is real, use Definition 2.1.1.(b), (2.32), $a^* = a$, and $\rho^* = \rho$.

This model should be contrasted with the corresponding classical version:

1. The *states* of a given classical system are represented by the probability measures μ on some phase space M associated to the system (i.e., $\mu(M) = 1$).
2. The *observables* of this system are bounded Borel functions $f : M \to \mathbb{R}$.
3. The *pairing* map is given by $< \mu, f > = \int_M d\mu\, f$ (cf. §2.6).

In both cases one has the notion of *pure* versus *mixed* states. In physics, a pure state gives maximal information about a system, whereas a mixed state displays a certain amount of ignorance. A precise mathematical definition based on convexity will be given in §3.3 below; for the moment, we note that:

- In classical physics pure states are identified with points x of the phase space M, which in the above setting should in turn be identified with the corresponding Dirac measures $\mu = \delta_x$, given by $< \delta_x, f >= f(x)$.
- In quantum mechanics, pure states are often erroneously identified with unit vectors Ψ in H, but in fact they are the corresponding one-dimensional projections $|\Psi\rangle\langle\Psi|$, seen as density matrices (these are Ψ "up to a phase").

Perhaps confusingly, such projections may also be regarded as two-valued *observables*, in that $p_\Phi = |\Phi\rangle\langle\Phi|$ corresponds to the yes-no question "is the state of the system Φ?" The expectation value of this observable in a state $p_\Psi = |\Psi\rangle\langle\Psi|$ is

$$\mathrm{Tr}\,(p_\Psi p_\Phi) = |(\Psi, \Phi)|^2, \tag{2.34}$$

which is lies in $[0, 1]$ and is called the **transition probability** between Ψ and Φ.

If we assume for simplicity that an observable a is *compact* (which is always the case if $H = \mathbb{C}^n$), then by Theorem 2.17 we have $a = \sum_i \lambda_i |\Phi_i\rangle\langle\Phi_i|$ for some o.n.b. (Φ_i) of H. Assuming each eigenvalue λ_i to be simple, the question "is the state of the system Φ?" then operationally amounts to asking "when a is measured, is its value found to be equal to λ_i?". In a pure state p_Ψ, according to (2.34) the answer "yes" then obtains with probability $|(\Psi, \Phi_i)|^2$, called the **Born probability**.

2.12 Unbounded operators

But what about the typical operators in quantum theory, like the position operator $\hat{x}$ on $L^2(\mathbb{R})$ (and similarly the triple $(\hat{x}^1, \hat{x}^2, \hat{x}^3)$ on $L^2(\mathbb{R}^3)$), the momentum operator $\hat{p} = -i\hbar d/dx$ on $L^2(\mathbb{R})$ (etc.), and the Schrödinger Hamiltonian $\hat{h} = -\frac{\hbar^2}{2m}\Delta + \hat{V}$? These will not play a big role in these notes, but it is good to know that they are *discontinuous* or **unbounded operators**. Such 'operators' are not initially defined on the entire Hilbert space H in question, but merely on some dense subspace $D \subset H$ of it, *which is not complete in the norm of* H. For example, each of the above expressions makes sense on the smooth functions with compact support $C_c^\infty(\mathbb{R}^n)$ (for appropriate n), or on the Schwartz space $\mathcal{S}(\mathbb{R}^n)$ of rapidly decreasing smooth functions on $\mathbb{R}^n$. Of course, one may initially also define a *bounded* operator on such dense subspaces. The fundamental difference between bounded and unbounded operators then becomes clear if one computes the supremum in (2.22), restricting to $v \in D$ in order for the numbers $\|av\|_H$ on the right-hand side to make sense:

- For a *bounded* operator $a : D \to H$ (i.e., the restriction of $a : H \to H$ to D), the supremum $\sup\{\|av\|_H,\, v \in D,\, \|v\|_H = 1\}$ is finite and equal to $\|a\|$ as defined in (2.22). The original operator $a : H \to H$ may then be recovered from its restriction $a : D \to H$ by continuity, in the sense that $af = \lim_n af_n$ for $f \in H$ and any sequence (f_n) in D converging to f (cf. Prop. 2.12).
- For an *unbounded* operator $a : D \to H$, $\sup\{\|av\|_H,\, v \in D,\, \|v\|_H = 1\} = \infty$.

It is possible to define the adjoint a^* of an unbounded operator a, and ask if $a^* = a$.

Definition 2.21

1. *The adjoint $a^* : D(a^*) \to H$ of an unbounded operator $a : D(a) \to H$ has domain $D(a^*)$ consisting of all $f \in H$ for which the functional $g \mapsto (f, ag)$ is bounded. By Riesz–Fischer, it follows that $(f, ag) = (h, g)$ for a vector $h \in H$ uniquely defined by f and a. Writing $a^*f := h$, we have $(a^*f, g) = (f, ag)$.*
2. *The operator a is called* **self-adjoint**,[19] *denoted $a^* = a$, when $D(a^*) = D(a)$ and $a^*f = af$ for all $f \in D(a)$.*

The operators mentioned above are not self-adjoint. Similarly, if $a \in C(\mathbb{R}^n)$ defines a multiplication operator $\hat{a}$ with $D(\hat{a}) = C_c^\infty(\mathbb{R}^n)$, then the domain of the adjoint is easily checked to be $D(\hat{a}^*) = \{f \in L^2(\mathbb{R}^n) \mid af \in L^2(\mathbb{R}^n)\}$, which is bigger than $C_c^\infty(\mathbb{R}^n)$. This suggests that it would have been better to define $\hat{a}$ on the larger domain $D(\hat{a}) = \{f \in L^2(\mathbb{R}^n) \mid af \in L^2(\mathbb{R}^n)\}$, which leads to the same expression for $D(\hat{a}^*)$. So in that case $D(\hat{a}^*) = D(\hat{a})$, and if also a is real-valued, then $\hat{a} = \hat{a}^*$.

More generally, suppose $a : D(a) \to H$ satisfies $D(a) \subset D(a^*)$ and $(af, g) = (f, ag)$ for all $f, g \in D(a)$. Can we find a *self-adjoint* operator $\tilde{a} : D(\tilde{a}) \to H$ such that $D(a) \subset D(\tilde{a})$ and $af = \tilde{a}f$ for all $f \in D(a)$? And if so, is this *self-adjoint extension* of a unique? If both answers are *yes*, then a is called **essentially self-adjoint**. This holds iff $a^{**} = a^*$, in which case the desired self-adjoint extension of a is simply its adjoint a^*. Indeed, this describes the example of $\hat{a}$ just given.

[19] If a is self-adjoint, then $(af, g) = (f, ag)$ for all $f, g \in D(a)$. If just this equality holds, in other words, if $D(a) \subset D(a^*)$ and $a^*f = af$ for all $f \in D(a)$, then a is called **symmetric**.

2.13 Stone's Theorem

Stone's Theorem provides a mathematical interpretation of the time-dependent Schrödinger equation, also explaining the role of self-adjointness. To state the theorem, we need to define the notion of time-evolution on a Hilbert space. We motivate this definition by noting that physicists solve the time-dependent Schrödinger equation with initial value $\psi(0) = \psi$ by $\psi(t) = u(t)\psi$, where $u(t) = \exp(-ith/\hbar)$. Heuristic reasoning then leads to the properties of u in the following definition.[20]

Definition 2.22 *A* **time-evolution** *on H is a map $t \mapsto u(t)$ associating a unitary operator $u(t)$ on H to each $t \in \mathbb{R}$, such that $u(0) = 1$, $u(s)u(t) = u(s+t)$ for all $s, t \in \mathbb{R}$, and $\lim_{t\to 0} u(t)\psi = \psi$ for each $\psi \in H$.*

Stone's theorem relates this to the Hamiltonian of quantum physics, as follows:

1. A time-evolution $\psi(t)$ defines a self-adjoint operator h (the 'Hamiltonian');
2. Conversely, a self-adjoint operator h defines a time-evolution $\psi(t)$.

Theorem 2.23 *(Stone's Theorem)*

1. *Let $t \mapsto u(t)$ be a time-evolution on H. Define a (possibly unbounded) operator h by $h\psi := i \lim_{s\to 0} \frac{u(s)-1}{s}\psi$, where the domain of h consists of all $\psi \in H$ for which this (norm) limit exists. Then $D(h)$ is dense in H and h is self-adjoint.*
2. *Provided $\psi \in D(h)$, for each $t \in \mathbb{R}$ the vector $\psi(t) = u(t)\psi$ lies in $D(h)$ as well and satisfies the time-dependent Schrödinger equation $h\psi(t) = id\psi(t)/dt$.*
3. *Given a (possibly unbounded) self-adjoint operator h on H, there exists a unique time-evolution $t \mapsto u(t)$ on H that is related to h in the above way.*

So far, we have thought of $t \mapsto u(t)\psi$ as the time-evolution of ψ. But nothing has relied on this interpretation: this is the power of abstraction in mathematics! Consider the following example. Take $H = L^2(\mathbb{R})$ and define the map $t \mapsto u(t)$ by

$$u(t)\psi(x) := \psi(x - t). \tag{2.35}$$

This satisfies Definition 2.22. The domain of h is $D(h) = \{\psi \in L^2(\mathbb{R}) \mid \psi' \in L^2(\mathbb{R})\}$, where the derivative ψ' is defined by $\psi'(x) := \lim_{s\to 0}(\psi(x+s) - \psi(x))/s$; the limit is *in the norm of* $L^2(\mathbb{R})$, rather than pointwise in x. Finally, the action is $h\psi = -i\psi'$. This 'Hamiltonian' is just the usual momentum operator $\hat{p}$ (with $\hbar = 1$). Stone's Theorem both provides its domain and states that $\hat{p}$ is self-adjoint on this domain.

[20] From a group-theoretical point of view, a time-evolution is a strongly continuous unitary representation of $\mathbb{R}$ (as an additive group). More generally, let G be a (topological) group. A **unitary representation** of G on a Hilbert space H is a (strongly continuous) homomorphism U from G into the group of all unitary operators on H. In other words, one has $U(xy) = U(x)U(y)$ and $U(e) = 1$ (and the map $(x, \psi) \mapsto U(x)\psi$ from $G \times H$ to H is continuous).

3 Operator algebras

So far, we have mostly studied operators in Hilbert space on their own. It was a fundamental insight of John von Neumann's that it is fruitful both for pure mathematics and for quantum physics to study *algebras of operators* on a Hilbert space,[21] also recognizing that *bounded* operators (simply called *operators* in what follows) provide the most convenient setting.[22] Indeed, in one of his papers on Hilbert space theory (1929), von Neumann defined a *ring of operators* M (nowadays called a *von Neumann algebra*) as a *-subalgebra of the algebra $B(H)$ of all bounded operators on a Hilbert space H that contains the unit 1 and is closed in the so-called weak operator topology.[23] In the same paper, von Neumann proved what is still the basic theorem of the subject: a *-subalgebra M of $B(H)$, containing the unit operator 1, is weakly closed iff $M'' = M$. Here the **commutant** M' of a collection M of bounded operators consists of all bounded operators that commute with all elements of M, and the **bicommutant** M'' is simply the iterated commutant $(M')'$. Subsequently, von Neumann went on to develop the theory of such algebras in the period 1936–1949, partly in collaboration with his assistant Murray [30].[24]

An important second step in the theory of operator algebras was the initiation of the theory of *C^*-algebras* by Gelfand and Naimark in 1943. It turns out that von Neumann's rings of operators ar special cases of C^*-algebras, but von Neumann algebras also continue to be studied on their own. A fruitful mathematical analogy is that C^*-algebras provide a noncommutative generalization of *topology*, whereas von Neumann algebras comprise noncommutative *measure theory*.[25] C^*-algebras were first applied to quantum theory by Segal in 1947, and have provided the basis for a mathematically rigorous study of especially infinite quantum systems ever since.

It is the modest purpose of this chapter to develop just enough knowledge and intuition on operator algebras (mostly C^*-algebras) to understand their applications to symmetry breaking. For more information, we refer to [4, 18, 48] (see also [21]).

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[21] Recall that an **algebra** is a vector space with an associative bilinear operation ('multiplication') $\cdot : A \times A \to A$; we usually write ab for $a \cdot b$. We call A **unital** if there is an element $1 \in A$, the **unit**, such that $1a = a1 = a$ for all $a \in A$. It is easy to see that a unit is unique when it exists.

[22] In contrast, the product of two unbounded operators is not necessarily defined. Nonetheless, there is a certain amount of literature on algebras of unbounded operators, partly in connection to quantum field theory. See, for example, [1, 39].

[23] All this means that M is a subalgebra of $B(H)$ with unit under operator mulitplication, that M is closed under the involution $a \mapsto a^*$, and that if for some sequence $\{a_n\} \subset M$ one has $|(v, (a_n - a)w)| \to 0$ for all $v, w \in H$, then $a \in M$. See also §§3.1 and 3.7 below.

[24] Von Neumann's reasons for studying rings of operators were plurifold, including representation theory and ergodic theory; as in his development of Hilbert spaces, important motivation certainly also came from quantum mechanics. Unlike many physicists then and even now, von Neumann knew that all Hilbert spaces of a given dimension are isomorphic (cf. Theorem 2.7), so that one cannot characterize a physical system by saying that 'its Hilbert space of (pure) states is $L^2(\mathbb{R}^3)$'. Instead, von Neumann hoped to characterize quantum-mechanical systems by algebraic conditions on the observables. He initiated a programme in this direction in the 1930s, partly in collaboration with Jordan and Wigner, but achieved little himself. After his death, von Neumann's goals in this direction have to some extent been realized by Haag and his followers in (algebraic) quantum statistical mechanics and quantum field theory (as discussed in the main part of this course).

[25] These analogies form the basis of *noncommutative geometry* as developed by Connes [7].

3.1 Basic definitions

If a and b are bounded operators on H, then so is their sum $a + b$, defined by $(a + b)(v) = av + bv$, and their product ab, given by $(ab)(v) = a(b(v))$. This follows from the triangle inequality for the norm and from (2.24), respectively. Also, homogeneity of the norm yields that ta is bounded for any $t \in \mathbb{C}$. Consequently, the set $B(H)$ of all bounded operators on a Hilbert space H forms an *algebra* over the complex numbers, having remarkable properties. To begin with (cf. (2.22)):

Proposition 3.1 *The space $B(H)$ of all bounded operators on a Hilbert space H is a Banach space in the operator norm*

$$\|a\| := \sup\{\|af\|_H,\ f \in H,\ \|f\|_H = 1\}. \tag{3.1}$$

This is a basic result from functional analysis; it even holds if H is a Banach space.

Definition 3.2 *A **Banach algebra** is a Banach space A that is simultaneously an algebra in which $\|ab\| \leq \|a\|\,\|b\|$ for all $a, b \in A$.*

According to (2.24), we see that $B(H)$ is not just a Banach *space* but even a Banach *algebra*. Also this would still be the case if H were merely a Banach space, but the fact that it is a Hilbert space gives a crucial further ingredient of the algebra $B(H)$.

Definition 3.3

1. *An **involution** on an algebra A is a real-linear map $A \to A^*$ such that $a^{**} = a$, $(ab)^* = b^*a^*$, and $(\lambda a)^* = \overline{\lambda}a^*$ for all $a, b \in A$ and $\lambda \in \mathbb{C}$. An algebra with involution is also called a* ***-algebra**.

2. *A **C^*-algebra** is a Banach algebra A with involution in which for all $a \in A$,*

$$\|a^*a\| = \|a\|^2. \tag{3.2}$$

3. *A* **homomorphism** *between C^*-algebras A en B is a linear map $\varphi : A \to B$ that satisfies $\varphi(ab) = \varphi(a)\varphi(b)$ and $\varphi(a^*) = \varphi(a)^*$ for all $a \in A$, $b \in B$.*

4. *An* **isomorphism** *between two C^*-algebras is an invertible homomorphism.*[26]

In view of (2.29), we conclude that $B(H)$ *is a C^*-algebra* (with the identity operator as its unit) with respect to the involution defined by the operator adjoint (2.27).

Similarly, if $A \subset B(H)$ is a norm-closed subalgebra of $B(H)$ such that if $a \in A$, then $a^* \in A$ (so that A is an algebra with involution), then A is obviously a C^*-algebra (not necessarily with unit). A case in point is $A = K(H)$, the C^*-algebra of *compact operators* on H. If $\dim(H) = \infty$, there is a strict inclusion $K(H) \subset B(H)$; for one thing, the unit operator lies in $B(H)$ but not in $K(H)$, which has no unit. If $\dim(H) < \infty$, though, one has $K(H) = B(H) = M_n(\mathbb{C})$, the $n \times n$ matrices.

On the other hand, the set $B_1(H)$ of trace-class operators satisfies (3.2) in the operator norm (3.1) but fails to be complete in that norm, whereas in the trace-norm $\|\cdot\|_1$ it is complete but (3.2) fails. Either way, $B_1(H)$ *fails to be a C^*-algebra.*

[26] It can be shown that an isomorphism is automatically isometric; see footnote 34.

3.2 Commutative C^*-algebras

The C^*-algebras $K(H)$ and $B(H)$ are highly noncommutative. For the opposite case, let X be a locally compact Hausdorff space (physicists may keep $X = \mathbb{R}^n$ in mind). The space $C_0(X)$ of all continuous functions $f : X \to \mathbb{C}$ that vanish at infinity[27] is an algebra under pointwise operations.[28] It has a natural involution

$$f^*(x) = \overline{f(x)}, \tag{3.3}$$

and a natural **supremum-norm** or **sup-norm** given by (cf. 2.12)

$$\|f\|_\infty := \sup\{|f(x)|, x \in X\}. \tag{3.4}$$

Then $C_0(X)$ is a commutative C^*-algebra; the axioms are easily checked. Let us note that $C_0(X)$ has a unit (namely the function equal to 1 for any x) iff X is compact. The converse, due to Gelfand and Naimark (1943), is a beautiful result:

Theorem 3.4 *Every commutative C^*-algebra A is isomorphic to $C_0(X)$ for some locally compact Hausdorff space X, which is unique up to homeomorphism.*

This space X is often denoted by $\Sigma(A)$ and is called the **Gelfand spectrum** of A. It may be realized as the set of multiplicative linear functionals on A, that is, as the set of all nonzero linear maps $\omega : A \to \mathbb{C}$ that satisfy $\omega(ab) = \omega(a)\omega(b)$.[29] The isomorphism $A \to C_0(\Sigma(A))$ is given by the **Gelfand transform** $a \mapsto \hat{a}$, where

$$\hat{a}(\omega) := \omega(a), \tag{3.5}$$

where $a \in A$ and $\omega \in \Sigma(A)$. For example, if A is already given as $A = C_0(X)$, then each $x \in X$ defines a functional ω_x on A by $\omega_x(f) = f(x)$, which is multiplicative by the pointwise definition of multiplication in A. Theorem 3.4 then implies $\Sigma(C_0(X)) \cong X$. In general, it follows from basic functional analysis that $\hat{a}$ is a continuous function on $\Sigma(A)$;[30] a more detailed analysis proves that it maps A into $C_0(\Sigma(A))$. Injectivity and surjectivity of the Gelfand transform both result from the difficult fact—whose proof relies on axiom (3.2)—that it is isometric, i.e., $\|\hat{a}\|_\infty = \|a\|$. Given this result, injectivity is trivial, and surjectivity follows from the Stone–Weierstrass Theorem. Finally, is immediately clear from the multiplicativity of $\omega \in \Sigma(A)$ that the Gelfand transform is an algebra homomorphism.

It follows from Theorem 3.4 that arbitrary commutative C^*-algebras are of the form $A \subset B(H)$ for some Hilbert space H (cf. the end of the preceding subsection). We have already seen this for $A = C_0(\mathbb{R}^n)$, which acts on $H = L^2(\mathbb{R}^n)$ by multiplication operators on; see text below (2.26). This construction, then, may be generalized to the case of $C_0(X)$ by putting $H = L^2(X, \mu)$ for some measure μ whose support is X.

[27] I.e., for each $\epsilon > 0$ there is a compact subset $K \subset X$ such that $|f(x)| < \epsilon$ for all x outside K.

[28] Addition is given by $(f + g)(x) = f(x) + g(x)$, multiplication is $(fg)(x) = f(x)g(x)$, etc.

[29] These functionals lie in the dual space A^* of A, but the topology in which Theorem 3.4 holds is not the (relative) norm-topology on X but the (relative) weak* topology, also called the **Gelfand topology** on X. These concepts are explained in the next subsection.

[30] Indeed, $a \mapsto \hat{a}$ maps A into the double dual $A^{**} := (A^*)^*$ of A, and $A \subset A^{**}$ precisely consists of all functionals on on A^* that are continuous with respect to the norm-topology on A^*.

3.3 States

A more systematic study of the connection between C^*-algebras and Hilbert spaces relies on the concept of a *state*, to which we now turn (see also subsection 2.11).

Definition 3.5 *A* ***state*** *on a unital C^*-algebra A is a linear map $\omega : A \to \mathbb{C}$ that is* ***positive****, in that $\omega(a^*a) \geq 0$ for all $a \in A$, and* ***normalized****, in that $\omega(1) = 1$.*

If we define the dual A^* of A as the space of linear maps $\varphi : A \to \mathbb{C}$ for which

$$\|\varphi\| = \sup\{|\varphi(a)|, a \in A, \|a\| = 1\} \tag{3.6}$$

is finite (cf. (2.22)), then it can be shown that any state ω on A lies in A^*, with $\|\omega\| = 1$. This leads to an extension of Definition 3.5 to general (i.e., not necessarily unital) C^*-algebras: *a state on a C^*-algebra A is a functional $\omega : A \to \mathbb{C}$ that is positive and normalized in the sense that $\|\omega\| = 1$.* This implies $\omega(1) = 1$ whenever A does have a unit, so that the two definitions are consistent when they overlap.

The state space $S(A)$ of A (i.e., the set of all states on A) is a *convex set*: if ω_1 and ω_2 are states, then so is $\lambda\omega_1 + (1-\lambda)\omega_2$ for any $\lambda \in [0,1]$. It follows that if $(\omega_1, \omega_2, \ldots, \omega_n)$ are states, and $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ are numbers in $[0,1]$ such that $\sum_i \lambda_i = 1$, then $\sum_i \lambda_i \omega_i$ is a state. This extends to infinite sums if we equip $S(A)$ with the weak* topology inherited from A^* (in which $\omega_n \to \omega$ if $\omega_n(a) \to \omega(a)$ for each $a \in A$).[31] If A has a unit, then $S(A)$ is a *compact convex set* in this topology.

Definition 3.6 *A state ω is* **pure** *if $\omega = \lambda\,\omega_1 + (1-\lambda)\omega_2$ for some $\lambda \in (0,1)$ and certain states ω_1 and ω_2 implies $\omega_1 = \omega_2$. The pure states on A comprise the* pure state space *of A, denoted by $P(A)$ or $\partial S(A)$. If a state is not pure, it is* **mixed**.

The convex structure of the state space is nicely displayed by $A = M_2(\mathbb{C})$, the C^*-algebra of 2×2 complex matrices. Put

$$\rho = \tfrac{1}{2} \begin{pmatrix} 1+z & x+iy \\ x-iy & 1-z \end{pmatrix}; \tag{3.7}$$

then ρ is a density matrix on $\mathbb{C}^2$ iff $(x,y,z) \in \mathbb{R}^3$ with $x^2 + y^2 + z^2 \leq 1$; this set is the three-ball B^3 in $\mathbb{R}^3$. It is easy to see that ρ defines a state ω_ρ on the $M_2(\mathbb{C})$ by

$$\omega_\rho(a) = \mathrm{Tr}\,(\rho a). \tag{3.8}$$

Conversely, every state on $M_2(\mathbb{C})$ is of this form (exercise). Hence the state space $S(M_2(\mathbb{C}))$ of a quantum 2-level system is isomorphic (as a convex set) to B^3. The pure states correspond to the points (x,y,z) for which $x^2 + y^2 + z^2 = 1$, i.e., to the two-sphere $S^2 = \partial B^3$ (also called the *Bloch sphere* in this context).

The classical analogue of this example is the phase space $M = \{x_1, x_2\}$ consisting of just two points; the corresponding commutative C^*-algebra is $C(M) = \mathbb{C} \oplus \mathbb{C}$. Each probability measure μ on M takes the form $\mu(x_1) = \lambda_1$ and $\mu(x_2) = \lambda_2$ with $\lambda_i \in [0,1]$ and $\lambda_1 + \lambda_2 = 1$. Hence the state space of $\mathbb{C} \oplus \mathbb{C}$ may be identified with the interval $[0,1]$ with its natural convex structure, in that $\lambda \in [0,1]$ corresponds to the probability measure $\lambda_1 = \lambda$, $\lambda_2 = 1 - \lambda$. Once again, the boundary points $\{0,1\} = \partial[0,1]$ yield the pure states in question.

[31] This is the weakest topology making all functions $\omega \mapsto \omega(a)$ from $S(A)$ to $\mathbb{C}$, $a \in A$, continuous.

3.4 The Born rule revisited

We will now see to what extent the previous example may be generalized. Two examples of basic importance to classical and quantum physics are (cf. §2.11):

• The Riesz–Markov Theorem 2.10 implies that any *probability measure* μ on X defines a state ω_μ on $A = C_0(X)$ by $\omega_\mu(f) = \int_X d\mu\, f$, and *vice versa*; the requirement $\|\varphi\| = 1$ in the definition of a state forces $\mu(X) = 1$. We often write ω_μ as $\mu(f)$.

The pure states are precisely the *Dirac measures* δ_x, defined for each $x \in X$ by $\delta_x(A) = 1$ if $x \in A$ and $\delta_x(A) = 0$ if $x \notin A$, for $A \subset X$. The corresponding integral, which we denote by ω_x or ev_x, then maps f to $f(x)$. Hence $P(C_0(X))$ is homeomorphic to X under the bijection $\mathrm{ev}_x \leftrightarrow x$. More generally, a nonzero functional on a commutative C^*-algebra defines a *pure* state iff it is *multiplicative*, and hence Theorem 3.4 implies that the pure state space of a commutative C^*-algebra is homeomorphic to its Gelfand spectrum, or $P(A) \cong \Sigma(A)$.

• Any density matrix ρ on a Hilbert space H defines a state ω_ρ on the C^*-algebra $B(H)$ by (3.8), i.e., $\omega_\rho(a) = \mathrm{Tr}\,(\rho a)$. Such a state is pure iff it is a **vector state**, i.e., if ρ is a one-dimensional projection $p_\Psi \equiv |\Psi\rangle\langle\Psi|$ for some unit vector $\Psi \in H$. Simply writing ψ for ω_{p_Ψ}, we then have

$$\psi(a) = \mathrm{Tr}\,(p_\Psi a) = (\Psi, a\Psi). \tag{3.9}$$

Indeed, the spectrum $\sigma(\rho)$ of $\rho = \sum_i \lambda_i p_i$ contains points different from $\lambda = 0$ or $\lambda = 1$ iff it is mixed, whereas $\sigma(p_\Psi) = \{0, 1\}$. However, this argument (for the purity of ψ) only shows that ψ has no nontrivial decomposition $\psi = \lambda\,\omega_1 + (1-\lambda)\omega_2$ *when* ψ *is taken to be a state on* $B(H)$, for in that case one has $\mathrm{Tr}\,(\rho_1 a) = \mathrm{Tr}\,(\rho_2 a)$ for all $a \in B(H)$ iff $\rho_1 = \rho_2$. This is still the case for $K(H)$ instead of $B(H)$ (exercise).

For more general C^*-algebras $A \subset B(H)$, however, it may no longer be the case that vector states as in (3.9) are pure. For example, if $H = \mathbb{C}^n$ and D_n consists of all diagonal $n \times n$ matrices, with elements $a = \mathrm{diag}(a_1, \ldots, a_n)$, $a_i \in \mathbb{C}$, then

$$\psi(a) = \sum_{i=1}^{n} |\Psi_i|^2 a_i. \tag{3.10}$$

So ψ, *as a state on the* C^**-algebra* D_n, coincides with $\sum_i \lambda_i |e_i\rangle\langle e_i|$, with coefficients $\lambda_i = \psi(|e_i\rangle\langle e_i|) = |(e_i, \Psi)|^2 = |\Psi_i|^2$, where (e_i) is the standard basis of $\mathbb{C}^n$. This state is pure on D_n iff $\Psi \sim e_i$, so in general it will be mixed. In quantum physics, λ_i is the Born probability for the outcome a_i of a measurement of a in the state Ψ.

An infinite-dimensional analogue of this example is $H = L^2(\mathbb{R}^n)$ and $A = C_0(\mathbb{R}^n)$, acting on H as multiplication operators (henceforth we omit the hat on a). Then

$$\psi(a) = \int_{\mathbb{R}^n} d^n x\, |\Psi(x)|^2 a(x), \tag{3.11}$$

is always mixed: this state corresponds to the probability measure on $\mathbb{R}^n$ with density $|\Psi(x)|^2$. As a limiting case, we may take a to be the characteristic function $a = \chi_\Delta$ of some region $\Delta \subset \mathbb{R}^n$, so that $\psi(\chi_\Delta) = \int_\Delta d^n x\, |\Psi(x)|^2$ is the Born probability for finding the particle within Δ (first written down in 1926 by Pauli).[32]

[32] Although $\chi_\Delta \notin C_0(\mathbb{R}^n)$, one has $\chi_\Delta \in C_0(\mathbb{R}^n)''$, to which algebra ψ extends; see §§3.6 and 3.7.

3.5 The spectrum revisited

In order to unify and generalize (3.10) and (3.11), we return to the *spectrum*, already encountered for normal operators in §2.9. We first generalize Definition 2.15.

Definition 3.7 *Let A be a C^*-algebra with unit 1 (or, more generally, a Banach algebra with unit).*[33] *The* ***spectrum*** *$\sigma(a)$ of $a \in A$ is the set of all $z \in \mathbb{C}$ for which $a - z \equiv a - z \cdot 1$ has no (two-sided) inverse in A.*

The spectrum $\sigma(a)$ is a closed subset of $\mathbb{C}$. One of the remarkable properties of C^*-algebras is that the norm may be recovered from the algebraic structure: if we define the **spectral radius** $r(a)$ of $a \in A$ by $r(a) := \sup\{|z|, z \in \sigma(a)\}$, then $\|a\| = r(a)$ if $a^* = a$, and $\|a\| = \sqrt{r(a^*a)}$ in general. Consequently, *if* an algebra with involution has a norm in which it is a C^*-algebra, then that norm is unique.[34]

If $a \in A$ is *normal*, then the C^*-algebra $C^*(a)$ generated by a *and the unit* within A (i.e., the norm-closure of all polynomials in a and a^*) is obviously commutative.

Theorem 3.8 *Let a be a normal element of a unital C^*-algebra A. Then the spectrum of a in A coincides with the spectrum of a in $C^*(a)$, so that we may unambiguously speak of* the *spectrum $\sigma(a)$. Moreover, there is a unique isomorphism*

$$C(\sigma(a)) \cong C^*(a) \tag{3.12}$$

under which the function $z \mapsto z$ on $\sigma(a) \subset \mathbb{C}$ is mapped to $a \in C^*(a) \subset A$.

This isomorphism $\varphi : C(\sigma(a)) \to C^*(a)$ maps a polynomial $p \equiv p(z, \overline{z}) \in C(\sigma(a))$ into the corresponding polynomial $p(a, a^*) \in C^*(a)$. If $f \in C(\sigma(a))$, then (by Stone–Weierstrass) there is a polynomial p on $\sigma(a)$ such that $p_n \to f$ in the sup-norm on $C(\sigma(a))$. Defining $f(a, a^*)$ as the norm-limit of $p_n(a, a^*)$ in A, we have $\varphi(f) = f(a, a^*)$. Since isomorphisms between C^*-algebras are isometric, one has $\|f(a, a^*)\| = \|f\|_\infty$. In addition, $\sigma(f(a, a^*))$ is just the image of $\sigma(a)$ under f.

In the context of Theorem 3.4, Theorem 3.8 states that the spectrum $\sigma(a)$ of $a \in A$ coincides with the Gelfand spectrum of the commutative C^*-algebra $C^*(a)$; indeed, $\lambda \in \sigma(a)$ provides the multiplicative functional $\omega_\lambda(f(a, a^*)) = f(\lambda)$ on $C^*(a)$.

Finally, the consistency between Definitions 3.7 and 2.15 whenever they overlap is guaranteed by the following result, whose proof is an exercise.

Proposition 3.9 *Let $a \in B(H)$ be normal. Then $\lambda \in \sigma(a)$ iff there exists a sequence (f_n) in H with $\|f_n\| = 1$ for all n such that $\lim_{n\to\infty} \|(a - \lambda)f_n\| = 0$.*

---

[33] If A does not have a unit, one has to add one in order to define spectra. This is done as follows. First, define $\dot{A} = A \oplus \mathbb{C}$ as a *vector space*, with elements $(a, z) \equiv a \dot{+} z$. The element $(0, 1)$ will be the unit of $\dot{A}$. Second, define $\dot{A}$ as an *algebra* with involution by putting $(a, w) \cdot (b, z) := (ab + wb + za, wz)$ and $(a, z)^* = (a^*, \overline{z})$. Third, define a *norm* on $\dot{A}$. This is the difficult step. To understand it, regard $\dot{A}$ as a subspace of $L(A)$, the Banach algebra of bounded linear maps from A to A, in the obvious way, that is, $(a, z)(b) = ab + zb$. This provides the norm $\|(a, z)\| = \sup\{\|ab + zb\|, b \in A, \|b\| = 1\}$ on $\dot{A}$. Thus defined, $\dot{A}$ is a C^*-algebra with unit, called the **unitization** of A. The spectrum of $a \in A$, then, is defined as the spectrum of $(a, 0)$ in $\dot{A}$.

[34] This proves the claim in footnote 26 that an isomorphism $\varphi : A \to B$ between C^*-algebras is isometric: considering the 'new' norm $\|a\|'_A = \|\varphi(a)\|_B$ on A, it must be that $\|a\|'_A = \|a\| \equiv \|a\|_A$.

3.6 Spectral Theorem

Combining the ideas in the previous two subsections, we now take a self-adjoint operator $a \in B(H)$ and a density matrix ρ on H. The restriction of the state ρ to $C^*(a)$ defines a unique probability measure μ_ρ on $\sigma(a)$ for which

$$\int_{\sigma(a)} d\mu_\rho(\lambda)\, f(\lambda) \equiv \mu_\rho(f) = \mathrm{Tr}\,(\rho f(a)) \;\text{ for all } f \in C(\sigma(a)). \tag{3.13}$$

We know from §2.6 that the *left*-hand side of (3.13) actually makes sense for any $f \in \mathcal{L}^1(\sigma(a), \mu_\rho)$. Since μ_ρ is a probability measure, this class includes all bounded (Borel) functions $f : \sigma(a) \to \mathbb{R}$. For example, the characteristic function χ_Δ of some Borel subset $\Delta \subset \sigma(a)$ yields $\int_{\sigma(a)} d\mu_\rho\, \chi_\Delta = \mu_\rho(\Delta)$, whose physical interpretation is given by the Born rule: regarding a as an observable and ρ as a state (cf. §2.11),

if a is measured in a state ρ, the probability of finding an outcome in Δ is $\mu_\rho(\Delta)$.

In particular, if $\rho = p_\Psi$ for some unit vector $\Psi \in H$, and $\lambda \in \sigma_d(a)$ is a simple eigenvalue of a with eigenvector e_λ, then by taking $\Delta = \{\lambda\}$ it follows[35] that the probability of finding λ is given by the well-known Born probability $|(\Psi, e_\lambda)|^2$.

We may ask if also the *right*-hand side of (3.13) makes sense for any bounded (Borel) function f, and, in particular, if there exists an operator $\chi_\Delta(a)$ such that

$$\mu_\rho(\Delta) = \mathrm{Tr}\,(\rho \chi_\Delta(a)). \tag{3.14}$$

This question cannot be answered in the context of Theorem 3.8, since χ_Δ is typically discontinuous, so that $\chi_\Delta(a)$ cannot be an element of $C^*(a)$. This problem may be resolved by completing the latter in a weaker topology on $B(H)$ than the operator norm topology. Many topologies suffice for this purpose; let us take the strong topology, in which $a_n \to a$ iff $a_n f \to af$ for all $f \in H$. Defining $W^*(a)$ as the (sequential) completion of $C^*(a)$ in the strong topology, it can be shown for any compact set $K \subset \mathbb{R}$ that each positive bounded (Borel) function $f : K \to \mathbb{R}$ is a pointwise limit of some bounded monotone increasing sequence p_n of polynomials on K. Applying this to $K = \sigma(a)$, we obtain a bounded monotone increasing sequence $p_n(a)$ of operators on H, which in turn can be shown to have a strong limit. This limit is by definition equal to $f(a)$, which by construction lies in $W^*(a)$. In particular, taking $f = \chi_\Delta$ this defines the so-called **spectral projections** $\chi_\Delta(a) \in W^*(a)$, which validate (3.14). A straightforward extension of this argument from self-adjoint operators a to normal ones then yields von Neumann's great **Spectral Theorem**:

Theorem 3.10 *Let $a \in B(H)$ be a normal operator, and let $\mathcal{B}(\sigma(a))$ be the (commutative) algebra of bounded Borel functions on $\sigma(a)$, with obvious involution. The isomorphism $C(\sigma(a)) \to C^*(a)$ of Theorem 3.8 has a unique extension to a homomorphism $\mathcal{B}(\sigma(a)) \to W^*(a)$ that satisfies $\|f(a)\| \leq \|f\|_\infty$ for each $f \in \mathcal{B}(\sigma(a))$.*

Note that both $\mathcal{B}(\sigma(a))$ and $W^*(a)$ are C^*-algebras. This result is stronger than Theorem 3.8 in that it applies to a much larger class of functions than just continuous ones, but it is weaker in that the ensuing homomorphism fails to be an isomorphism.

[35] We assume that λ is separated from $\sigma_c(a)$, in case a has some continuous spectrum. In that case, δ_λ is a continuous function on $\sigma(a)$ and (in the context of Theorem 3.8) $\delta_\lambda(a) = |e_\lambda\rangle\langle e_\lambda|$.

3.7 Von Neumann algebras

As already mentioned, von Neumann saw that strong operator completions of the type $C^*(a) \rightsquigarrow W^*(a)$ within $B(H)$ may equivalently be done algebraically. For any Hilbert space H, let $A \subset B(H)$ be some subset. The **commutant** of A, defined by

$$A' := \{b \in B(H) \mid ab = ba \, \forall a \in A\}, \tag{3.15}$$

is a subalgebra of $B(H)$. Similarly, one has the **bicommmutant** $A'' = (A')'$ of A.

Definition 3.11 *A *-algebra $M \subset B(H)$ is a* **von Neumann algebra** *if $M'' = M$.*

This condition forces M to be a C^*-algebra with unit (exercise), and is always satisfied if $\dim(H) < \infty$ (another exercise). If $\dim(H) = \infty$, on the other hand, we have $K(H)'' = B(H)$, so that the compact operators do not form a von Neumann algebra. On the commutative side, the C^*-algebra $C_0(\mathbb{R}^n)$ of multiplication operators on $L^2(\mathbb{R}^n)$ yields $C_0(\mathbb{R}^n)'' = L^\infty(\mathbb{R}^n)$, i.e., the algebra of (a.e.) bounded Borel functions on $\mathbb{R}^n$, and so $C_0(\mathbb{R}^n)$ is not a von Neumann algebra either.

In order to state von Neumann's famous double commutant theorem, we review a few of the most important topologies on $B(H)$ (using sequences for simplicity):[36]

- The **norm-topology** corresponds to $a_n \to a$ iff $\|(a_n - a)\| \to 0$ (cf. (3.1)).
- The **strong (operator) topology** has $a_n \to a$ iff $\|(a_n - a)f\| \to 0 \, \forall \, f \in H$.
- The **weak (operator) topology** has $a_n \to a$ iff $|(f, (a_n - a)g)| \to 0 \forall \, f, g \in H$.

None of these topologies coincide on infinite-dimensional Hilbert spaces. For example, if (e_i) is an o.n.b. of H, then $p_n = \sum_{i=1}^n |e_i\rangle\langle e_i|$ does not converge in the norm topology as $n \to \infty$, whereas $p_n \to 1$ in the two others. If $H = L^2([0,1])$, then the multiplication operators $e_n(t) = \exp(2\pi i n t)$ converge to zero in the weak operator topology but not in the strong one. So here is the **double commutant theorem**:

Theorem 3.12 *Let M be a unital *-algebra in $B(H)$. Then $M'' = M$ iff M is closed in the strong topology, which in turn holds iff M is closed in the weak topology.*

However, next to the norm topology, the second intrinsic topology on a von Neumann algebra in both a mathematical and a physical sense is neither the strong nor the weak one, but the **σ-weak topology**, in which $a_n \to a$ iff $|\mathrm{Tr}\,(\rho(a_n - a))| \to 0$ for each $\rho \in B_1(H)$. This results from a deep characterization theorem for von Neumann algebra due to Sakai: *a C^*-algebra is a von Neumann algebra iff it is the dual of a Banach space.* The latter is called the **predual** of M, denoted by M_*, so that $M = M_*^*$. The σ-weak topology on M then coincides with the weak*-topology with respect to M_*, i.e., one has $a_n \to a$ iff $|\rho(a_n - a)| \to 0$ for each $\rho \in M_*$. For example, one has $B(H)_* = B_1(H) = K(H)^*$, so that $B(H) = B_1(H)^* = K(H)^{**}$.

[36] Defining a topology in terms of convergence should really be done using nets or filters.

3.8 Characterization of states

With the concept of a von Neumann algebra at hand, we return to our discussion of states on C^*-algebras. We saw in §3.3 that all states on the 2×3 matrices are given by density matrices. This conclusion easily extends to the $n \times n$ matrices (seen as $M_n(\mathbb{C}) = B(\mathbb{C}^n)$), and also—though less easily—to the C^*-algebra of compact operators $K(H)$ on an arbitrary Hilbert space H (exercise). To state the far more substantial Theorem 3.15 below (due to von Neumann), we need some preparation.

Definition 3.13 *A* **normal state** *on a von Neumann algebra M is an element of the* **normal state space** $S_n(M) := S(M) \cap M_*$.

If $M \subset B(H)$, each density matrix on H almost by definition yields a normal state. Less trivially, it can be shown that a state ω is normal iff $\omega(\bigvee_i p_i) = \sum_i \omega(p_i)$ for arbitrary families of mutually orthogonal projections (p_i) in M (i.e. $p_i p_j = 0$ if $i \neq j$), where the supremum $\bigvee_i p_i$ is defined with respect to the ordering on projections given by $p \leq q$ iff $pH \subseteq pH$, that is, iff $\mathrm{ran}(p) \subseteq \mathrm{ran}(q)$.[37]

One reason why the continuity condition defining normal states may be reformulated in terms of projections, is that (unlike general C^*-algebras) von Neumann algebras have lots of them. Let $\mathrm{Proj}(A)$ be the set of projections in a *-algebra A.

Proposition 3.14 *If M is a von Neumann algebra, then $M = \mathrm{Proj}(M)''$.*

In particular, by Theorem 3.12 any element of M may be weakly or strongly approximated by linear combinations of projections within M.[38] To see that this is not true for C^*-algebras, a look at the commutative case suffices: if $A = C(X)$, then X is connected iff $\mathrm{Proj}(A) = \{0, 1\}$. So if a commutative von Neumann algebra M is regarded as a commutative C^*-algebra, then the Gelfand isomorphism $M \cong C(\Sigma(M))$ involves a highly disconnected ('Stonean') topological space $\Sigma(M)$.

This abundance of projections is useful, for example, if $M = A'$ is the commutant of some C^*-algebra $A \subset B(H)$.[39] Namely, for each $p \in \mathrm{Proj}(A')$ the closed subspace pH of H is stable under A (and even under A''). Taking $H_i = p_i H$ for a *complete* family (p_i) of mutually orthogonal projections in A' (i.e., $\sum_i p_i = 1$ strongly), one may therefore *decompose* H under the action of A (or even of A'') as $H = \oplus_i H_i$.[40]

We close this subsection with a characterization of normal states.

Theorem 3.15

1. *Every* normal *state on $B(H)$ is given by a density matrix on H.*[41]
2. *More generally, every* normal *state on a von Neumann algebra $M \subset B(H)$ is given by a density matrix on H (and* vice versa*).*

[37] In other words, $(\bigvee_i p_i)H$ is the smallest closed subpace containing all subspaces $p_i H$.

[38] Indeed, an old-fashioned way of stating Theorem 3.10 is that a normal operator a can be approximated by its spectral projections $\chi_\Delta(a)$ in a suitable way, which then lie in $M = W^*(a)$).

[39] Exercise: $A''' = A'$ for any *-algebra A, so that A' is indeed a von Neumann algebra.

[40] We say that $H = \oplus_i H_i$ under $A \subset B(H)$ if $a\psi_i \in H_i$ for each $a \in A$ and $\psi_i \in H_i$. See §3.13.

[41] In the literature on the foundations of quantum mechanics this is called von Neumann's *no hidden variable theorem*, since it proves that (weakly continuous) quantum-mechanical averages $a \mapsto \omega(a)$ cannot be dispersion-free (i.e. cannot satisfy $\omega(a^2) = \omega(a^2)$ for all $a^* = a \in B(H)$).

3.9 The GNS-construction

As in the case of groups, it is natural to look at representations of C^*-algebras.

Definition 3.16 *A **representation** of a C^*-algebra A on a Hilbert space H is a linear map $\pi : A \to B(H)$ such that $\pi(ab) = \pi(a)\pi(b)$, and $\pi(a^*) = \pi(a)^*$, $\forall a, b \in A$.*

- *A representation $\pi : A \to B(H)$ is called* **cyclic** *if there is a vector $\Omega \in H$ for which $\overline{\pi(A)\Omega} = H$;[42] in other words, each $\Psi \in H$ is the limit of a sequence $\pi(a_n)\Omega$ in H, where $a_n \in A$. In that case, Ω is called a* **cyclic vector** *for π.*

Physically, the idea behind cyclicity would be that each state arises by 'filling up' the ground state Ω with 'excitations' $\pi(a)\Omega$. There is a beautiful connection between cyclic *representations* of A and *states* on A, given by the **GNS-construction**.[43] In quantum physics, this construction provides the bridge between the usual Hilbert space formalism and the abstract C^*-algebraic approach, so it is quite important.

Theorem 3.17 *Let ω be a state on a C^*-algebra A. There exists a cyclic representation π_ω of A on a Hilbert space H_ω with cyclic unit vector Ω_ω such that*

$$\omega(a) = (\Omega_\omega, \pi_\omega(a)\Omega_\omega) \quad \forall a \in A. \tag{3.16}$$

The idea is to construct H_ω from A and subsequently define π_ω by left-multiplication:

1. Define a sesquilinear form $(-,-)_0$ on A by $(a,b)_0 := \omega(a^*b)$. This form almost defines an inner product on A, except that it may not be positive definite (i.e., it might be that $\omega(a^*a) = 0$ for some $a \neq 0$). Hence we remove the null space $N_\omega = \{a \in A \,|\, \omega(a^*a) = 0\}$ by forming the quotient A/N_ω. The form

$$([a],[b]) := \omega(a^*b) \tag{3.17}$$

   on A/N_ω (where $a \mapsto [a]$ denotes the canonical projection $A \to A/N_\omega$) is positive definite by construction and defines an inner product $(-,-)$. The Hilbert space H_ω, then, is the completion of A/N_ω in the corresponding norm.

2. The representation $\pi_\omega(A)$ is initially defined on $A/N_\omega \subset H_\omega$ by

$$\pi_\omega(a)[b] := [ab]. \tag{3.18}$$

   It is trivial that π_ω is linear and satisfies $\pi_\omega(ab) = \pi_\omega(a)\pi_\omega(b)$; to prove that $\pi_\omega(a)^* = \pi_\omega(a^*)$, take inner products with vectors $[b]$ and $[c]$ in A/N_ω. The technical point of the proof, which we omit, is that each $\pi_\omega(a)$ is well defined and *bounded* on A/N_ω, so that it may be extended to all of H_ω by continuity.

3. If A has a unit, define $\Omega_\omega = [1]$; then (3.16) follows by a simple computation.[44]

The GNS-construction simplifies when ω is **faithful** in that $\omega(a^*a) = 0$ iff $a = 0$; since N_ω is zero, H_ω is just the completion of A in the inner product $(a,b) = \omega(a^*b)$.

[42] Here $\overline{\pi(A)\Omega}$ is the closure of the linear span of the subset $\{\pi(a)\Psi, a \in A, \Psi \in H\}$ of H.

[43] Named after three founding fathers of the field: I.M. Gelfand, M. Naimark, and I.E. Segal.

[44] If A has no unit, the GNS-construction is applied to the unitization $\dot{A}$ of A (see footnote 33), in terms of the state $\dot{\omega}$ on $\dot{A}$ given by $\dot{\omega}(a,z) = \omega(a) + z$. The representation $\pi_\omega(A)$ is then simply the restriction of $\pi_{\dot{\omega}}(\dot{A})$ to A. Alternatively, one may use a so-called approximate unit of A.

3.10 Easy examples of the GNS-construction

• Let $A = D_n$ be the diagonal $n \times n$ matrices, and let ψ be the state (3.10). Then N_ψ consists of all $a = \mathrm{diag}(a_1, \ldots, a_n)$ for which $\psi(a^*a) = \sum_{i=1}^n |\Psi_i|^2 |a_i|^2 = 0$. Hence each component $\Psi_j = 0$ (if it exists) kills the corresponding j'th copy of $\mathbb{C}$ in passing from $A \cong \mathbb{C}^n$ to $H_\psi = A/N_\psi$, for if $\Psi_j = 0$, then $\mathrm{diag}(0, \ldots, 0, a_j, 0, \ldots, 0) \in N_\psi$. It follows that $H_\psi = \mathbb{C}^m$, where $m \leq n$ is the number of i for which $\Psi_i \neq 0$, with the peculiar inner product $(z, w) = \sum_i |\Psi_i|^2 \overline{z}_i w_i$. However, the map $u : H_\psi \to \mathbb{C}^m$, given by $u(z_i) = \Psi_i z_i$, is clearly unitary for the usual inner product on $\mathbb{C}^m$, and the resulting representation π_ψ on $\mathbb{C}^m$ is simply given by $\pi_\psi(a) z_i = a_i z_i$. The cyclic vector Ω_ψ in H_ψ is $(1, \ldots, 1)$, whose image in $\mathbb{C}^m$ under u is simply Ψ itself *with zeros omitted*. If $\psi_i = e_j$ for $i = j$ and zero otherwise, then $H_\psi = \mathbb{C}$. If, on the other hand, $\Psi_i \neq 0$ for all i, then $H_\psi = \mathbb{C}^n$, and π_ψ recovers the defining representation.

• The previous example (reinterpreted as $D_n = C(\underline{n})$) generalizes to arbitrary commutative C^*-algebras $A = C_0(X)$; cf. §3.4. Seen as a state, a probability measure μ is on X induces the sesquilinear form $(f, g)_0 = \int_X d\mu(x)\, \overline{f(x)} g(x)$ on A, so that $H_\mu = L^2(X, \mu)$ and $\pi_\mu(f)\Psi(x) = f(x)\Psi(x)$. The cyclic vector Ω_μ is the function identically equal to 1; we verify $(\Omega_\mu, \pi_\mu(f)\Omega_\mu) = \int_X d\mu(x)\, f(x) = \mu(f)$. If $\mu = \delta_x$, i.e., $\mu(f) = f(x)$, then $H_\mu = \mathbb{C}$ with $\pi_{\omega_x}(f) = f(x)$. In the opposite case, the support of μ is X, as is typically the case for $d\mu(x) = |\Psi(x)|^2 d^n x$, see (3.11).

• For a noncommutative example, take $A = M_n(\mathbb{C})$, with a state necessarily of the form $\omega_\rho(a) = \mathrm{Tr}\,(\rho a)$, for some density matrix ρ. Writing N_ρ for N_{ω_ρ}, etc., it follows that $N_\rho = \{a \in A \mid \mathrm{Tr}\,(\rho a^* a) = 0\}$. If we expand $\rho = \sum_i \lambda_i p_i$ (cf. §2.10), and for simplicity assume that $p_i = |e_i\rangle\langle e_i|$ with respect to the standard basis (e_i) of $\mathbb{C}^n$, then once again two cases of special interest arise:

1. If $\rho = |e_j\rangle\langle e_j|$ is pure, the null space is $N_\rho = \{a \in A \mid a e_j = 0\}$. Hence $a \in N_\rho$ iff the j'th column $C_j(a)$ of a vanishes, so that $a - b \in N_\rho$ iff $C_j(a) = C_j(b)$. Thus the equivalence class $[a] \in A/N_\rho$ may be identified with $C_j(a)$, so that $H_\rho = \mathbb{C}^n$ with the standard inner product. Indeed, representing $z \in \mathbb{C}^n$ by a matrix a with $C_j(a) = z$ and zeros elsewhere, and likewise $C_j(b) = w$, we have (no sum over j):

$$(z, w) = ([a], [b]) = \rho(a^* b) = \sum_i \overline{a_{ij}} b_{ij} = \sum_i \overline{z}_i w_i = (z, w).$$

Similarly, (3.18) reads $\pi_\rho(a) w_i = [ab]_i = \sum_k [a_{ik} b_{kj}] = \sum_k a_{ik} w_k$, or $\pi_\rho(a) w = aw$. The cyclic vector Ω_ρ is $[1_n] = e_j$. More generally, for a pure state ψ the GNS-representation $\pi_\psi(M_n(\mathbb{C}))$ induced by ψ is equal to the defining representation on $\mathbb{C}^n$, with cyclic vector $\Omega_\psi = \Psi$. To verify (3.16), $(\Omega_\psi \pi_\psi(a) \Omega_\psi) = (\Psi, a\Psi) = \psi(a)$.

2. If $\lambda_i > 0$ for all i (as in an equilibrium state $\rho = Z^{-1} \exp(-\beta h)$, where $Z = \mathrm{Tr} \exp(-\beta h)$ for some Hamiltonian h), then $N_\rho = 0$ and $H_\rho = M_n(\mathbb{C})$, equipped with the inner product $(a, b) = \mathrm{Tr}\,(\rho\, a^* b)$. The GNS-representation is given by $\pi_\rho(a) b = ab$, with $\Omega_\rho = 1_n$; note that $\|\Omega_\rho\|^2 = (1_n, 1_n) = \mathrm{Tr}\,(\rho) = 1$. The unitary transformation $u(a) = a\rho^{1/2}$ maps H_ρ into $M_n(\mathbb{C})$ with inner product $(a, b) = \mathrm{Tr}\,(a^* b)$, with inverse $u^*(b) = b\rho^{-1/2}$. For the corresponding representation $\tilde{\pi}_\rho = u \pi_\rho u^*$, we obtain $\tilde{\pi}_\rho(a) b = ab$, too. The cyclic vector in $M_n(\mathbb{C})$ becomes $\tilde{\Omega}_\rho = u\Omega_\rho = \rho^{1/2}$; note that $(\tilde{\Omega}_\rho, \tilde{\pi}_\rho(a) \tilde{\Omega}_\rho) = \mathrm{Tr}\, \rho^{1/2} a \rho^{1/2} = \mathrm{Tr}\,(\rho a)$, verifying (3.16).

3.11 Irreducible representations and pure states

As for group representation, there is a natural notion of irreducibility for C^*-algebras.

Definition 3.18 *A representation $\pi : A \to B(H)$ is called* **irreducible** *when H has no nontrivial closed subspaces stable under $\pi(A)$. In other words, if $K \subset H$ is a closed subspace such that $\pi(a)\Psi \in K$ for all $a \in A$, $\Psi \in K$, then $K = 0$ or $K = H$.*

If π is *not* irreducible, then we do have such a subspace K, and since $\pi(a^*) = \pi(a)^*$ it follows that also $K^\perp$ is stable under π. Thus we may *reduce* $H = K \oplus K^\perp$, with $\pi(A)K^{(\perp)} \subset K^{(\perp)}$. For example, the defining representation of $A = M_n(\mathbb{C})$ is irreducible, but its restriction to D_n is not: each subspace $\mathbb{C} \cdot e_i$ is stable under D_n.

Proposition 3.19 *The following conditions on $\pi : A \to B(H)$ are equivalent:*

1. *π is irreducible;*
2. *Each nonzero vector $\Omega \in H$ is cyclic;*
3. *$\pi(A)' = \mathbb{C} \cdot 1$, or, equivalently, $\pi(A)'' = B(H)$.*

To get some idea of the proof, if $\pi(A)' \neq \mathbb{C} \cdot 1$, then $\pi(A)'$ contains a nontrivial projection p (since it is a von Neumann algebra), and hence $K = pH$ is stable under A. This proves $\neg 3 \Rightarrow \neg 1$ and hence $1 \Rightarrow 3$. The rest of the proof is a useful exercise.

There is a beautiful characterization of irreducibility of GNS-representations.

Theorem 3.20 *The GNS-representation $\pi_\omega(A)$ is irreducible iff ω is pure.*

We just prove the easy direction. When ω is pure yet $\pi_\omega(A)$ reducible, there is a *nontrivial* projection $p \in \pi_\omega(A)'$. If $p\Omega_\omega = 0$, then $ap\Omega_\omega = pa\Omega_\omega = 0$ for all $a \in A$, so that $p = 0$, since π_ω is cyclic. $p\Omega_\omega \neq 0$. Similarly, $p^\perp\Omega_\omega \neq 0$ (with $p^\perp = 1 - p$). But in that case $\omega = \lambda\psi + (1 - \lambda)\psi^\perp$, where ψ is the **vector state**

$$\psi(a) = (\Psi, \pi_\omega(a)\Psi) \tag{3.19}$$

defined by the unit vector $\Psi := p\Omega_\omega / \|p\Omega_\omega\|$, the state $\psi^\perp$ is defined likewise by the unit vector $\Psi^\perp := p^\perp\Omega_\omega / \|p^\perp\Omega_\omega\|$, and $\lambda = \|p^\perp\Omega_\omega\|^2 \notin \{0, 1\}$. Hence ω is mixed.

The following result applies to general representations, but it is particularly useful for irreducible ones. We say that two representations $\pi_1 : A \to B(H_1)$ and $\pi_2 : A \to B(H_2)$ are **equivalent** ($\pi_1 \cong \pi_2$) if there is a unitary operator $u : H_1 \to H_2$ intertwining π_1 and π_2, in the sense that $\pi_2(a) = u\pi_1(a)u^*$ for all $a \in A$.

Proposition 3.21 *If $\pi : A \to B(H)$ has a cyclic vector Ω, then the GNS-representation induced by the vector state $\omega(a) = (\Omega, \pi(a)\Omega)$ is equivalent to π.*

Indeed, initially define $u : H_\omega \to H$ on $\pi_\omega(A)\Omega_\omega$ by $u\pi_\omega(a)\Omega_\omega = \pi(a)\Omega$, and extend u to all of H_ω by continuity (since $\overline{\pi_\omega(A)\Omega_\omega} = H_\omega$). This u intertwines π_ω and π.

So if π is irreducible, *each* unit vector in H defines a GNS-representation equivalent to the given one. Another corollary of Proposition 3.21 is that if one has two cyclic representations π_i with cyclic vectors Ω_i ($i = 1, 2$) such that the equality $(\Omega_1, \pi_1(a)\Omega_1) = (\Omega_2, \pi_2(a)\Omega_2)$ holds for all $a \in A$, then π_1 and π_2 are equivalent.

3.12 Primary states

Pure *states* are states about which everything possible is known. To recapitulate, combining Proposition 3.19 and Theorem 3.20, we have the equivalences

$$\omega \text{ pure} \leftrightarrow \omega \text{ has no nontrivial decomposition} \leftrightarrow \pi_\omega \text{ irreducible} \leftrightarrow \pi_\omega(A)' = \mathbb{C} \cdot 1.$$

In physics, one also has pure thermodynamical *phases*. These are mixed states described by so-called *primary states*, which yields an analogous chain of equivalences:

$$\begin{aligned} \omega \text{ primary} &\leftrightarrow \omega \text{ has no nontrivial decomposition into } \textit{disjoint} \text{ states} \\ &\leftrightarrow \pi_\omega \text{ factorial} \leftrightarrow \pi_\omega(A)' \cap \pi_\omega(A)'' = \mathbb{C} \cdot 1. \end{aligned}$$

The first double arrow states a definition, as does the last one, which says that the center of the von Neumann algebra $\pi_\omega(A)''$ is trivial. In general, the *center* of a von Neumann algebra M is $M \cap M'$, and M is called a *factor* if $M \cap M = \mathbb{C} \cdot 1$. Thus a representation $\pi(A)$ is *factorial* if the associated von Neumann algebra $\pi(A)''$ is a factor. If π is a direct sum of irreducible representations, then it is factorial iff all of these are equivalent, so that π is equivalent to some multiple n of a single irreducible representation π_ω. Factorial representations may arise in many other ways, though, because representations of C^*-algebras are rarely completely reducible.

To complete the definitions, we call two states ω_1 and ω_2 on A *disjoint*, *quasi-equivalent*, or *equivalent*, if the corresponding GNS-representations π_{ω_1} and π_{ω_2} have the said property. We know what equivalence means (cf. §3.11). For the other two, we first call some representation $\pi'(A)$ on a Hilbert space $H' \subset H$ a *subrepresentation* of a representation $\pi(A)$ on H, written $\pi' \subset \pi$, if $\pi' = \pi_{|H'}$. It follows that $\pi_1(A)$ and $\pi_2(A)$ have equivalent subrepresentations iff there exists a nonzero partial isometry $v : H_1 \to H_2$ such that $v\pi_1(a) = \pi_2(a)v$ for all $a \in A$.

Definition 3.22 *Two representations $\pi_1(A)$ and $\pi_2(A)$ are called:*

1. disjoint *if they do not have any equivalent subrepresentations;*[45]
2. quasi-equivalent *if every subrepresentation of π_1 has a subrepresentation that is equivalent to some subrepresentation of π_2, and* vice versa.[46]

Two factorial representations (and hence two primary states) are either disjoint or quasi-equivalent. In the completely reducible case $\pi_i \cong n_i \cdot \pi_{\omega_i}$, the latter occurs iff $\omega_1 \cong \omega_2$. The technical result underlying the above equivalences, then, is as follows:

Proposition 3.23 *For any state ω, if $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ for some $\lambda \in (0,1)$, then ω_1 and ω_2 are disjoint iff there is a projection $p \in \pi_\omega(A)' \cap \pi_\omega(A)''$ such that:*

$$\pi_\omega(A)_{|pH_\omega} \cong \pi_{\omega_1}(A); \tag{3.20}$$

$$\pi_\omega(A)_{|(1-p)H_\omega} \cong \pi_{\omega_2}(A). \tag{3.21}$$

The physical significance of primary states will be further analyzed in §4.4.

[45] In other words, there exists no representation of A that is equivalent both to some subrepresentation of π_1 and to some subrepresentation of π_2.

[46] Equivalently, π_1 has no subrepresentations disjoint from π_2, and *vice versa*. π_1 and π_2 are quasi-equivalent iff there is a (normal) isomorphism $\varphi : \pi_1(A)'' \to \pi_2(A)''$ of von Neumann algebras for which $\varphi(\pi_1(a)) = \pi_2(a)$ for all $a \in A$, and this is the case iff the set of states on A of the form $a \mapsto \mathrm{Tr}\,(\rho\pi_i(a))$, where ρ is a density matrix on H_i, is the same for $i = 1$ as it is for $i = 2$.

3.13 Characterization of C^*-algebras

Next to Theorem 3.4, the second most famous result about C^*-algebras (also due to Gelfand and Naimark) gives a complete characterization of them.

Theorem 3.24 *A C^*-algebra A admits an injective representation $\pi : A \to B(H)$ on some Hilbert space H. In other words, each C^*-algebra is isomorphic to a norm-closed *-algebra in $B(H)$, for some Hilbert space H.*

Given a state ω on A, the GNS-construction provides us with a representation $\pi_\omega : A \to B(H_\omega)$. If this representation were injective, we would be finished, but firstly we do not know that any state exists on A at all, and secondly we have no guarantee that π_ω is indeed injective. The first problem is quickly resolved: for any normal $a \in A$ and $\lambda \in \sigma(a)$, there is a state ω_λ on A for which $\omega_\lambda(a) = \lambda$. To prove this, start by constructing ω_λ on $C^*(a)$ (as in §3.5), and rely on the Hahn–Banach Theorem of functional analysis (i.e., on the Axiom of Choice) to extend ω to all of A. Since $\sigma(a)$ is closed, there is a $\lambda \in \sigma(a)$ for which the spectral radius $r(a)$ equals $|\lambda|$. For this λ, we therefore have $|\omega_\lambda(a)| = |\lambda| = r(a) = \|a\|$. This proves:

Lemma 3.25 *For any selfadjoint element $a \in A$ (i.e., $a^* = a$), there exists a state ω_a on A such that $|\omega_a(a)| = \|a\|$.*

To solve the second problem, we introduce the **universal representation**[47]

$$H_u := \oplus_{\omega \in S(A)} H_\omega; \tag{3.22}$$

$$\pi_u(A) := \oplus_{\omega \in S(A)} \pi_\omega(A). \tag{3.23}$$

The Hilbert space H_u will be the H in the statement of Theorem 3.24. To prove that $\pi = \pi_u$ is injective, take some fixed $\rho \in S(A)$, and define the vector Ω as having components $\Omega_\omega = 0$ for $\omega \neq \rho$, and Ω_ρ equal to the cyclic vector of the GNS-construction for ρ. This vector clearly lies in H_u. Then $(\pi_u(a)\Omega)_\omega = \pi_\omega(a)\Omega_\rho$ for $\omega = \rho$, and zero otherwise. Now suppose that $\pi_u(a) = 0$ for some $a \in A$. Then $\pi_u(a)\Omega = 0$, hence $\pi_\rho(a)\Omega_\rho = 0$, hence $\|\pi_\rho(a)\Omega_\rho\|^2 = \rho(a^*a) = 0$ by the GNS-construction. Taking $\rho = \omega_{a^*a}$, Lemma 3.25 (with a^*a instead of a) implies

$$\|a\|^2 = \|a^*a\| = \omega_{a^*a}(a^*a) = 0.$$

Hence $a = 0$, so that π_u is injective. This concludes the proof of Theorem 3.24.[48]

Each C^*-algebra A has an **enveloping von Neumann algebra** $\pi_u(A)'' \subset B(H_u)$. An element $b \in \pi_u(A)''$ defines a linear map $\hat{b} : S(A) \to \mathbb{C}$ by $\hat{b}(\omega) = (\Omega_\omega, b\Omega_\omega)$, where $\Omega_\omega \in H_\omega \subset H_u$. Recalling that $S(A) \subset A^*$, this extends to a continuous map $\hat{b} : A^* \to \mathbb{C}$ (indeed, $\|\hat{b}\| = \|b\|_{B(H_u)}$). Hence $\hat{b} \in A^{**}$, and the ensuing map $b \mapsto \hat{b}$ from $\pi_u(A)''$ to A^{**} turns out to be an isomorphism of Banach spaces.

[47] If (H_i) is a family of Hilbert spaces, then $H = \bigoplus H_i$ consists of all sequences (Ψ_i) with $\Psi_i \in H_i$ and $\sum_i \|\Psi_i\|^2_{H_1} < \infty$, with componentwise linear structure (if the index set is uncountable, the sums are defined as in §2.4). Writing $\sum_i \Psi_i$ for (Ψ_i), the inner product on H is given by $(\sum_i \Psi_i, \sum_j \Phi_j) = \sum_i (\Psi_i, \Phi_i)_{H_i}$. If $\pi_i : A \to B(H_i)$ are representations of A, the **direct sum** $\pi = \bigoplus \pi_i$ on $H = \bigoplus H_i$ is defined by $\pi(a) \sum_i \Psi_i = \sum_i \pi_i(a)\Psi_i$, where $\Psi_i \in H_i$.

[48] It should be noted that H_u is often larger than necessary. For $A = M_n(\mathbb{C})$, for example, any vector state in $\mathbb{C}^n$ already gives rise to an injective representation, namely the defining one.

4 Symmetry breaking in quantum theory

We now apply the abstract formalism above to concrete quantum systems [5, 10, 13, 20, 38, 40, 41, 42, 45, 49]. The C^*-algebra A plays the role of the 'algebra of observables' of some quantum system (i.e., its observables will be the self-adjoint elements of A). If $A = B(H)$, all (self-adjoint) operators on H are deemed observable: we are typically dealing with a 'small' quantum system, without any restriction on what can be observed (in the lab). In large systems, on the other hand, we impose the restriction that the observables be *localized* in finite regions [13].

The simplest large systems are defined on a lattice $\mathbb{Z}^d$ in d-dimensional space, with some finite-dimensional Hilbert space $H_0 \cong \mathbb{C}^n$ associated to each site $x \in \mathbb{Z}^d$. For example, in order to describe magnetism one takes $H_0 = \mathbb{C}^2$, assuming that each site of some crystal lattice is occupied by an immobile electron (or other spin-$\frac{1}{2}$ particle) whose only degree of freedom is its spin. Thus the algebra of observables of a single site x is just $A_x = B(H_0) \cong M_n(\mathbb{C})$. For any *finite* subset $\Lambda \subset \mathbb{Z}^d$, put

$$A(\Lambda) = \otimes_{x\in\Lambda} A_x = \otimes_{x\in\Lambda} B(H_0) \cong B(\otimes_{x\in\Lambda} H_0) \equiv B(H_\Lambda). \tag{4.1}$$

If $a \in B(H_0)$ and $y \in \Lambda$, we write $a(y)$ for the element $\otimes_{x\in\Lambda} c_x$ of $A(\Lambda)$ with $c_y = a$ and $c_x = 1$ (i.e., the unit of $B(H_0)$) for all $x \neq y$. The product $a(y)b(z)$ in $A(\Lambda)$ is $\otimes_{x\in\Lambda} d_x$, with $d_y = ab$ and $d_x = 1$ for all $x \neq y$ whenever $y = z$, whereas if $y \neq z$, then $d_y = a$, $d_z = b$, and $d_x = 1$ for all $x \neq y$ and $x \neq z$ (linear combinations of $a(y)$ and $b(z)$ are not of this 'elementary tensor' form, however). Clearly, for all a, b,

$$[a(x), b(y)] = 0 \text{ if } x \neq y. \tag{4.2}$$

Then $A(\Lambda)$ consists of all polynomials in such elements, where y varies over Λ and a varies over $B(H_0)$. Each $A(\Lambda)$ is a C^*-algebra through the identifications in (4.1).

For $\Lambda \subset \tilde{\Lambda}$ (both finite) we have an inclusion $A(\Lambda) \subset A(\tilde{\Lambda})$, defined on the generators $a(y)$, $y \in \Lambda$, by saying that $a(y) \in A(\tilde{\Lambda})$ is the element $\otimes_{x\in\tilde{\Lambda}} \tilde{c}_x$ of $A(\Lambda)$ with $\tilde{c}_x = 1$ for all $x \neq y$ and $\tilde{c}_y = a$. Physically, this means that an observable localized in Λ stays the same if we extend the region (but not the observable). Hence the set-theoretic union $A_{\rm loc} = \cup_\Lambda A(\Lambda)$ over all *finite* regions Λ is well-defined, consisting of all operators that are localized in *some* finite Λ. Thus $A_{\rm loc}$ inherits all algebraic operations as well as the norm of the $A(\Lambda)$, but it fails to be complete in that norm and hence—unlike the $A(\Lambda)$— it is not a C^*-algebra. The completion

$$A = \overline{A_{\rm loc}} \equiv \overline{\cup_\Lambda A(\Lambda)} \tag{4.3}$$

in the underlying norm is the *C^*-algebra of quasi-local observables* of the given system. It contains all $A(\Lambda)$, but also certain other elements that by definition can be approximated (in norm) by localized operators.[49] The *Einstein locality* condition

$$[A(\Lambda_1), A(\Lambda_2)] = 0 \text{ if } \Lambda_1 \cap \Lambda_2 = \emptyset,\ A(\Lambda_i) \subset A, \tag{4.4}$$

then follows from (4.2). For lattice systems the sharper condition $A(\Lambda)' = A(\Lambda')$ (*Haag duality*) holds (cf. [42, Prop. IV.1.6]), where the left-hand side denotes the commutant of $A(\Lambda)$ in A, and the right-hand side means $A(\mathbb{Z}^d\backslash\Lambda) \equiv \overline{\cup_{\Lambda_1\subset\mathbb{Z}^d\backslash\Lambda} A(\Lambda_1)}$.

[49] Compare (4.3) with the definition of the commutative C^*-algebra $C_0(\mathbb{R}^n)$ as the completion of $\cup_O C_c(O)$, where $O \subset \mathbb{R}^n$ is open, and $C_c(O) \subset C_c(O')$ for $O \subset O'$ by extension with value zero.

4.1 Symmetry in elementary quantum mechanics

In elementary quantum mechanics in a Hilbert space H, in which the algebra of observables is simply taken to be the C^*-algebra $B(H)$, the concept of symmetry revolves around the mathematical notion of a unitary operator $u : H \to H$. Physically, however, unitary operators play (at least) three conceptually distinct roles, namely as symmetries of: *1. pure states*, *2. general states*, and *3. observables*.

Ad 1. Since pure states are unit vectors *up to a phase*, the pure state space of an elementary quantum system is the *projective* Hilbert space $\mathbb{P}\mathcal{H}$, defined as $\mathbb{P}\mathcal{H} = \{\Psi \in H \mid \|\Psi\| = 1\}/\sim$, where $\Phi \sim \Psi$ iff $\Psi = z\Phi$ for some $z \in \mathbb{C}$, $|z| = 1$. The defining action of a unitary operator u on H descends to an action $u_P : \mathbb{P}\mathcal{H} \to \mathbb{P}\mathcal{H}$, which, like u itself, is clearly a bijection, with inverse $(u_P)^{-1} = (u^{-1})_P$. Moreover, the physically relevant structure on $\mathbb{P}\mathcal{H}$ that is preserved by u_P so as to qualify as a symmetry, is that of a *transition probability*. This is a map $P : \mathbb{P}\mathcal{H} \times \mathbb{P}\mathcal{H} \to [0, 1]$, given by $P(\psi, \varphi) = |(\Psi, \Phi)|^2$, where we have denoted the image of $\Psi \in H$ in $\mathbb{P}\mathcal{H}$ by ψ, etc. Unitarity immediately gives $P(u_P(\psi), u_P(\varphi)) = P(\psi, \varphi)$. Conversely, *Wigner's Theorem* [6] states that any bijection of $\mathbb{P}\mathcal{H}$ that preserves transition probabilities is necessarily of the form u_P, for some unitary *or anti-unitary* operator $u : H \to H$.

Ad 2. In elementary quantum mechanics on H, states are density matrices on H. Denoting the set of all density matrices on H by $\mathbb{S}\mathcal{H}$, a unitary u on H defines a map $u_S : \mathbb{S}\mathcal{H} \to \mathbb{S}\mathcal{H}$ by $u_S(\rho) = u\rho u^*$. This is a bijection (with inverse $(u_S)^{-1} = (u^{-1})_S$), which moreover is *affine* in the sense for each $\lambda \in (0, 1)$ and $\rho_1, \rho_2 \in \mathbb{S}\mathcal{H}$ one has

$$u_S(\lambda\rho_1 + (1 - \lambda)\rho_2) = \lambda u_S(\rho_1) + (1 - \lambda)u_S(\rho_2). \tag{4.5}$$

Thus u_S is an *affine bijection* of the state space $\mathbb{S}\mathcal{H}$. Conversely, a straightforward extension of Wigner's Theorem (cf. [6]) states that each affine homeomorphism of $\mathbb{S}\mathcal{H}$ is necessarily of the form u_S, for some unitary *or anti-unitary* operator $u : H \to H$.

Ad 3. An *automorphism* of the C^*-algebra $B(H)$ of observables is an invertible homomorphism $\alpha : B(H) \to B(H)$ (i.e., α is linear, $\alpha(ab) = \alpha(a)\alpha(b)$, and $\alpha(a^*) = \alpha(a)^*$). Clearly, each unitary $u : H \to H$ defines an automorphism $\alpha_u : B(H) \to B(H)$ by putting $\alpha_u(a) = uau^*$. Conversely, Kadison proved that each automorphism of $B(H)$ is of the form α_u, for some *unitary* $u : H \to H$ (cf. [4]). To find a place for anti-unitary operators, look at $B(H)_{sa} = \{a \in B(H) \mid a^* = a\}$ as a *real* vector space, equipped with the *Jordan product* $a \circ b = \frac{1}{2}(ab + ba)$. A *Jordan isomorphism* of $B(H)$ is an invertible *real*-linear map $\alpha : B(H)_{sa} \to B(H)_{sa}$ that preserves the Jordan product (or, equivalently, preserves squares in that $\alpha(a^2) = \alpha(a)^2$). Kadison's (extended) Theorem then states that any Jordan isomorphism of $B(H)$ is of the form α_U, where $u : H \to H$ is either unitary or anti-unitary.

In conclusion, though conceptually quite different, each of the three notions of symmetry in quantum mechanics we discussed is reducible to the action of a unitary or anti-unitary operator on H, so that they are equivalent to one another. For example, the restriction of u_S to $\mathbb{P}\mathcal{H}$ is u_P, which in turn has a unique extension to an affine bijection of $\mathbb{S}\mathcal{H}$, and u_S and α_U are related by $\mathrm{Tr}\,(u_S(\rho)a) = \mathrm{Tr}\,(\rho\alpha_{u^*}(a))$.

4.2 Symmetry in algebraic quantum theory

We now generalize the preceding discussion to the case where the observables form an arbitrary C^*-algebra A. Once again, we distinguish three notions of symmetry.

1. Pure states. Let $P(A)$ be the pure state space of A. The notion of a transition probability may be defined as a function $P : P(A) \times P(A) \to [0, 1]$, given by [36]

$$P(\rho, \sigma) = 1 - \tfrac{1}{4}\|\rho - \sigma\|^2. \tag{4.6}$$

This definition has two attractive features. First, if ρ and σ are equivalent, we may assume, without loss of generality, that the GNS-representations π_ρ and π_σ are defined on the same Hilbert space, which, then, contains both cyclic vectors Ω_ρ and Ω_σ. In that case, $P(\rho, \sigma) = |(\Omega_\rho, \Omega_\sigma)|^2$. Second, if ρ and σ (and hence π_ρ and π_σ) are inequivalent, we have $P(\rho, \sigma) = 0$. Thus we would like to define a symmetry of $P(A)$ as a bijection $\upsilon_P : P(A) \to P(A)$ that satisfies $P(\upsilon_P(\psi), \upsilon_P(\varphi)) = P(\psi, \varphi)$. However, in order to prove that our three notions of symmetry are equivalent, we require υ_P to be *uniformly continuous* with respect to the weak*-topology on $P(A)$ inherited from the dual A^* (in which $\omega_n \to \omega$ iff $|\omega_n(a) - \omega(a)| \to 0$ for each $a \in A$).

2. General states. A symmetry of the state space $S(A)$ is defined as an affine homeomorphism $\upsilon_S : S(A) \to S(A)$ with respect to the weak*-topology; see (4.5).

3. Observables. A symmetry of A itself is a *Jordan isomorphism* of A, that is, an invertible *real*-linear map $\alpha : A_{sa} \to A_{sa}$ such that $\alpha(a \circ b) = \alpha(a) \circ \alpha(b)$. A special case of this is an *automorphism* $\alpha : A \to A$, which is (the restriction of) an invertible *complex*-linear map satisfying $\alpha(ab) = \alpha(a)\alpha(b)$, and $\alpha(a^*) = \alpha(a)^*$.

Theorem 4.1 *Let A be a C^*-algebra. There is a bijective equivalence between:*

- *uniformly continuous bijections of $P(A)$ that preserve* (4.6)*;*
- *affine homeomorphisms of $S(A)$;*
- *Jordan isomorphisms of A:*

1. *A Jordan isomorphism $\alpha : A_{sa} \to A_{sa}$ defines an affine homeomorphism $\alpha^* : S(A) \to S(A)$ by (complex linear extension of) $\alpha^*\omega(a) = \omega(\alpha^{-1}(a))$. Conversely, for every affine homeomorphism $\varphi : S(A) \to S(A)$ there is a unique Jordan isomorphism $\alpha : A_{sa} \to A_{sa}$ such that $\varphi = \alpha^*$.*

2. *The restriction of an affine homeomorphism $\alpha^* : S(A) \to S(A)$ to the pure states $P(A) \subset S(A)$ is a uniformly continuous bijection of $P(A)$ preserving* (4.6)*. Conversely, every uniformly continuous bijections of $P(A)$ preserving* (4.6) *has a unique extension to an affine homeomorphism of $S(A)$.*

The conclusion is the same as for elementary quantum mechanics: our three notions of symmetry are equivalent,[50] but in general there is no unitary operator to impose this equivalence. So what is the technical link between symmetry and unitarity?

[50]The only easy part is the passage from α to α^*. The reason why $\varphi_{|P(A)}$ preserves transition probabilities is that $P(\rho, \sigma) = \inf\{\rho(a), a \in A_{sa}, 0 \leq a \leq 1, \sigma(a) = 1\}$, so that (4.6) follows from the convex structure of $S(A)$. The extension of $\upsilon_P : P(A) \to P(A)$ to $S(A)$ relies on the Krein–Milman Theorem , according to which $S(A)$ is the convex hull of $P(A)$. See [20] for all this.

4.3 Unitary implementation of symmetries

From now on, we will only deal with the special class of symmetries that are given by *automorphisms* of A; this excludes Jordan isomorphisms that satisfy $\alpha(ab) = \alpha(b)\alpha(a)$ for some a, b (for $A = B(H)$, this corresponds to looking at *unitary* operators alone). One reason for this restriction is that we often deal with a *symmetry group* G of A, that is, we have a group homomorphism $\alpha : G \to \mathrm{Aut}(A)$, where $\mathrm{Aut}(A)$ is the group of all automorphisms of A. We will write α_g for $\alpha(g)$ and say that G is an *automorphism group of* G. Now, if G is a connected Lie group, $g \in G$ may be connected to the unit $e \in G$ by a continuous path. Since the unit corresponds to $\alpha_e = \mathrm{id}$, which maps every $a \in A$ to itself, α_e is clearly an automorphism. Requiring continuity of α (in the sense that for each fixed $a \in A$ the map $g \mapsto \alpha_g(a)$ from G to A is continuous) then forces each α_g to be an automorphism.

A homomorphism $\alpha : G \to \mathrm{Aut}(B(H))$ is always given by a family u_g of unitary operators on H, in that $\alpha_g(a) = u_g a u_g^*$ for all $g \in G$. The property $\alpha_g \alpha_h = \alpha_{gh}$ does not necessarily enforce $u_g u_h = u_{gh}$ (for one may have a 'projective' unitary representation $g \mapsto u_g$ of G on H), but one may always pass to a central extension $\overline{G}$ of G for which this problem does not arise (e.g., $\overline{SO(3)} = SU(2)$). In Theorem 4.4 below (describing unbroken symmetry), even such a passage is not necessary.

For general C^*-algebras A (especially those modeling large quantum systems), one rarely has $\alpha(a) = uau^*$ for some $u \in A$ even for single automorphisms α, let alone for a whole group of them. What may happen, however, is the following.

Definition 4.2 *Let $\pi : A \to B(H)$ be a representation of A. An automorphism $\alpha : A \to A$ is* implemented *in π if there exists a unitary operator $u : H \to H$ with*

$$\pi(\alpha(a)) = u\pi(a)u^* \quad \textit{for all } a \in A. \tag{4.7}$$

Theorem 4.3 *An automorphism $\alpha : A \to A$ can be implemented in the GNS-representation π_ω defined by a state ω on A iff $\pi_{\alpha^*\omega}$ and π_ω are equivalent.*

Whether or not this is true, define $w : H_\omega \to H_{\alpha^*\omega}$ by $w\pi_\omega(a)\Omega_\omega = \pi_{\alpha^*\omega}(\alpha(a))\Omega_{\alpha^*\omega}$. This operator is well defined and unitary, and satisfies $w\Omega_\omega = \Omega_{\alpha^*\omega}$ as well as $w\pi_\omega(a)w^* = \pi_{\alpha^*\omega}(\alpha(a))$; these properties even characterize w. If $\pi_{\alpha^*\omega} \cong \pi_\omega$, there exists a unitary $v : H_\omega \to H_{\alpha^*\omega}$ satisfying $v\pi_\omega(a)v^* = \pi_{\alpha^*\omega}(a)$, $a \in A$. Then $u = v^*w$ satisfies (4.7) for $\pi = \pi_\omega$. The converse is similar. An important special case is:

Theorem 4.4 *Suppose that $\alpha^*\omega = \omega$, that is, $\omega(\alpha(a)) = \omega(a)$ for all $a \in A$. Then α can be implemented by a unitary operator $u : H_\omega \to H_\omega$ satisfying $u\Omega_\omega = \Omega_\omega$. In particular, if G is a continuous automorphism group of A and $\alpha_g^*\omega = \omega$ for all $g \in G$, we obtain a family of unitaries $u_g : H_\omega \to H_\omega$ that for all $g \in G$ satisfy*

$$u_g\Omega_\omega = \Omega_\omega; \tag{4.8}$$

$$\pi_\omega(\alpha_g(a)) = u_g\pi_\omega(a)u_g^*, \tag{4.9}$$

and form a continuous unitary representation of G on H_ω, in that $u_e = 1$, $u_g u_h = u_{gh}$, and the function $g \mapsto u_g\Psi$ is continuous from G to H_ω for each fixed $\Psi \in H_\omega$.

For fixed α, one easily shows that the operator defined by $u\pi_\omega(a)\Omega_\omega = \pi_\omega(\alpha(a))\Omega_\omega$ does the job. For α_g, $g \in G$, it is a similar exercise to check the claims.

4.4 Cluster properties

Through the associated GNS-representation $\pi_\omega : A \to B(H_\omega)$, a state ω on a quasi-local C^*-algebra A as in (4.3) defines two interesting subalgebras of $B(H_\omega)$:

- the *center* $A^c_\omega := \pi_\omega(A)'' \cap \pi_\omega(A)'$;
- the *algebra at infinity* $A^\infty_\omega := \cap_\Lambda \pi_\omega(A(\Lambda'))''$, with $A(\Lambda') = \overline{\cup_{\Lambda_1 \subset \mathbb{Z}^d \setminus \Lambda} A(\Lambda_1)}$.

It is easy to show from locality (4.4) that $A^\infty_\omega \subseteq A^c_\omega$. If one also has Haag duality $A(\Lambda)' = A(\Lambda')$ and if each $A(\Lambda)$ and hence A is simple, then one also has the opposite inclusion, so that $A^\infty_\omega = A^c_\omega$. This is the case, for example, If H_0 and hence each $A(\Lambda)$ are finite-dimensional; see [42, Thm. IV.1.7] for a complete proof.

The algebra at infinity (and hence the center) is home to the *macroscopic observables* in π_ω, such as the average $w - \lim_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \sum_{x \in \Lambda} \pi_\omega(b(x))$ of some $b \in B(H_0)$, or, more generally of expressions like the left-hand side of (4.13) below. Therefore, if A^∞_ω is trivial, macroscopic observables are 'c-numbers', i.e., multiples of the unit operator. In particular, they do not fluctuate, which is among the defining properties of *pure* thermodynamic phases (cf. §3.12). So this is the case in particular when the center A^c_ω is trivial, in other words, when ω is *primary*.

The main result in this area, due to Lanford and Ruelle [24], is as follows.

Theorem 4.5 *A state ω on a C^*-algebra A of quasi-local observables (cf.* (4.3)*) has trivial algebra at infinity, i.e., $A^\infty_\omega = \mathbb{C} \cdot 1$, iff it is clustering, in that for all $a \in A$ and all $\varepsilon > 0$ there is a finite $\Lambda \subset \mathbb{Z}^d$ such that for all $b \in A(\Lambda')$, $\|b\| = 1$, one has*

$$|\omega(ab) - \omega(a)\omega(b)| \leq \varepsilon. \tag{4.10}$$

In particular, if ω is primary, then it is clustering and (4.10) *holds.*

The complete proof is quite technical [42, Cor. IV.1.8], but the main idea is as follows. Choose finite regions Λ_n moving to infinity (i.e., eventually avoiding any given Λ), and pick elements $c_n \in A(\Lambda_n)$, $\|c_n\| = 1$. The sequence $(\pi_\omega(c_n))$ in $B(H_\omega)$ has a weakly convergent subsequence,[51] with limit $c \in B(H_\omega)$.

- By von Neumann's Bicommutant Theorem 3.12,[52] we have $c \in \pi_\omega(A)''$.
- By locality (4.4) and the delocalization of the Λ_n, also $c \in \pi_\omega(A)'$.

Hence $c \in A^c_\omega$, and by a more refined argument (which is unnecessary if if $A^\infty_\omega = A^c_\omega$), even $c \in A^\infty_\omega$. So if $A^\infty_\omega = \mathbb{C} \cdot 1$ we have $c = (\Omega_\omega, c\Omega_\omega) \cdot 1$. On the other hand, we have $(\Omega_\omega, c\Omega_\omega) = \lim_n (\Omega_\omega, \pi_\omega(c_n)\Omega_\omega) = \lim_n \omega(c_n)$, so that we may compute

$$\lim_n \omega(ac_n) = \lim_n (\Omega_\omega, \pi_\omega(a)\pi_\omega(c_n)\Omega_\omega) = (\Omega_\omega, \pi_\omega(a)c\Omega_\omega) = \omega(a) \lim_n \omega(c_n).$$

Thus for any $\varepsilon > 0$ there is an N such that $|\omega(ac_n) - \omega(a)\omega(c_n)| \leq \varepsilon$ for all $n > N$. To derive (4.10) from this, an easy *reductio ad absurdum* argument suffices. The converse direction of Theorem 4.5 uses the technical Kaplansky Density Theorem.

[51] This follows from the Banach–Alaoglu Theorem of functional analysis, applied to $B(H_\omega)$ seen as the dual space of $B_1(H_\omega)$. On the unit ball, the corresponding weak*-topology on $B(H_\omega)$ coincides with the weak operator topology, so that the unit ball in $B(H_\omega)$ is weakly compact.

[52] The weak closure $\overline{M}$ of any unital *-algebra M in $B(H)$ then coincides with M''.

4.5 Uniqueness of translation-invariant states

Further clustering results follow if we equip A in (4.3) with an automorphic action $\tau : \mathbb{Z}^d \to \mathrm{Aut}(A)$ of $\mathbb{Z}^d$, defined as follows: for $x \in \mathbb{Z}^d$, define $\tau_x : A(\Lambda) \to A(x+\Lambda)$ by $\tau_x(a(y)) = a(x+y)$, using the notation explained below (4.1), and extend to $\tau_x : A \to A$ by continuity. The following property then holds:[53]

Definition 4.6 *An automorphic action τ of $\mathbb{Z}^d$ on a C^*-algebra A is (uniformly)* asymptotically abelian *if in the sense that $\lim_{x\to\infty}[a, \tau_x(b)] = 0$ for all $a, b \in A$.*

Theorem 4.7 *Let A be a C^*-algebra A equipped with an asymptotically abelian action τ of $\mathbb{Z}^d$, and let ω be a translation-invariant primary state on A (i.e., $\tau_x^*\omega = \omega$ for all $x \in \mathbb{Z}^d$). Then Ω_ω is the only translation-invariant vector in H_ω. Moreover,*[54]

$$\lim_{x\to\infty} \omega(a\tau_x(b)) = \omega(a)\omega(b); \tag{4.11}$$

$$w - \lim_{x\to\infty} \pi_\omega(\tau_x(b)) = \omega(b)\cdot 1; \tag{4.12}$$

$$w - \lim_{\Lambda\uparrow\mathbb{Z}^d} |\Lambda|^{-1} \sum_{x\in\Lambda} \pi_\omega(\tau_x(b)) = \omega(b)\cdot 1. \tag{4.13}$$

The proof is quite instructive: If ω is primary, $\lim_{x\to\infty} |\omega(a\tau_x(b)) - \omega(a)\omega(\tau_x(b))| = 0$ either from Theorem 4.5, or directly, from the same argument. Translation-invariance then yields (4.11). We then compute $\omega(a\tau_x(b))$ in terms of the projection

$$P_0 = s - \lim_{\Lambda\uparrow\mathbb{Z}^d} |\Lambda|^{-1} \sum_{x\in\Lambda} U(x) \tag{4.14}$$

onto the translation-invariant subspace of H_ω, where U is the unitary representation of $\mathbb{Z}^d$ on H_ω from Theorem 4.4 (with $G = \mathbb{Z}^d$).[55] Since $P_0\Omega_\omega = \Omega_\omega$, we have

$$\omega(a\tau_x(b)) = (\Omega_\omega, \pi_\omega(a)\pi_\omega(\tau_x(b))\Omega_\omega) = (\Omega_\omega, \pi_\omega(a)([\pi_\omega(\tau_x(b)), P_0] + P_0\pi_\omega(b))\Omega_\omega).$$

We now let $x \to \infty$, upon which the commutator vanishes, because the weak limit of $\pi_\omega(\tau_x(b))$ lies in the center of $\pi_\omega(A)''$, which is assumed trivial. The remaining term is compatible with (4.11) iff P_0 is one-dimensional, so that Ω_ω is the only translation-invariant vector in H_ω. A similar trick, now using $P_0 = |\Omega_\omega\rangle\langle\Omega_\omega|$, yields

$$\pi_\omega(\tau_x(b))\pi_\omega(a)\Omega_\omega = ([\pi_\omega(\tau_x(b)), \pi_\omega(a)] + \pi_\omega(a)([\pi_\omega(\tau_x(b)), P_0] + \omega(b)))\Omega_\omega.$$

Both commutators vanish (weakly) as $x \to \infty$, proving (4.12). Similarly, write

$$\pi_\omega(\tau_x(b))\pi_\omega(a)\Omega_\omega = ([\pi_\omega(\tau_x(b)), \pi_\omega(a)] + \pi_\omega(a)U(x)\pi_\omega(b))\Omega_\omega,$$

and use (4.14) and once again $P_0 = |\Omega_\omega\rangle\langle\Omega_\omega|$, to prove (4.13).

[53] The condition means that $\lim_{n\to\infty} \|[a, \tau_{x_n}(b)]\| = 0$ for any sequence (x_n) with $|x_n| \to \infty$.

[54] This time, (4.11) means that any sequence (x_n) with $|x_n| \to \infty$ has a subsequence (x_n') for which $\lim_{n\to\infty} \omega(a\tau_{x_n'}(b)) = \omega(a)\omega(b)$, and analogously for (4.12) in the weak operator topology on $B(H_\omega)$. The limit $\Lambda \uparrow \mathbb{Z}^d$ in (4.13) is meant (for example) to be taken along an increasingly largely sequence of hypercubes Λ_n whose number of points goes as $|\Lambda_n| \sim n^d$ for $n \to \infty$.

[55] Eq. (4.14) is a special case of von Neumann's L^2 ergodic theorem, which generalizes the Peter–Weyl–Schur relation $P_0 = \int_G dg\, U(g)$ for compact groups G to *amenable* groups like $\mathbb{Z}^d$ or $\mathbb{R}^d$.

4.6 Dynamics

In a quantum system with a finite-dimensional Hilbert space H_Λ, the algebra of observables is $A(\Lambda) = B(H_\Lambda)$; for example, one may have $H_\Lambda = \otimes_{x\in\Lambda} H_x$ with $H_x = H_0 = \mathbb{C}^n$ for all $x \in \Lambda \subset \mathbb{Z}^d$, as before. Dynamics is given by a Hamiltonian $h_\Lambda \in A(\Lambda)$, giving rise to an automorphism group $\alpha^\Lambda : \mathbb{R} \to \mathrm{Aut}(A(\Lambda))$ by

$$\alpha_t^\Lambda(a) = e^{ith_\Lambda} a e^{-ith_\Lambda}, \tag{4.15}$$

where $a \in A(\Lambda)$. In the situation (4.3), we would like to assemble the family α^Λ into a single automorphism group $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$, which describes the dynamics of the corresponding infinite quantum system. This can be done if:

1. The local Hamiltonians h_Λ are of the form $h_\Lambda = \sum_{X\subset\Lambda} \Phi(X)$, where the sum is over all sublattices X of Λ, with a 'potential' $\Phi(X) \in B(H_X) \subset B(H_\Lambda)$.

2. The limit of $\alpha_t^\Lambda(a)$ as $\Lambda \uparrow \mathbb{Z}^d$ (which may be taken to mean that one chooses increasingly large cubes Λ_n for Λ and lets $n \to \infty$) exists for each $a \in A(\Lambda')$ and each Λ'. This is the case for short-range interactions (such as the typical nearest-neighbour interactions of the Ising and Heisenberg models, see below.)

For nearest-neighbour interactions, $\Phi(X)$ is nonzero iff $X = \{x, y\}$ is a pair of neighbours, and in the presence of an external magnetic field one also has terms $\Phi(\{x\})$. For example, in the Ising model one has $H_0 = \mathbb{C}^2$ and $\Phi(\{x, y\}) = \sigma_3(x)\sigma_3(y)$; an external field gives rise to additional terms $\Phi(\{x\}) = B\sigma^{(i)}$ ($i = 1, 2$ or 3). In $d = 1$ with periodic boundary conditions and $i = 1$, the total Hamiltonian, then, is

$$h_\Lambda = -\sum_{x=1}^{|\Lambda|} (\sigma_3(x)\sigma_3(x+1) + B\sigma_1(x). \tag{4.16}$$

Similarly, the Heisenberg model for (anti)ferromagnetism is given by $H_0 = \mathbb{C}^2$ and

$$h_\Lambda = J\sum_{x=1}^{|\Lambda|}\sum_{i=1}^{3} \sigma_i(x)\sigma_i(x+1) \equiv J\sum_x \vec{\sigma}(x)\cdot\vec{\sigma}(x+1), \tag{4.17}$$

where $J < 0$ yields ferromagnetism, whereas $J > 0$ gives rise to anti-ferromagnetism.

In any case, if the limit in no. 2 exists, we write

$$\alpha_t(a) = \lim_{\Lambda\uparrow\mathbb{Z}^d} \alpha_t^\Lambda(a); \tag{4.18}$$

a simple approximation argument then shows that each map $\alpha_t : \cup_\Lambda A(\Lambda) \to \cup_\Lambda A(\Lambda)$ thus defined for fixed $t \in \mathbb{R}$, may be extended to a map $\alpha_t : A \to A$ by continuity (i.e., for general $a \in A$, one defines $\alpha_t(a)$ as $\lim_n \alpha_t(a_n)$ for any sequence (a_n) converging to a in norm). Simple computations then show that each α_t is an automorphism of A, and that the ensuing map $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$, $t \mapsto \alpha_t$, is a homomorphism of groups, which is continuous in that $t \mapsto \alpha_t(a)$ is continuous from $\mathbb{R}$ to A for $a \in A$.

In conclusion, under the assumption of short-range interactions the local (or 'finite-volume) Hamiltonians h_Λ ultimately define a dynamics on A. This detour seems necessary, because formal expressions like $\lim_{\Lambda\uparrow\mathbb{Z}^d} h_\Lambda$ are *a priori* meaningless.

4.7 Ground states: definition

A ground state of a finite system $A(\Lambda) = B(H_\Lambda)$ is simply an eigenstate of the local Hamiltonian h_Λ with the lowest eigenvalue.[56] For infinite systems, no Hamiltonian is yet defined, so we need to define ground states in terms of the dynamics (cf. §4.6).

Definition 4.8 *Let A be a C^*-algebra with a given automorphism group $\mathbb{R}$, i.e., a continuous homomorphism $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$, which gives the dynamics of the underlying physical system. A* ground state *of (A, α) is a state ω on A such that:*

1. *ω is time-independent, i.e. $\alpha_t^* \omega = \omega$ (or $\omega(\alpha_t(a)) = \omega(a)$ for all $a \in A$) $\forall t \in \mathbb{R}$;*
2. *The generator h_ω of the ensuing continuous unitary representation $t \mapsto u_t$ of $\mathbb{R}$ on H_ω (cf. Theorem 4.4) has positive spectrum (with $u_t = \exp(ith_\omega)$).*[57]

It follows from this definition, (4.8), and (4.9), that if ω is a ground state, then

$$h_\omega \Omega_\omega = 0; \tag{4.19}$$

$$\pi_\omega(\alpha_t(a)) = e^{ith_\omega} \pi_\omega(a) e^{-ith_\omega}. \tag{4.20}$$

Since $\sigma(h_\omega) \subseteq \mathbb{R}^+$, the unit vector Ω_ω of the GNS-representation π_ω induced by a ground state ω is a ground state for the Hamiltonian h_ω in the usual sense.

In quantum mechanics, the 'Heisenberg equation of motion' $da(t)/dt = i[h, a(t)]$ plays a role as the infinitesimal of the unitary evolution $a(t) = \exp(ith) a \exp(-ith)$. In the C^*-algebraic formalism, we have to use the language of derivations.

Definition 4.9 *A* derivation *on a C^*-algebra A is a linear map $\delta : A \to A$ satisfying the* Leibniz rule $\delta(ab) = \delta(a)b + a\delta(b)$. *An* unbounded derivation *is a linear map $\delta : \mathrm{Dom}(\delta) \to A$ satisfying theLeibniz rule, where $\mathrm{Dom}(\delta) \subset A$ of δ is dense in A. We call δ* symmetric *if $\mathrm{Dom}(\delta)^* = \mathrm{Dom}(\delta)$ and $\delta(a^*) = \delta(a)^*$ for all $a \in \mathrm{Dom}(\delta)$.*

In fact, (bounded) derivations are quite rare; in the classical case $A = C_0(M)$ for some phase space M, nonzero derivations do not even exist (Sakai), all *unbounded* derivations being of the form $\delta_X(f) = Xf$ for some smooth vector field X on M. In the quantum-mechanical case $A = B(H)$, any (closed, strongly continuous) symmetric derivation $\delta : B(H) \to B(H)$ is of the form $\delta(a) = i[h, a]$ for some self-adjoint operator h on H (Kadison), so that δ is bounded iff h is a bounded operator.

Given some dynamics α on A, we define an (unbounded) derivation δ on A by

$$\delta(a) = \frac{d}{dt} \alpha_t(a)_{|t=0} \equiv \lim_{t \to 0} \frac{\alpha_t(a) - a}{t}, \tag{4.21}$$

where $a \in \mathrm{Dom}(\delta) \subset A$ iff this (norm-) limit exists. If $\alpha_t(a) = \exp(ith) a \exp(-ith)$, then clearly $\delta(a) = i[h, a]$. It is an exercise to prove an alternative to Definition 4.8:

Proposition 4.10 *ω is a ground state iff $-i\omega(a^* \delta(a)) \geq 0$ for all $a \in \mathrm{Dom}(\delta)$.*

The idea is that $-i\omega(a^*\delta(a)) = (\Omega_\omega, \pi_\omega(a)^*[h_\omega, \pi_\omega(a)]\Omega_\omega) = (\pi_\omega(a)\Omega_\omega, h_\omega \pi_\omega(a)\Omega_\omega)$. Since $\mathrm{Dom}(\delta)$ is dense in A and Ω_ω is cyclic for $\pi_\omega(A)$, positivity of this expression yields $(\Psi, h_\omega \Psi) \geq 0$ for all $\Psi \in \mathrm{Dom}(h_\omega)$, so that $\sigma(h_\omega) \subseteq \mathbb{R}^+$ (and *vice versa*).

At last, the Heisenberg equation then resurfaces as $\pi_\omega(\delta(a)) = i[[h_\omega, \pi_\omega(a)]$.

[56] Because $\dim(H_\Lambda) < \infty$, the spectrum of h_Λ is discrete and hence local ground states exist.

[57] Physicists usually write u_t for $\exp(-ith)$, so that $a(t) = \exp(ith) a \exp(-ith) = u_t^* a u_t$.

4.8 Ground states: Ising model in $d = 1$

Ground states of finite systems typically are, but *need not be* unique. For example, the Ising Hamiltonian (4.16) in $d = 1$ with $B = 0$ has a doubly degenerate ground state $\Psi_0^{\pm}(\Lambda) \in H_\Lambda$ in the usual sense (all spins up or all spins down), but has a unique ground state $\Psi_B(\Lambda)$ if $0 < B < B_c$ for some critical value $B_c > 0$ [31]. The latter is similar to the nondegenerate ground state of the double-well potential discussed in the Introduction. Indeed, for any B the Ising model has a $\mathbb{Z}_2$-symmetry $\sigma_1 \mapsto \sigma_1$, $\sigma_2 \mapsto -\sigma_2$, $\sigma_3 \mapsto -\sigma_3$, given by a 180-degree rotation around the x-axis, which is implemented by the unitary operator $u^\Lambda = \otimes_{x\in\Lambda}\sigma_1(x)$ on H_Λ. The unique ground state is obviously symmetric, i.e., $u^\Lambda\Psi_B(\Lambda) = \Psi_B(\Lambda)$, whereas $u^\Lambda\Psi_0^{\pm(\Lambda)} = \Psi_0^{\mp}(\Lambda)$.

For the corresponding *infinite* system, the infinite-volume relic of u_Λ is the unique automorphism γ of A that for each $a \in A(\Lambda)$ is given by $\gamma(a) = u_\Lambda a u_\Lambda^*$. The property $[u^\Lambda, h_\Lambda] = 0$ then becomes $[\alpha_t, \gamma] = 0$ for each $t \in \mathbb{R}$, which implies that $\gamma^*\omega$ is a ground state whenever ω is one. The situation is then as follows [2, 5, 19].

- For $B = 0$, there are two translation-invariant pure ground states $\omega_0^{\pm}$ in the sense of Definition 4.8. These are the $\Lambda \to \infty$ limit of $\Psi_0^{\pm}(\Lambda)$, in that for each Λ and $a \in A(\Lambda)$ one has $\omega_0^{\pm}(a) = (\Psi_0^{\pm}(\Lambda), a\Psi_0^{\pm}(\Lambda))_{H_\Lambda}$. The states ω_0^+ and ω_0^- are inequivalent,[58] and the counterpart of the relation $u^\Lambda\Psi_0^{\pm(\Lambda)} = \Psi_0^{\mp}(\Lambda)$ is $\gamma^*\omega_0^{\pm} = \omega_0^{\mp}$. Any mixture $\lambda \cdot \omega_0^+ + (1-\lambda)\cdot\omega_0^-$ is also a ground state.[59]

- If $0 < B < B_c$, there are two translation-invariant pure ground states $\omega_B^{\pm}$, related by $\gamma^*\omega_B^{\pm} = \omega_B^{\mp}$, as opposed to the single one in finite volume. This is a typical situation, in which SSB only occurs in infinite-volume. The unique symmetric translation-invariant ground state is $\omega_B \equiv \frac{1}{2}(\omega_B^+ + \omega_B^-)$, which is mixed and hence does not have good clustering properties; for example, macroscopic observables fluctuate. The restriction $\omega_B(\Lambda)$ of ω_B to each $A(\Lambda)$ remains mixed, but for each $a \in A(\Lambda)$ the difference between $\omega_B(\Lambda)(a)$ and the ground state expectation value $\omega_B^\Lambda(a) \equiv (\Psi_B(\Lambda), a\Psi_B(\Lambda))_{H_\Lambda}$ vanishes (even exponentially fast) as $\Lambda \to \infty$. In this sense, the mixture ω_B is the (weak) $\Lambda \to \infty$ limit of the pure ground states ω_B^Λ: as in the case of Schrödinger's cat, the point is that in the macroscopic limit, quantum interference terms vanish [15].

This begs the question which finite-volume states converge to the pure ground states $\omega_B^{\pm}$. There is a complete analogy with the double-well potential here, in that for each finite Λ the local Hamiltonian h_Λ has a low-energy state $\tilde{\Psi}_B(\Lambda)$, such that the pure vector states on $A(\Lambda)$ defined by $(\Psi_B(\Lambda) \pm \tilde{\Psi}_B(\Lambda))/\sqrt{2}$ converge to $\omega_B^{\pm}$ [19].

[58] Taking $b = \sigma_3(y)$ at some fixed $y \in \Lambda$ we have $\omega_0^{\pm}(\sigma_3(y)) = \pm 1$, so that either (4.12) or (4.13) precludes the existence of a unitary operator $u : H_{\omega_0^+} \to H_{\omega_0^-}$ satisfying $u\pi_0^+(a) = \pi_0^-(a)u$ for all $a \in A$. This argument wal already presented in the Inroduction. The same conclusion follows from the uniqueness of a translation-invariant vector in $H_{\omega_0^\pm}$ according to Theorem 4.7.

[59] All this is unsurprising. However, there is an additional family ω_0^x, $x \in \mathbb{Z}$, of non-translation-invariant pure ground states, described by a 'kink' at site x, in that all spins to the left of x are up and those to the right are down. These states are all equivalent to each other, being related by a finite number of spin flips σ_1, but each is inequivalent to both ω_0^+ and ω_-^+. The restriction of ω_0^x to $A(\Lambda)$ is not a ground state, but the energy difference with $\Psi_0^{\pm}(\Lambda)$ vanishes as $\Lambda \to \infty$.

4.9 Equilibrium states and the KMS condition

It is a bit more difficult to find an appropriate definition of thermal equilibrium states of infinite quantum systems. The problem is similar to the definition of ground states, in that it is clear what to do for finite systems, namely writing down

$$\omega_\beta^\Lambda(a) = \frac{1}{\mathrm{Tr}\,(e^{-\beta h_\Lambda})}\mathrm{Tr}\,(e^{-\beta h_\Lambda}a), \tag{4.22}$$

but that subsequently the lack of a global Hamiltonian in some representation of A causes trouble.[60] This problem was solved in 1967 by Haag, Hugenholtz, and Winnink [14], who used an earlier observation of Kubo and independently Martin and Schwinger to the effect that for any $a, b \in A(\Lambda)$ in terms of (4.15) one has

$$\omega_\beta^\Lambda(\alpha_t(a)b) = \omega_\beta^\Lambda(b\alpha_{t+i\beta}(a)). \tag{4.23}$$

Definition 4.11 *Let A be a C^*-algebra with an automorphism group $\mathbb{R}$. A* KMS-state *at inverse temperature $\beta \in \mathbb{R}$ is a state ω on A wit the following property:*

1. *For any $a, b \in A$, the function $F_{a,b} : t \mapsto \omega(b\alpha_t(a))$ from $\mathbb{R}$ to $\mathbb{C}$ has an analytic continuation to the strip $S_\beta = \{z \in \mathbb{C} \mid 0 \leq \mathrm{Im}\,(z) \leq \beta\}$, where it is holomorphic in the interior and continuous on the boundary $\partial S_\beta = \mathbb{R} \cup (\mathbb{R} + i\beta)$;*

2. *The boundary values of $F_{a,b}$ are related, for all $t \in \mathbb{R}$, by*

$$F_{a,b}(t) = \omega(b\alpha_t(a)); \tag{4.24}$$

$$F_{a,b}(t + i\beta) = \omega(\alpha_t(a)b). \tag{4.25}$$

Initially, the mathematical characterization of equilibrium states by the KMS condition was somewhat tentative, but in the 1970s and '80s it became clear that it was spot on, being equivalent to local and global thermodynamic stability (against perturbations of the dynamics), the maximum entropy principle, etc. [5, 41, 42]. The states ω_β^Λ are KMS at β. The following properties generalize their properties.

Proposition 4.12 *1. A KMS-state at $\beta \in \mathbb{R}\backslash\{0\}$ is time-independent.*

2. *A KMS-state at $\beta \in \mathbb{R}$ is faithful, in that $\omega(a^*a) = 0$ iff $a = 0$.*

3. *In the GNS-rep π_ω induced by a KMS-state the vector $\Omega_\omega \in H_\omega$ is both cyclic (cf. Definition 3.16) and* separating*, in that $\pi_\omega(a)\Omega_\omega = 0$ iff $a = 0$.*

We omit the proof (cf. [5, §§5.3.3,5.3.9]); note that 3 is an easy consequence of 2.

If $A = M_n(\mathbb{C})$ the last example of §3.10 evidently applies, i.e., for $\omega = \omega_\beta^\Lambda$ as in (4.23) we have (up to unitary isomorphism) $H_\omega = M_n(\mathbb{C})$, $\pi_\omega(a)b = ab$, and $\Omega_\omega = \rho^{1/2}$, where $\rho = Z^{-1}\exp(-\beta h)$ with $h \equiv h_\Lambda$. It is worth verifying that the 'Hamiltonian' h_ω that satisfies (4.19) and (4.20) is *not* given by $\pi_\omega(h)$, which meets (4.20) but fails (4.19)), but by $h_\omega = \pi_\omega(h) - J\pi_\omega(h)J$, where the anti-unitary operator $J : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ is given by $Ja = a^*$. Indeed, because $[\pi_\omega(a), J\pi_\omega(b)J] = 0$ for all $a, b \in M_n(\mathbb{C})$ one still has (4.20), but in addition we now have $h_\omega\Omega_\omega = (\pi_\omega(h) - J\pi_\omega(h)J)\rho^{1/2} = h\rho^{1/2} - (h\rho^{1/2})^* = 0$.

[60] One might be tempted to use the global Hamiltonian h_ω of a ground state, but in that case $\exp(-\beta h_\omega)$ typically will not be in the trace-class $B_1(H_\omega)$, so that (4.22) is not defined.

4.10 Decomposition of states

Abstracting the previous discussion, spontaneous symmetry breaking involves:

- a C^*-algebra A (e.g., of the form (4.3)) with time-evolution $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$;
- a symmetry group $\gamma : G \to \mathrm{Aut}(A)$ such that $\alpha_t \gamma_g = \gamma_g \alpha_t$ for all $t \in \mathbb{R}, g \in G$.
- a ground- or KMS-state ω on A for which $\omega_g \equiv \gamma_g^* \omega \neq \omega$ for some $g \in G$.

Naively, one would conversely say that SSB is absent if a symmetric ground- or KMS-state exists, but this is incorrect: as we have seen in the Ising model with $G = \mathbb{Z}_2$, the symmetry-breaking ground states $\omega_0^{\pm}$ may be combined into a new ground state $\frac{1}{2}(\omega_0^+ + \omega_0^-)$, which is symmetric! In fact, combining asymmetric ground states into a symmetric one by an averaging procedure of ω_g over G is possible whenever G is amenable (this includes the case where G is compact). Moreover, the $\Lambda \uparrow \mathbb{Z}^d$ limit of symmetric ground- or KMS-states ω_Λ (obtained upon choosing symmetric boundary conditions for the Hamiltonian h_Λ and hence for the canonical density matrix ρ_Λ) is a symmetric ground/KMS state, even when asymmetric ground/KMS-states exist.

To handle this, we need a good notion of decomposition of states, to the effect that even though a ground- or KMS-state may happen to be symmetric, SSB occurs just in case some of its components in a 'canonical' decomposition break the symmetry. The question, then, is what these 'canonical' component states are.

The answer is given by convexity theory. Recall (cf. §3.3) that the state space $S(A)$ is a compact convex set in the weak*-topology inherited from A^* (assuming A to have a unit), and that the pure state space $P(A)$ is just its *boundary* $\partial S(A)$. It can be shown that the set $S_\beta(A)$ of KMS-states at β is a compact convex subset of $S(A)$, as is the set $S_\infty(A)$ of ground states. The 'canonical' states, then, are the elements of $\partial S_\beta(A)$, which consists of those $\omega' \in S_\beta(A)$ for which $\omega' = \lambda \omega_1' + (1-\lambda)\omega_2'$ for some $\lambda \in (0,1)$ and certain ω_1' and ω_2' *in* $S_\beta(A)$ implies $\omega_1' = \omega_2' = \omega'$ (cf. Definition 3.6). Such *extremal* decompositions may involve integrals instead of sums; this typically means that there is a probability measure μ on $\partial S_\beta(A)$, such that for each $a \in A$,

$$\omega(a) = \int_{\partial S_\beta(A)} d\mu(\lambda)\, \omega_\lambda(a) S_\beta(A). \tag{4.26}$$

In case of SSB, the measure μ is typically supported on some G-orbit in $\partial S_\beta(A)$.

1. For *KMS-states* one has $\partial S_\beta(A) = S_\beta(A) \cap S_p(A)$, where $S_p(A)$ is the set of *primary* states on A (cf. §3.12), so that the extremal decomposition of a KMS state coincides with its decomposition into *primary* KMS states. Moreover, *this decomposition is unique* [5, Theorem 5.3.30]. This is quite perfect!

2. For *ground states*, the analogous result would be $\partial S_\infty(A) = S_\infty(A) \cap \partial S(A)$, where $\partial S(A)$ is the set of *pure* states on A, so that the extremal decomposition of a ground state within the set of all ground states coincides with its decomposition into pure ground states. This is physically expected and holds in realistic models, but is provably the case only under additional assumptions.[61]

[61] See [5, Theorem 5.3.37]. The strongest such assumption is weak asymptotic abeliannes of the dynamics, i.e., $\lim_{t\to\infty} \omega([\alpha_t(a), b]) = 0$, and a weaker condition is that $\pi_\omega(A)'$ is commutative.

4.11 Order parameters

On the basis of the preceding discussion, one may define SSB as a property of the dynamics and the symmetry alone by the condition $(\partial S_\beta(A))^G = \emptyset$, where, for any $K \subset S(A)$, the set K^G consists of the G-invariant elements of A. Rephrasing this definition as $S_\beta(A)^G \cap S_p(A) = \emptyset$, we here have the essence of SSB: *an invariant ground/KMS state cannot be primary, whereas a primary ground/KMS state cannot be invariant.*[62] However, one may also define SSB as a property of a given state ω, as in the previous subsection. Leaving the self-evident case of an asymmetric state apart, we now turn to the problem of detecting SSB in an invariant state [41].

Definition 4.13 *Let A be a quasilocal C^*-algebra A with symmetry group G. A* (strong) order parameter *in A is an n-tuple $\vec{\phi} = (\phi_1, \ldots, \phi_n) \in A^n$ for which $\omega(\vec{\phi}) = 0$ if (and only if) ω is G-invariant, for any* translation-invariant *state ω on A.*

An order parameter defines an accompanying vector-field $x \mapsto \vec{\phi}(x)$ by $\phi_i(x) = \tau_x(\phi)$. Since ω is translation-invariant, $\omega(\vec{\phi}) = 0$ is equivalent to $\omega(\vec{\phi}(x)) = 0$ for all x.

In the Ising model, with $G = \mathbb{Z}_2$, $\sigma_3(0)$ is an order parameter, which can be extended to a strong one $\vec{\phi} = (\sigma_2(0), \sigma_3(0))$. In the Heisenberg model, where $G = SO(3)$, the triple $(\sigma_1(0), \sigma_2(0), \sigma_3(0))$ provides a strong order parameter.

Theorem 4.14 *Suppose that $\vec{\phi}$ is a (strong) order parameter, as in Definition 4.13. Then a G-invariant and translation-invariant ground/KMS state $\omega \in S_\beta(A)^G$ displays SSB—in the sense that some of the components in its extremal decomposition fail to be G-invariant—if (and only if) the following positivity requirement holds:*[63]

$$\lim_{x\to\infty} \omega\left(\sum_{i=1}^{n} \phi_i(0)^* \phi_i(x)\right) > 0. \tag{4.27}$$

The "if" part of the theorem is equivalent to the claim that the limit in question vanishes in the absence of SSB. Let (4.26) be the extremal decomposition of ω. If (almost) each extremal state ω_λ is invariant, then $\omega_\lambda(\underline{\phi_i(x)) = 0}$ for all i by definition of an order parameter, and similarly $\omega_\lambda(\phi_i(x)^*) = \overline{\omega_\lambda(\phi_i(x))} = 0$. Interchanging $\lim_{x\to\infty}$ with the integral over $\partial S_\beta(A)$ (which is allowed because μ is a probability measure), and using (4.11) then shows that the left-hand side of (4.27) vanishes.

To avoid difficult measure-theoretic aspects of the extremal decomposition theory, and also for pedagogical purposes, we prove the "only if" part only in the special case that $\omega = \int_G dg\, \rho_g$ (weakly), where $\rho \in \partial S_\beta(A)$ and $\rho_g = \gamma_g^* \rho$, as before. Since $\rho_g(\sum_{i=1}^n \phi_i(0)^* \phi_i(x))$ is independent of g (by definition of an order parameter), we may replace ρ_g by ρ in the expression for ω; the term $\int_G dg$ then factors out and is equal to unity. Thus we may replace ω in (4.27) by ρ. Since ρ is a primary state, we may now use (4.11) once again, so that the left-hand side of (4.27) becomes $\sum_{i=1}^n |\rho(\phi_i)|^2$. By assumption, ρ is not G-invariant, so that (by definition of a strong order parameter) at least one of the terms $|\rho(\phi_i)|$ is nonzero. Q.E.D.

[62] A weaker definition would be $S_\beta(A)^G \neq S_\beta(A)$, which implies $(\partial S_\beta(A))^G \neq \partial S_\beta(A)$ and hence forces the existence of asymmetric extremal KMS/ground states, but leaves open the possibility that symmetric extremal KMS/ground states exist.

[63] In that case, we say that the two-point function on the left-hand side exhibits *long-range order*.

4.12 Mean-field theories

In order to illustrate the abstract material so far, we now discuss a class of explicitly solvable models that display SSB. We work in de the setting of §4.6. Our running examples are the *Weisz-model* for ferromagnetism and the *BCS-model* for superconductivity, the latter in the so-called strong coupling limit. Both have arbitrary dimension d and $n = 2$, so that $H_0 = \mathbb{C}^2$, and are given by the local Hamiltonians

$$h_\Lambda^W = -\tfrac{1}{2}\frac{J}{|\Lambda|}\sum_{x,y\in\Lambda}\sigma_3(x)\sigma_3(y) - \vec{B}\cdot\sum_{x\in\Lambda}\vec{\sigma}(x); \tag{4.28}$$

$$h_\Lambda^{BCS} = \tfrac{1}{2}\varepsilon\sum_{x\in\Lambda}(1-\sigma_3(x)) - \frac{\lambda}{|\Lambda|}\sum_{x,y\in\Lambda}\sigma_-(x)\sigma_+(y). \tag{4.29}$$

In (4.28), $J > 0$ determines the strength of the spin-spin coupling, and $\vec{B}$ is an external magnetic field. The symmetry group of h_Λ^W is at least $G = \mathbb{Z}_2 = \{1, -1\}$, represented on H_0 (and thence on H_Λ) in a way that depends on the direction of $\vec{B}$. We will just consider the two cases where $\vec{B}$ lies in either the z-direction or the x-direction; in both cases we represent $\mathbb{Z}_2$ on $\mathbb{C}^2$ by $1 \mapsto u_1 = 1_2$ and $-1 \mapsto u_{-1} = \sigma_1$. For any group G represented on H_0 by $g \mapsto u_g$, we then put

$$u_g^\Lambda = \otimes_{x\in\Lambda} u_g(x), \tag{4.30}$$

which is a unitary operator on H_Λ. Clearly, with (4.28), $[h_\Lambda^W, u_g^\Lambda] = 0$ for $g \in \mathbb{Z}_2$.

In (4.29), the lattice Λ actually does not lie in physical space; it represents some labelling of states near the Fermi surface of the material in question. The idea is that the vectors $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ in $H_x \cong \mathbb{C}^2$ are states with one and zero Cooper pairs, respectively; the former has energy ε, whereas the latter—the unoccupied state—has zero energy.[64] The second term denotes the two-body interaction between Cooper pairs. The symmetry group of h_Λ^{BCS} is $G = U(1)$, realized on $\mathbb{C}^2$ through $u_g = \exp(\frac{1}{2}ig\sigma_3)$, $g \in [0, 4\pi)$, and extended to a unitary representation $g \mapsto u_g^\Lambda$ on H_Λ by (4.30); with $\sigma_\pm = \frac{1}{2}(\sigma_1 \pm i\sigma_2)$, one has $[h_\Lambda^{BCS}, u_g^\Lambda] = 0$ for all $g \in U(1)$.

A general (homogeneous) mean-field theory is defined by the local Hamiltonians

$$h_\Lambda = |\Lambda|\tilde{h}(T_1^\Lambda, \ldots, T_{n^2-1}^\Lambda), \tag{4.31}$$

where the $(T_i)_{i=1}^{n^2-1}$ together with $T_0 \equiv 1_n$ form a basis of the real vector space $M_n(\mathbb{C})_h$ of traceless hermitian $n \times n$ matrices, that is, of the Lie algebra $su(n)$,[65]

$$T_i^\Lambda = \frac{1}{|\Lambda|}\sum_{x\in\Lambda} T_i(x), \tag{4.32}$$

and $\tilde{h}$ is a polynomial expression (sensitive to operator ordering). Clearly, (4.28) and (4.29) are of this form. In the next subsection we will see that $\tilde{h}$ really defines a function on the vector space $u(n)^*$ dual to the Lie algebra $u(n)$.

[64] A Cooper pair consists of two electrons whose spins and momenta are anti-alligned.

[65] The Lie group $SU(n)$ consists of all unitary $n \times n$ matrices u with $\det(u) = 1$. Its Lie algebra $su(n)$ consists of all traceless hermitian $n \times n$ matrices. For $n = 2$ one has $T_i = \frac{1}{2}\sigma_i$, $i = 1, 2, 3$.

4.13 Mean-field Hamiltonian

Given the quantum-mechanical Hamiltonians (4.31), we define a single classical "Hamiltonian" $\tilde{h} \in C^\infty(su(n)^*, \mathbb{R})$ on the "phase space" $su(n)^*$. This is simply accomplished by replacing each T_i^Λ in (4.31) by the corresponding coordinate function θ_i on $su(n)^*$, defined by $\theta_i(\theta) = \theta(T_i)$. For our running examples, this yields

$$\tilde{h}^W(\theta) = -2J\theta_3^2 - 2\vec{B}\cdot\vec{\theta}; \tag{4.33}$$

$$\tilde{h}^{BCS}(\theta) = \varepsilon(\tfrac{1}{2} - \theta_3) - \lambda(\theta_1^2 + \theta_2^2 - \theta_3). \tag{4.34}$$

In general, for arbitrary $\overline{\theta} \in su(n)^*$, with coordinates $(\overline{\theta}_1, \ldots, \overline{\theta}_{n^2-1})$, $\overline{\theta}_i = \overline{\theta}(T_i)$,

$$\tilde{h}_{\overline{\theta}} := \tilde{h}(\overline{\theta}) + \sum_{i=1}^{n^2-1} \frac{\partial \tilde{h}}{\partial \theta_i}(\overline{\theta}) \cdot T_i \tag{4.35}$$

defines an hermitian operator $\tilde{h}_{\overline{\theta}}$ on H_0, called the *mean-field Hamiltonian*. E.g.,

$$\tilde{h}_{\overline{\theta}}^W = \tilde{h}^W(\overline{\theta}) - 2J\overline{\theta}_3\sigma_3 - \vec{B}\cdot\vec{\sigma}; \tag{4.36}$$

$$\tilde{h}_{\overline{\theta}}^{BCS} = \tilde{h}^{BCS}(\overline{\theta}) + \tfrac{1}{2}\varepsilon(1-\sigma_3) - \lambda(\overline{\theta}_1\sigma_1 + \overline{\theta}_2\sigma_2 - \tfrac{1}{2}\sigma_3). \tag{4.37}$$

For any (inverse temperature) $\beta = T^{-1}$, the *self-consistency* equation for $\overline{\theta}$ is

$$\tilde{\omega}_\beta^{\overline{\theta}} = \overline{\theta}, \text{ or } \tilde{\omega}_\beta^{\overline{\theta}}(T_i) = \overline{\theta}_i, \ (i = 1, \ldots, n^2-1); \tag{4.38}$$

$$\tilde{\omega}_\beta^{\overline{\theta}}(a) := \frac{\mathrm{Tr}_{H_0}(e^{-\beta\tilde{h}_{\overline{\theta}}}\, a)}{\mathrm{Tr}_{H_0}(e^{-\beta\tilde{h}_{\overline{\theta}}})}. \tag{4.39}$$

Clearly, the constant $\tilde{h}(\overline{\theta})$ in (4.35) drops out of this equation and may be ignored. For example, if we take (4.36) with $\vec{B} = 0$, then (4.38) forces $\overline{\theta}_1 = \overline{\theta}_2 = 0$, whereas the mean magnetization $m \equiv 2\overline{\theta}_3 = \tilde{\omega}_\beta^{\overline{\theta}}(\sigma_3)$ satisfies the famous equation $\tanh(\beta J m) = m$. This has a solution $m = 0$ for any β, and for $T \geq T_c = J$ (so that $\beta_c J = 1$) this is the only solution. For $T < T_c$, two additional solutions $\pm m_\beta$ with $m_\beta > 0$ appear. Similarly, for the mean-field Hamiltonian (4.34) of the BCS-model, eq. (4.38) has a critical temperature above which $\overline{\theta} = 0$ is the only solution, and below which there is an additional family of nonzero solutions parametrized by $U(1)$.

Proposition 4.15 *The self-consistency equation* (4.38) *has at least one solution.*

To see this, we embed the state space $S(M_n(\mathbb{C})) \equiv S_n$, i.e. the compact convex set of $n \times n$ density matrices, in $su(n)^*$ in the obvious way: $\rho \in S_n$ maps $X \in su(n)$ to $\mathrm{Tr}\,(\rho X) \equiv \rho(X)$. This is indeed an embedding, since $\rho \in su(n)^*$ determines $\rho \in S_n$ and *vice versa*: for $\rho(a^*) = \overline{\rho(a)}$ and $\rho(1) = 1$, and the complex linear span of 1 and $su(n)$ is $M_n(\mathbb{C})$. (For example, for $n = 2$, the embedding $S_2 \hookrightarrow su(2)^* \cong \mathbb{R}^3$ is just given by realizing S_2 as the three-ball B^3 in $\mathbb{R}^3$, cf. (3.7).) According to (4.38), $\overline{\theta}_i$ is precisely of this form, with $\rho = \tilde{\omega}_\beta^{\overline{\theta}}$. Thus $\overline{\theta} \in su(n)^*$ is constrained to lie in $S_n \subset su(n)^*$, and by (4.38) it is a fixed point of the continuous function $f : S_n \to S_n$ defined by $f(\rho) = \tilde{\omega}_\beta^\rho$. The claim then follows from Brouwer's Theorem stating that any continuous map from a compact compact set in $\mathbb{R}^k$ to itself has a fixed point.

4.14 Exactness of the mean-field approximation

The symmetries of h_Λ are reflected by the solution set of (4.38). The first point is that $G \subset U(n)$ acts not only on $H_0 = \mathbb{C}^n$ by $g \mapsto u_g$, but also on the state space S_n, viz. by $g \mapsto (\gamma_g^0)^*$, where $\gamma_g^0 : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ is the automorphism $\gamma_g^0(a) = u_g a u_g^*$, so that $(\gamma_g^0)^* \rho = \rho \circ \gamma_{g^{-1}}^0 = u_g \rho u_g^*$.[66] For example, for $G = SU(2)$ this action is just the defining action of $SO(3) = SU(2)/\mathbb{Z}_2$ on $\mathbb{R}^3$ (with $\mathbb{Z}_2 = \{1_2, -1_2\}$). For $G = \mathbb{Z}_2 = \{1_2, \sigma_1\} \equiv \{1, -1\}$, as in the Weisz-model, the nontrivial element $g = -1$ acts like a rotation of π around the x-axis, so that $(\gamma_{-1}^0)^*(x, y, z) = (x, -y, -z)$.

Under this action, any symmetry group G of the local Hamiltonians h_Λ also leaves $\tilde{h} \in C^\infty(S_n)$ invariant in the sense that $\tilde{h} \circ (\gamma_g^0)^* = \tilde{h}$, restricting $\tilde{h}$ to $S_n \subset su(n)^*$.[67]

Lemma 4.16 *If $\tilde{h} \in C^\infty(S_n)$ is G-invariant under the above G-action on S_n, then any $g \in G$ maps a solution $\overline{\theta}$ of (4.38) into another solution $(\gamma_g^0)^* \overline{\theta} \equiv \overline{\theta}_g$ of (4.38). In other words, the solution set of (4.38) is a union of G-orbits in S_n.*

This follows from $(\gamma_g^0)^* \tilde{\omega}_\beta^{\overline{\theta}} = \tilde{\omega}_\beta^{\overline{\theta}_g}$, which is immediate from (4.39) and (4.35). Q.E.D.

The mean-field approximation—i.e. of the local Hamiltonians (4.31) by the single-site mean-field Hamiltonians (4.35)—is exact in the following sense [3, 11]:

Theorem 4.17 *Let ω_β a limit point of the net (ω_β^Λ) defined by (4.22) and (4.31), as $\Lambda \uparrow \mathbb{Z}^d$. Then the decomposition (4.26) of ω_β into primary states is given by*

$$\omega_\beta = \int_{S_n} d\mu_\beta(\overline{\theta})\, \omega_\beta^{\overline{\theta}}, \tag{4.40}$$

$$\omega_\beta^{\overline{\theta}} := \otimes_{x \in \mathbb{Z}^d} \tilde{\omega}_\beta^{\overline{\theta}}(x), \tag{4.41}$$

for some probability measure μ_β on S_n, where the state $\tilde{\omega}_\beta^{\overline{\theta}}(x)$ on $B(H_x) \cong M_n(\mathbb{C})$ is given by (4.39), applied to site $x \in \mathbb{Z}^d$, with $h_{\overline{\theta}}$ given by (4.35), and $\overline{\theta} \in S_n$ satisfies (4.38). In particular, each state $\omega_\beta^{\overline{\theta}}$ defined by (4.41), (4.35), and (4.38) is primary.

In most examples, including the Weisz- and BCS-models, the limit state ω_β is actually unique, and in addition the pure thermodynamic states contributing to the primary decomposition (4.26) of ω_β form a single G-orbit in S_n. For $T \geq T_c$ there is just one term in (4.40), namely ω_β^0 at $\overline{\theta} = 0$. In the Weisz-model this is the unique tracial state tr on A, given on $A(\Lambda)$ by $\mathrm{tr}(a) = \mathrm{Tr}\,(a)/\dim(H_\Lambda)$, and extended to A by continuity (the β-independence of this state seems a pathology of the model). At $T < T_c$ the $\mathbb{Z}_2$-orbit carrying the measure in (4.40) is $\{(0, 0, \pm 2m_\beta)\}$.

To see SSB in these models, we extend each automorphism γ_g^0 of $B(H_0)$ to an automorphism $\gamma_g^\Lambda = \otimes_{x \in \Lambda} \gamma_g^x$ of $A(\Lambda)$, which yields an automorphism γ_g of A by continuity. The G-invariance $(\gamma_g^\Lambda)^* \omega_\beta^\Lambda = \omega_\beta^\Lambda$ of each Gibbs state ω_β^Λ then implies $\gamma_g^* \omega_\beta = \omega_\beta$ for each limit state, but (cf. the proof of Lemma 4.16) we have $\gamma_g^* \omega_\beta^{\overline{\theta}} = \omega_\beta^{\overline{\theta}_g}$, so that a primary state $\omega_\beta^{\overline{\theta}}$ breaks the G-symmetry whenever $\overline{\theta}_g \neq \overline{\theta}$ for some $g \in G$.

[66] This is a double restriction of the coadjoint action of $U(n)$ on $u(n)^*$, defined by $\mathrm{Co}_g(\theta) = \theta \circ \mathrm{Ad}_{g^{-1}}$, with $\mathrm{Ad}_g : u(n) \to u(n)$ given by $\mathrm{Ad}_g(X) = u_g X u_g^*$. First, $S_n \subset u(n)^*$ is stable under this action, and second, the coadjoint action of $U(n)$ on S_n is restricted to the subgroup $G \subset U(n)$.

[67] In fact, the full $\tilde{h} \in C^\infty(u(n)^*)$ is invariant under the G-action defined in the previous footnote.

4.15 KMS-condition in mean-field theories

One would expect the states ω_β and $\omega_\beta^{\overline{\theta}}$ in (4.40) to satisfy the KMS-condition: the former is a limit of local Gibbs states (4.22), and as to the the latter, primary states in the decomposition of a state automatically satisfy the KMS-condition if that state does. However: KMS with respect to which time-evolution? Indeed, the Hamiltonians (4.31) of mean-field models are long-range, which implies that the local time-evolutions (4.15), fail to extend to an automorphism group α on A.

The solution is to enlarge A to $A \otimes C$, where C is some algebra generated by the average values (4.32) in the limit $\Lambda \to \mathbb{Z}^d$. Since the expression (4.32) yields

$$[T_i^\Lambda, T_j^\Lambda] = \frac{1}{|\Lambda|}[T_i, T_j]^\Lambda, \tag{4.42}$$

this algebra should be *commutative*. Consider the set $S(A)^P$ of all *permutation-invariant states* on A, defined in the obvious way.[68] This is a compact convex set in $S(A)$, whose boundary $\partial S(A)^P$ is isomorphic to S_n, in that $\rho \in S_n$ defines a product state $\rho^\otimes = \otimes_{x\in\mathbb{Z}^d}\rho(x)$ in $\partial S(A)^P$, and each element of $\partial S(A)^P$ is of this form [43]. Each $\omega \in S(A)^P$ defines a probability measure μ_ω on S_n such that the integral

$$\omega = \int_{S_n} d\mu_\omega(\rho)\, \rho^\otimes \tag{4.43}$$

yields both the extremal and the primary decomposition of ω. The form of the mean-field Hamiltonians (4.31) then implies that the state ω_β in (4.40) lies in $S(A)^P$, and according to (4.41) each of its components $\omega_\beta^{\overline{\theta}}$ is an element of $\partial S(A)^P$. In each GNS-representation $\pi_\omega(A)$ defined by $\omega \in S(A)^P$, the limits $T_i^\omega := \lim_{\Lambda\uparrow\mathbb{Z}^d}\pi_\omega(T_i^\Lambda)$ exist in the strong operator topology, lie in the closure $\pi_\omega(A)''$, and generate a commutative C^*-algebra. If $\omega = \rho^\otimes \in \partial S(A)^P$, then T_i^ω is a multiple $\rho(T_i)$ of the identity (since it is easily seen to lie in the center of $\pi_\omega(A)''$, which by definition is trivial if ω is primary). Thus we abstractly define $\lim_{\Lambda\uparrow\mathbb{Z}^d} T_i^\Lambda$ as the function $\hat{T}_i(\rho) = \rho(T_i)$ on S_n, and identify the C^*-algebra C introduced above with $C(S_n)$. The above GNS-representation $\pi_\omega(A)$ then extends to $A \otimes C(S_n)$ by putting $\pi_\omega(\hat{T}_i) := T_i^\omega$.

Theorem 4.18 *1. There is a unique time-evolution α on $A \otimes C(S_n)$ such that for any $\omega \in S(A)^P$, $a \in A$, and $T_i \in su(n)$ (and hence $\hat{T}_i \in \hat{C}(S_n)$) one has*

$$s\text{-}\lim_{\Lambda\uparrow\mathbb{Z}^d} \pi_\omega(e^{ith_\Lambda} a e^{-ith_\Lambda}) = \pi_\omega(\alpha_t(a)); \tag{4.44}$$

$$s\text{-}\lim_{\tilde{\Lambda}\uparrow\mathbb{Z}^d}\lim_{\Lambda\uparrow\mathbb{Z}^d} \pi_\omega(e^{ith_\Lambda} T_i^{\tilde{\Lambda}} e^{-ith_\Lambda}) = \pi_\omega(\alpha_t(\hat{T}_i)). \tag{4.45}$$

2. The states ω_β and $\omega_\beta^{\overline{\theta}}$ in (4.40), extended to $A \otimes C(S_n)$ by $\omega(a \otimes \hat{T}_i) = \omega(a)\mu_\omega(\hat{T}_i)$, cf. (4.43), satisfy the KMS-condition at β with respect to α.

See [3] for the proof. Unlike A, C is actually stable under each α_t, so that one obtains a classical time-evolution on its Gelfand spectrum S_n, seen as a phase space.[69]

[68] I.e., the expectation value of an elementary tensor $\otimes_{x\in\Lambda} a_x(x)$ in $\omega \in S(A)^P$ is unchanged under permutation of the terms (a_x). For $\Lambda = \{x, y\}$ this means $\omega(a_x \otimes a_y) = \omega(a_y \otimes a_x)$.

[69] This time-evolution is truly classical, in being the Hamiltonian flow of $\tilde{h} \in C^\infty(S_n)$ with respect to the canonical Lie–Poisson bracket S_n inherits from $su(n)^*$ [3, 23].

5 Goldstone Theorem and Higgs Mechanism

The Goldstone Theorem and the Higgs Mechanism are two aspects of SSB that apparently contradict each other. In any case both require very careful treatment. The former results when the broken symmetry group G is a Lie group (of dimension ≥ 1), and the latter arises when it is an infinite-dimensional gauge group (see below).

Let us start with the simple case $G = SO(2)$, acting on $\mathbb{R}^2$ by rotation. This induces the obvious action on the classical phase space $T^*\mathbb{R}^2$, i.e., $R(p,q) = (Rp, Rq)$ as well as on the quantum Hilbert space $H = L^2(\mathbb{R}^2)$, that is, $U_R\psi(x) = \psi(R^{-1}x)$. Let us see what changes with respect to the action of $\mathbb{Z}_2$ on $\mathbb{R}$ considered in the Introduction. We now regard the potential V in (1.1) as an $SO(2)$-invariant function on $\mathbb{R}^2$ through the reinterpretation of q^2 as $q_1^2 + q_2^2$. This is the famous 'Mexican hat potential'. Thus the classical Hamiltonian $h(p,q) = p^2/2m + V(q)$, with $p^2 = p_1^2 + p_2^2$, is $SO(2)$-invariant, and the set of classical ground states

$$\mathcal{E}_0 = \{(p,q) \in T^*\mathbb{R}^2 \mid p = 0, q^2 = (\omega/\lambda)^2\} \tag{5.1}$$

is the SO(2)-orbit through e.g. the point $(p_1 = p_2 = 0, q_1 = \omega/\lambda, q_2 = 0)$. Compared to the one-dimensional case, the two-point set of ground states with $\mathbb{Z}_2$-symmetry is now connected and forms a circle in phase space. The intuition behind the Goldstone Theorem is that a particle can freely move in this circle at no cost of energy. If we look at mass as inertia, such motion is 'massless', as there is no obstruction. However, this intuition is only fully realized in quantum field theory.

In quantum mechanics, the ground state of the Hamiltonian (1.2) (now acting on $L^2(\mathbb{R}^2)$) remains unique, as in the one-dimensional case. In polar coordinates (r, ϕ) we have

$$h = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right) + V(r), \tag{5.2}$$

with $V(r) = -\frac{1}{2}\omega^2 r^2 + \frac{1}{4}\lambda^2 r^4$. With $L^2(\mathbb{R}^2) \cong L^2(\mathbb{R}^+) \otimes \ell^2(\mathbb{Z})$ under Fourier transformation in the angle variable, this becomes

$$h\Psi(r,n) = \left(-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2}\right) + V(r)\right)\Psi(r,n). \tag{5.3}$$

Since $\hbar^2 n^2/2mr^2$ is positive, the ground state Ψ_0 has $\Psi_0(r,n) = 0$ for all $n \neq 0$, and hence it is $SO(2)$-invariant, since the $SO(2)$-action on $L^2(\mathbb{R}^2)$ Fourier-transforms to the action $U_\theta\Psi(r,n) = \exp(in\theta)\Psi(r,n)$. Indeed, from a group-theoretical point of view, the unitary isomorphism $L^2(\mathbb{R}^2) \cong L^2(\mathbb{R}^+) \otimes \ell^2(\mathbb{Z})$ is nothing but the decomposition $L^2(\mathbb{R}^2) \cong \bigoplus_{n\in\mathbb{Z}} H_n$ where $H_n = L^2(\mathbb{R}^+)$ for all n, but with $\Phi_n \in H_n$ transforming under $SO(2)$ as $U_\theta\Phi_n(r) = \exp(in\theta)\Phi_n(r)$, $\theta \in [0, 2\pi]$. The $SO(2)$-invariant subspace of $L^2(\mathbb{R}^2)$, then, is precisely the space H_0 in which Ψ_0 lies. This is analogous to the situation occurring in one dimension higher (i.e. $\mathbb{R}^3$) with e.g. the hydrogen atom: in that case, the symmetry group is $SO(3)$, and $L^2(\mathbb{R}^3)$ decomposes accordingly as $L^2(\mathbb{R}^3) \cong \bigoplus_{j\in\mathbb{N}} H_j$, where $H_j = L^2(\mathbb{R}^+) \otimes \mathbb{C}^{2j+1}$. The ground state for a spherically symmetric potential then typically lies in H_0 and is $SO(3)$-invariant.

For our purpose, however, the relevant comparison is with the one-dimensional case: the decomposition of $L^2(\mathbb{R})$ under the natural $\mathbb{Z}_2$-action $U_{-1}\Psi(x) = \Psi(-x)$ is

$$L^2(\mathbb{R}) = H_0 \oplus H_1 \tag{5.4}$$

$$H_i = \{\Psi \in L^2(\mathbb{R}) \mid \Psi(x) = (-1)^i \Psi(-x)\}, \ \ i = 0, 1. \tag{5.5}$$

This time, H_+ is the $\mathbb{Z}_2$-invariant subspace containing the ground state Ψ_0. Being $\mathbb{Z}_2$-invariant, Ψ_0 is has peaks above both classical minima $\pm q_0$; in fact, Ψ_0 is real-valued and strictly positive. The ground state of the corresponding two-dimensional system, seen as an element of $L^2(\mathbb{R}^2)$, is just this Ψ_0 extended from $\mathbb{R}$ to $\mathbb{R}^2$ by rotational invariance. Hence the ground state remains real-valued and strictly positive, with peaks about the circle of classical minima in $\mathbb{R}^2$.

For $d = 1$, the first excited state Ψ_1 lies in H_1; it is real-valued, like Ψ_0, but since it has to satisfy $\Psi_1(-x) = -\Psi(x)$, it cannot be positive. Indeed, with a suitable choice of phase, Ψ_1 has one positive peak above q_0 and the same peak but now negative below $-q_0$. Using advanced semiclassical analysis, it can be shown that

$$\Psi_\pm = (\Psi_0 \pm \Psi_1)\sqrt{2} \tag{5.6}$$

is peaked above $\pm q_0$ alone (i.e., the negative peak of $\pm\Psi_1$ below $\mp q_0$ exactly cancels the corresponding peak of Ψ_0). The classical limit of Ψ_0 comes out as the mixed state $\frac{1}{2}(\omega_+ + \omega_-)$, where $\omega_\pm = (p = 0, \pm q_0)$, but each state $\Psi_\pm$ has the pure state $\omega_\pm$ as its classical limit. The latter are ground states, and hence in particular they are time-independent; to understand this, note that according to the WKB-approximation, the energy difference $E_0 - E_1$ beween Ψ_0 and Ψ_1 vanishes exponentially fast as $\hbar \to 0$, so that in the classical limit the states $\Psi_\pm$ rapidly approach energy eigenstates.

A similar but more complicated situation arises in $d = 2$. The role of the pair $(\Psi_0 \in H_0, \Psi_1 \in H_1)$ is now played by an infinite tower $(\Psi_n \in H_n, n \in \mathbb{Z})$, where Ψ_n is the lowest energy eigenstate (for h in (5.3)) in $H_n \subset L^2(\mathbb{R}^2)$. The state Ψ_+ for $d = 1$ now should be something like $\lim_{N\to\infty} \Psi^{(N)}$, with the unit vectors

$$\Psi^{(N)} = \frac{1}{\sqrt{2N+1}} \sum_{n=-N}^{N} \Psi_n, \tag{5.7}$$

but unfortunately this limit does not exist in $L^2(\mathbb{R}^2)$. The simplest way to proceed is to keep N finite but large, and define $\Psi_\theta^{(N)} = U_\theta \Psi^{(N)}$ as the analogue of Ψ_-; the upshot is that the set (5.1) of classical ground states emerges as the double limit $\lim_{N\to\infty} \lim_{\hbar\to 0}$ applied to $\Psi_\theta^{(N)}$, seen as a vector state in the algebraic sense. The easiest way of making this idea precise is to introduce Weyl's quantization prescription of classical functions on phase space: for $f \in C_c^\infty(T^*\mathbb{R}^n)$, the formula

$$Q_\hbar(f)\Psi(x) = \int_{T^*\mathbb{R}^n} \frac{d^n p d^n y}{(2\pi\hbar)^n} \, e^{ip(x-y)/\hbar} f\left(p, \tfrac{1}{2}(x+y)\right) \Psi(y) \tag{5.8}$$

defines a bounded operator $Q_\hbar(f)$ on $L^2(\mathbb{R}^n)$. For all $f \in C_c^\infty(T^*\mathbb{R}^n)$, we then have

$$\lim_{N\to\infty} \lim_{\hbar\to 0} (\Psi_\theta^{(N)}, Q_\hbar(f)\Psi_\theta^{(N)}) = \omega_\theta(f), \tag{5.9}$$

where ω_θ is a pure state on $C_0(T^*\mathbb{R}^2)$ corresponding to a suitable point in (5.1).

5.1 SSB in classical field theory

In this subsection we illustrate SSB in classical field theory through a simple example, where the symmetry group is $G = SO(N)$, but whenever possible we write things down in such a way that the generalization to arbitrary scalar field theories is obvious. Suppose we have N real scalar fields $\varphi \equiv (\varphi_1, \ldots, \varphi_N)$, on which $SO(N)$ acts in the defining representation on $\mathbb{R}^N$. Let the usual relativistic Lagrangian,[70]

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu \varphi_i \partial^\mu \varphi_i - V(\varphi), \tag{5.10}$$

contain an $SO(N)$-invariant potential V, typically of the form (with $\varphi^2 \equiv \sum_{i=1}^N \varphi_i^2$)

$$V(\varphi) = -\frac{m^2}{2}\varphi^2 + \frac{\lambda}{4}\varphi^4, \tag{5.11}$$

where $\lambda > 0$, but m^2 may have either sign. If $m^2 < 0$, the minimum of V lies at $\varphi = 0$, but if $m^2 > 0$ the minima form the $SO(N)$-orbit through

$$\varphi^c = (v, 0, \cdots, 0); \tag{5.12}$$

$$v \equiv m/\sqrt{\lambda} = \|\varphi^c\|. \tag{5.13}$$

The idea is that the physical fields are excitations of the 'vacuum state' φ^c, so that, instead of φ, as the appropriate 'small oscillation' field one should use

$$\chi(x) = \varphi(x) - \varphi^c. \tag{5.14}$$

Consequently, the potential is expanded in a Taylor series for small χ as

$$V(\varphi) = V(\varphi^c) + \tfrac{1}{2}V''_{ij}\chi_i\chi_j + O(\chi^3); \tag{5.15}$$

$$V''_{ij} \equiv \frac{\partial^2 V}{\partial\varphi_i \partial\varphi_j}(\varphi^c). \tag{5.16}$$

Note that the linear term vanishes because $V'(\varphi^c) = 0$. We now use the $SO(N)$-invariance of V, i.e., $V(g\varphi) = V(\varphi)$ for all $g \in SO(N)$. For $T^a \in \mathfrak{g}$ (i.e. the Lie algebra of G, realized by anti-symmetric traceless $N \times N$ matrices) this yields

$$\frac{d}{dt}V(e^{tT_a}\varphi)_{t=0} = 0 \Leftrightarrow \frac{\partial V(\varphi)}{\partial\varphi_i}T^a_{ij}\varphi_j = 0. \tag{5.17}$$

Differentiation with respect to φ_k and putting $\varphi = \varphi^c$ then gives

$$V''_{ik}T^a_{ij}\varphi^c_j = 0. \tag{5.18}$$

In general, let $H \subset G$ be the stabilizer of φ^c, i.e., $g \in H$ iff $g\varphi^c = \varphi^c$. In our example (5.11) - (5.12), we evidently have $H = SO(N-1)$. Then $T^a\varphi^c = 0$ for all generators T^a of the Lie algebra $\mathfrak{h}$ of H, so that there are

$$M \equiv \dim(G) - \dim(H) = \dim(G/H) = \dim(G \cdot \varphi^c) \tag{5.19}$$

linearly independent null eigenvectors of V'' (seen as an $N \times N$ matrix). This number equals the dimension of the submanifold of $\mathbb{R}^N$ where V assumes its minimum. In our example we have $M = N - 1$, since $\dim(SO(N)) = \frac{1}{2}N(N-1)$.

[70] From now on, we sum over repeated indices like i and μ (Einstein summation convention).

5.2 Goldstone Theorem in classical field theory

We now perform an affine field redefinition, based on an affine coordinate transformation in $\mathbb{R}^N$ that diagonalizes the matrix V''. The original (real) fields were $\varphi = (\varphi_1, \ldots, \varphi_N)$, and the new (real) fields are $(\chi_1, \theta_2, \cdots, \theta_N)$, with $\chi_1 = \varphi_1 - v$ as in (5.14), and the famous *Goldstone boson* fields are defined, also in general, by

$$\theta_a = \frac{1}{v}\langle T^a\varphi^c, \varphi\rangle = \frac{1}{v}T^a_{ij}\varphi^c_j\varphi_i. \tag{5.20}$$

Here $\langle\cdot,\cdot\rangle$ denotes the inner product in $\mathbb{R}^N$, and we have chosen a basis of $\mathfrak{g}$ in which the elements $(T^1, \ldots, T^{\dim(H)})$ form a basis of $\mathfrak{h}$, completed by M further elements $(T^{\dim(H)+1}, \ldots T^{\dim(G)+1})$, so as to have basis of $\mathfrak{g}$. The index a in (5.20), then, runs from $\dim(H)+1$ to $\dim(G)$, so that there are M Goldstone bosons, cf. (5.19). In our running example, this number was shown to be $M = N-1$, and in view of (5.12), the field $\theta_a = T^a_{i1}\varphi_i$ is a linear combination of the φ_2 till φ_N.

The simplest example is $N = 2$ with potential (5.11) and $m^2 > 0$. With the single generator $T = -i\sigma_2$, we obtain $\theta = \varphi_2$. Since $V'' = \mathrm{diag}(2m^2, 0)$, we see that the mass term $-\frac{1}{2}m^2\varphi_1^2$ in (5.11) (with $\varphi^2 = \varphi_1^2 + \varphi_2^2$) changes from the 'wrong' sign $-m^2$ to the 'right' sign $+2m^2$ in (5.15), whilst $-\frac{1}{2}m^2\varphi_2^2$ in (5.11) simply disappears, so that the field θ comes out to be massless. Indeed, this is the whole point of the introduction of the Goldstone bosons: in view of (5.18) and (5.20), the Goldstone fields do not occur in the quadratic term in (5.15) and hence are they are massless, in satisfying a field equation of the form $\partial_\mu\partial^\mu\theta_a = \cdots$, where $\cdots$ does not contain any term linear in any field. In general, the Goldstone Theorem states:

Theorem 5.1 *Suppose that a compact Lie group $G \subset SO(N)$ acts on N real scalar fields $\varphi = (\varphi_1, \ldots, \varphi_N)$, leaving the potential V in the Lagrangian* (5.10) *invariant. If G is spontaneously broken to an unbroken subgroup $H \subset G$, then there are at least* $\dim(G/H)$ *massless fields. Here the assumption means that V assumes a minimum at φ^c whose stability group is H, and the conclusion states that there exists a transformation from the original fields $(\varphi_1, \ldots, \varphi_N)$ to new fields $(\chi_1, \ldots, \chi_{N-M}, \theta_1, \ldots, \theta_M)$, $M = \dim(G) - \dim(H)$, which is invertible in a neighborhood of $\varphi = \varphi^c$, such that the potential $V(\varphi)$, re-expressed in the fields χ and θ, has no quadratic terms in θ.*

The local invertibility of the field redefinition around $\varphi^c \neq 0$ is crucial; in our example, where $\chi \equiv \chi_1 = \varphi_1 - v$ and $\theta_a = T^a_{i1}\varphi_i$, this may be checked explicitly.

An alternative proof uses a nonlinear definition of the Goldstone bosons, namely

$$\varphi(x) = e^{\frac{1}{v}\theta_a(x)T^a}(\varphi^c + \chi(x)), \tag{5.21}$$

where the sum over a ranges from 1 to M, $v = \|\varphi^c\|$, and the fields $\chi = (\chi_1, \ldots, \chi_{N-M})$ are chosen orthogonal (in $\mathbb{R}^N$) to the $T^a\varphi_c$, $a = 1, \ldots, M$, and hence to the θ_a.

Provided the generators of $SO(N)$ (and hence of $G \subset SO(N)$) have been chosen such that $\langle T^a\varphi^c, T^b\varphi^c\rangle = v^2\delta^{ab}$, the fields θ^a defined by (5.21) coincide with the fields in (5.20) up to quadratic terms in χ and θ; to see this, expand the exponential and also use $\langle T^a\varphi^c, \varphi^c\rangle = \langle T^a\varphi^c, \chi\rangle = 0$. This transformation is only well defined if $v \neq 0$, i..e., if SSB from G to H occurs, and its existence immediately implies the Goldstone Theorem 5.1, for by (5.21) and G-invariance, $V(\varphi)$ is independent of θ.

5.3 Higgs Mechanism in classical field theory I

We now proceed to a discussion of SSB in gauge theories, especially with an eye on the *Higgs Mechanism*, which plays a central role in the so-called *Standard Model* of high-energy physics. We look at the *Abelian Higgs Model*, given by the Lagrangian

$$\mathcal{L} = -\tfrac{1}{4}F_A^2 + \tfrac{1}{2}\langle D_\mu^A\varphi, D_\mu^A\varphi\rangle - V(\varphi), \tag{5.22}$$

where $\varphi = (\varphi_1, \varphi_2)$ is a scalar field, the usual electromagnetic field strength is $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, in terms of which $F_A^2 = F_{\mu\nu}F^{\mu\nu}$, and the covariant derivative is

$$D_\mu^A\varphi \equiv (\partial_\mu - eA_\mu \cdot T)\varphi = \left(\partial_\mu \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - eA_\mu \cdot \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\right) \cdot \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{5.23}$$

Here e is some coupling constant, identified with the unit of electrical charge. We still assume that V only depends on $\|\varphi\|^2 = \langle\varphi,\varphi\rangle$ and hence is $SO(2)$-invariant.

The novel situation compared to (5.10) and the like is that, whereas (5.10) is invariant under *global* $SO(2)$ transformations, the Lagrangian (5.22) is invariant under *local* $SO(2)$ "gauge" transformations that depend on x, namely

$$\varphi(x) \;\mapsto\; e^{\alpha(x)\cdot T}\varphi(x) = \begin{pmatrix} \cos\alpha(x) & -\sin\alpha(x) \\ \sin\alpha(x) & \cos\alpha(x) \end{pmatrix} \cdot \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix}; \tag{5.24}$$

$$A_\mu(x) \;\mapsto\; A_\mu(x) + \frac{1}{e}\partial_\mu\alpha(x). \tag{5.25}$$

We say that the gauge group $\mathcal{G} = C^\infty(\mathbb{R}^d, U(1))$ acts on the space of fields (A,φ) by (5.24) - (5.25). Now suppose V has a minimum at some constant value $\varphi^c \neq 0$. In that case, any field configuration ($\varphi(x) = \exp(\alpha(x)\cdot T)\varphi^c$, $A_\mu(x) = (1/e)\partial_\mu\alpha(x)$), $\alpha \in \mathcal{G}$, minimizes the action. Hence the possible 'vacua' of the model comprise the (infinite-dimensional) orbit $\mathcal{V}$ of the gauge group through $(A = 0, \varphi = \varphi^c)$. Note that $D_\mu^A\varphi = 0$ for $(A,\varphi) \in \mathcal{V}$, i.e., φ is *covariantly* constant along the vacuum orbit (whereas for global symmetries it is constant full stop). Relative to the (arbitrary) choice $(0,\varphi^c) \in \mathcal{V}$, we then introduce real fields χ and θ, called the *Higgs field* and the *would-be Goldstone boson*, respectively, by (5.21), which now simply reads

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = e^{\frac{1}{v}\theta(x)\cdot T} \cdot \begin{pmatrix} v + \chi(x) \\ 0 \end{pmatrix}. \tag{5.26}$$

After this redefinition of the scalar fields, the Lagrangian (5.22) becomes

$$\mathcal{L} = -\tfrac{1}{4}F_B^2 + \tfrac{1}{2}\partial_\mu\chi\partial^\mu\chi + \tfrac{1}{2}e^2(v+\chi)^2 B_\mu B^\mu - V(v+\chi, 0), \tag{5.27}$$

where $B_\mu = A_\mu - (1/ev)\partial_\mu\theta$, and $F_B^2 = F_{\mu\nu}F^{\mu\nu}$ for $F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$. This describes a vector boson B with mass term $\frac{1}{2}m_B^2 B_\mu B^\mu$, with $m_B^2 = \frac{1}{2}e^2v^2 > 0$ (as opposed to the massless vector field A), and a scalar field χ with mass term $\frac{1}{2}m_\chi^2\chi^2$, with $m_\chi^2 = (\partial^2 V/\partial\phi_1^2)_{|(v,0)} > 0$ (since V supposedly has a minimum at $\varphi^c = (v,0)$).

This is the *Higgs Mechanism*: the gauge field becomes massive, whilst the massless ('would-be') Goldstone boson disappears from the theory: it is (allegedly) 'eaten' by the gauge field. Thus the scalar degree of freedom θ that seems lost is recovered as the longitudinal component of the massive vector field (which for a gauge field would merely have been an unphysical 'gauge degree of freedom', see below).

5.4 Higgs Mechanism in classical field theory II

In the description just given, the Higgs Mechanism in classical field theory is seen as a consequence of SSB under special conditions. Remarkably, there is an alternative account of the Higgs Mechanism, according to which it has nothing to do with SSB!

We now perform a field redefinition analogous to (5.26) etc. straight away, viz.

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = e^{\theta(x)\cdot T} \cdot \begin{pmatrix} \rho(x) \\ 0 \end{pmatrix}; \tag{5.28}$$

$$A_\mu = B_\mu + (1/e)\partial_\mu \theta, \tag{5.29}$$

defined and invertible in a neighbourhood of any $(\rho_0 > 0, \theta_0 \in (-\pi, \pi), B_0)$, where B_0 is arbitrary. Each of these new fields is gauge-invariant: for (5.24) becomes $\theta(x) \mapsto \theta(x) + \alpha(x)$ with $\rho(x) \mapsto \rho(x)$, so that according to (5.25), B does not transform at all. As in (5.27), the Lagrangian becomes

$$\mathcal{L} = -\tfrac{1}{4}F_B^2 + \tfrac{1}{2}\partial_\mu\rho\partial^\mu\rho + \tfrac{1}{2}e^2\rho^2 B_\mu B^\mu - V(\rho), \tag{5.30}$$

with $V(\rho) \equiv V(\rho, 0)$. This is a Lagrangian without any internal symmetries at all (not even $\mathbb{Z}_2$, since $\rho > 0$), but of course one can still look for 'classical vacua' that minimize the energy and hence the potential $V(\rho)$. If $\rho = 0$ is the absolue minimum, then the above field redefinition is *a fortiori* invalidated, but if $V'(v) = 0$ for some $v > 0$, we proceed as before, introducing a Higgs field $\chi(x) = \rho(x) - v$, and recovering the Lagrangian (5.27). This once again leads to the Higgs Mechanism.

This can be generalized to the nonabelian case; we explain the $SU(2)$ case. In (5.22), the scalar field $\varphi = (\varphi_1, \varphi_2)$ is now complex, forming an $SU(2)$ doublet, the brackets $\langle \cdot, \cdot \rangle$ now denote the inner product in $\mathbb{C}^2$ (taken linear in the second variable, as usual), the nonabelian gauge field is $A = A^a\sigma_a$ (where the Pauli matrices σ_a, $a = 1, 2, 3$, form a hermitian basis of the Lie algebra of $SU(2)$), with associated field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + g[A_\mu, A_\nu]$ and covariant derivative $D_\mu^A = \partial_\mu + igA_\mu$. With $F_A^2 = F_{\mu\nu}^a F_a^{\mu\nu}$, the Lagrangian (5.22) is invariant under the transformations

$$\varphi(x) \mapsto e^{i\alpha_a(x)\sigma_a(x)}\varphi(x); \tag{5.31}$$

$$A_\mu(x) \mapsto e^{i\alpha_a(x)\sigma_a(x)}(A_\mu(x) - (i/g)\partial_\mu)e^{-i\alpha_a(x)\sigma_a(x)}. \tag{5.32}$$

The definition of the gauge-invariant fields B and ρ à la (5.28) - (5.29) is obviously

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = e^{i\theta_a(x)\cdot\sigma_a} \cdot \begin{pmatrix} \rho(x) \\ 0 \end{pmatrix}; \tag{5.33}$$

$$A_\mu(x) = e^{i\theta_a(x)\sigma_a(x)}(B_\mu(x) - (i/g)\partial_\mu)e^{-i\theta_a(x)\sigma_a(x)}, \tag{5.34}$$

which leads, *mutatis mutandis*, to the very same Lagrangian (5.30); cf. [17, 28, 37].

As a compromise between these two derivations of the Higgs Mechanism, it is also possible to fix the gauge by picking the representative (φ, A) in each $\mathcal{G}$-orbit for which $\varphi_2(x) = 0$ and $\varphi_1(x) > 0$; note that this so-called 'unitary' gauge is ill-defined if $\varphi_1(x) = 0$. Calling this unique representative (ρ, B), we are again led to (5.30).

5.5 Constrained Hamiltonian systems: electromagnetism

Gauge field theories are constrained systems, in which the apparent degrees of freedom in the Lagrangian are not the physical ones. For free electromagnetism, the Lagrangian for the gauge field A_μ is $\mathcal{L}(A) = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$, with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. In terms of the usual gauge-invariant fields $E_i = F_{i0} = \partial_i A_0 - \partial_0 A_i$ and $\vec{B} = \nabla \times \vec{A}$, the corresponding Euler–Lagrange equation for A_0 gives Gauss' Law $\nabla \cdot \vec{E} = 0$, whereas the one for A_i gives $\partial\vec{E}/\partial t = \nabla \times \vec{B}$ (the remaining Maxwell equations $\partial\vec{B}/\partial t = -\nabla \times \vec{E}$ and $\nabla \cdot \vec{B} = 0$ follow from the definitions of $\vec{B}$ and $\vec{E}$ out of A).

The first-order nature of the Maxwell equations suggests they are in Hamiltonian form. The canonical momenta are given by $\Pi_\mu = \partial\mathcal{L}/\partial\dot{A}_\mu$, which yields $\Pi_i = -E_i$, as well as the *primary constraint* $\Pi_0 = 0$. Nonetheless, the canonical Hamiltonian

$$h = \int d^3x \, \Big(\Pi_\mu(x)\dot{A}_\mu(x) - \mathcal{L}(x)\Big) = \int d^3x \, (\tfrac{1}{2}\vec{E}^2(x) + \tfrac{1}{2}\vec{B}^2(x) - A_0(x)\nabla \cdot \vec{E}(x))$$

is well defined. In the Hamiltonian formalism, Gauss' Law resurfaces as the *secondary constraint* stating that the primary constraint be preserved in time, viz.

$$\dot{\Pi}_0(x) = -\frac{\delta h}{\delta A_0(x)} = \nabla \cdot \vec{E}(x) \equiv 0. \tag{5.35}$$

Since $\frac{d}{dt}\nabla \cdot \vec{E}(x) = -\partial_i(\delta h/\delta A_i(x)) = -\partial_i(\Delta A_i - \partial_i \nabla \cdot \vec{A}) = 0$, there are no 'tertiary' constraints. Thus we have canonical (or 'phase space') variables $(\vec{E}, \vec{A})$ and (Π_0, A_0), subject to the constraints $\Pi_0(x) = 0$ and $\nabla \cdot \vec{E}(x) = 0$ for all x. Equivalently,

$$\Pi_0(\lambda_0) \equiv \int d^3x \, \Pi_0(x)\lambda_0(x) = 0; \;\; \Pi(\lambda) \equiv \int d^3x \, \nabla \cdot \vec{E}(x)\lambda(x) = 0, \tag{5.36}$$

for all functions λ_0 and λ on $\mathbb{R}^3$, forms an infinite set of constraints, one for each choice of λ_0 or λ. The constraints (5.36) are *first class*, meaning that their Poisson brackets are equal to existing constraints (or zero). In the Hamiltonian formalism, the role of the space-time dependent gauge transformations of the Lagrangian theory is played by the canonical transformations generated by the first class constraints, that is, $\delta_{\lambda_0}A_0(x) = \{\Pi_0(\lambda_0), A_0(x)\} = \lambda_0(x)$ and $\delta_{\lambda_0}A_i(x) = \delta_{\lambda_0}E_i(x) = 0$, and similarly $\delta_\lambda \vec{A}(x) = \nabla\lambda(x)$ and $\delta_\lambda \vec{E}(x) = 0$, $\delta_\lambda A_0(x) = 0$.

The holy grail of the Hamiltonian formalism is to find variables that are both *gauge invariant* and *unconstrained*. In our case, $A_\mu = (A_0, \vec{A})$ are unconstrained but gauge variant, whilst $\Pi_\mu = (\Pi_0, -\vec{E})$ are gauge invariant but constrained! Now write some vector field $\vec{V}$ as $\vec{V} = \vec{V}^L + \vec{V}^T$, where $\vec{V}^L = \Delta^{-1}\nabla(\nabla \cdot \vec{V})$ is the longitudinal component, so that $V_i^T = (\delta_{ij} - \Delta^{-1}\partial_i\partial_j)V_j$ is the transverse part. Then the physical variables of free electromagnetism are $\vec{A}^T$ and $\vec{E}^T$. The physical Hamiltonian

$$h = \tfrac{1}{2}\int d^3x \, (\vec{E}^T \cdot \vec{E}^T - \vec{A}^T \cdot \Delta\vec{A}^T), \tag{5.37}$$

then, is well defined on the physical (or 'reduced') phase space, which is the subset of all (A_μ, Π_μ) where the constraints (5.36) hold, modulo gauge equivalence.

5.6 Hamiltonian description of the Higgs Mechanism

After this preparation, we now analyze the abelian Higgs model as a constrained Hamiltonian system. It is convenient to combine the two real scalar fields φ_1 and φ_2 into a single complex scalar field $\varphi = (\varphi_1 + i\varphi_2)/\sqrt{2}$ and treat φ and its complex conjugate $\overline{\varphi}$ as independent variables. The Lagranigian (5.22) then becomes

$$\mathcal{L} = -\tfrac{1}{4}F_A^2 + \overline{D_\mu^A\varphi}\cdot D_\mu^A\varphi - V(\varphi,\overline{\varphi}), \tag{5.38}$$

with $D_\mu^A\varphi = (\partial_\mu - ieA_\mu)\varphi$, etc. The conjugate momenta Π_μ to A_μ are the same as for free electromagnetism, i.e., $\Pi_0 = 0$ and $\Pi_i = -E_i$, and for the scalar field we obtain $\pi = \partial\mathcal{L}/\partial\dot{\varphi} = \overline{D_0^A\varphi}$ and $\overline{\pi} = \partial\mathcal{L}/\partial\dot{\overline{\varphi}} = D_0^A\varphi$. The associated Hamiltonian is

$$h = \int d^3x\,\left(\tfrac{1}{2}\vec{E}^2 + \tfrac{1}{2}\vec{B}^2 - A_0(\nabla\cdot\vec{E} - j_0) + \overline{\pi}\pi + \overline{D_i^A\varphi}\cdot D_i^A\varphi + V(\varphi,\overline{\varphi})\right), \tag{5.39}$$

where $j_0 = ie(\pi\varphi - \overline{\pi\varphi})$ is the zero'th component of the Noether current. Hence the primary constraint remains $\Pi_0 = 0$, but the secondary constraints picks up an additional term and becomes $\nabla\cdot\vec{E} = j_0$ (which remains Gauss' law!). The physical (i.e., gauge invariant and unconstrained) variables can be computed as [26, 46]

$$\varphi_A = e^{ie\Delta^{-1}\nabla\cdot\vec{A}}\varphi,\ \overline{\varphi}_A = e^{-ie\Delta^{-1}\nabla\cdot\vec{A}}\overline{\varphi}; \tag{5.40}$$

$$\pi_A = e^{-ie\Delta^{-1}\nabla\cdot\vec{A}}\varphi,\ \overline{\pi}_A = e^{ie\Delta^{-1}\nabla\cdot\vec{A}}\overline{\pi}, \tag{5.41}$$

plus the same transverse fields $\vec{A}^T$ and $\vec{E}^T$ as in free electromagnetism. In terms of the transverse covariant derivative $D_i^T = \partial_i - ieA_i^T$, the physical Hamiltonian h is

$$\int d^3x\,\left(\tfrac{1}{2}(\vec{E}^T\cdot\vec{E}^T - \vec{A}^T\cdot\Delta\vec{A}^T - j_0^A\Delta^{-1}j_0^A) + \overline{\pi}_A\pi_A + \overline{D_i^T\varphi_A}\cdot D_i^T\varphi_A + V(\varphi_A,\overline{\varphi}_A)\right). \tag{5.42}$$

Physically, the third term in (5.42) is just the Coulomb energy, in which the charge density $j_0^A = ie(\pi_A\varphi_A - \overline{\pi}_A\overline{\varphi}_A)$ is the same as j_0 (since the latter is gauge invariant).

Remarkably, the physical field variables carry a residual $U(1)$-symmetry, viz.

$$\varphi_A \mapsto \exp(i\alpha)\varphi_A,\ \pi_A \mapsto \exp(-i\alpha)\pi_A,\ \overline{\varphi}_A \mapsto \exp(-i\alpha)\overline{\varphi}_A,\ \overline{\pi}_A \mapsto \exp(i\alpha)\overline{\pi}_A,$$

and no change for $\vec{A}^T$ and $\vec{E}^T$, under which the Hamiltonian (5.42) is invariant. If V has a minimum at $\varphi = \overline{\varphi} = v$, then we recover the Higgs Mechanism: after the field redefinition $\varphi_A = \exp(i\theta/v)(v+\chi)$ (and complex conjugate) and the reintroduction of the longitudinal component $A_i^L = -(1/ev)\partial_i\theta$ of the gauge field, along with (-) its conjugate momentum $E_i^L = -ev\Delta^{-1}\partial_i\pi_\theta$, the Hamiltonian (5.42) becomes [46]

$$\tfrac{1}{2}\int d^3x\,\left(\vec{E}^2 + \vec{B}^2 + \pi_\chi^2 + \partial_i\chi\partial_i\chi + \frac{1}{e^2v^2}(\nabla\cdot\vec{E})^2 + e^2v^2\vec{A}^2 + V(v+\chi)\right), \tag{5.43}$$

where $\vec{A} = \vec{A}^T + \vec{A}^L$ and $\vec{E} = \vec{E}^T + \vec{E}^L$. This describes a massive vector field, and the would-be Goldstone boson θ has disappeared, as befits the Higgs Mechanism!

5.7 Goldstone Theorem in QFT: assumptions

The Goldstone Theorem can be derived in quantum field theory, provided some assumptions are accepted in the absence of mathematically rigorous models [45]. The notation and assumptions underlying the Goldstone Theorem, then, are:

1. A is a *-algebra generated by the fields $\hat{\varphi}$ of some quantum field theory;
2. Space-time $\mathbb{R}^{d+1}$ acts on A by automorphisms $\alpha_{(x,t)}$, with $a(x,t) \equiv \alpha_{(x,t)}(a)$;
3. A compact Lie group G acts on A by automorphisms γ_g, $g \in G$;
4. G is a 'global symmetry', i.e., $\gamma_g \circ \alpha_{(x,t)} = \alpha_{(x,t)} \circ \gamma_g$ for all $(x,t) \in \mathbb{R}^{d+1}, g \in G$;
5. ω is an $\mathbb{R}^{d+1}$-invariant state on A, i.e., $\omega \circ \alpha_{(x,t)} = \omega$ for all $(x,t) \in \mathbb{R}^{d+1}$;
6. $\omega \circ \gamma_g \neq \omega$ for all $g \in G_a \subset G$, $G_a = \{\exp(sT^a), s \in \mathbb{R}, T^a \in \mathfrak{g}\}$;
7. $\delta^a \hat{\varphi}_\alpha(x) \equiv (d/ds)\gamma_{\exp(sT^a)}(\hat{\varphi}_\alpha)_{|s=0}$ is an order parameter, i.e., $\omega(\delta^a \hat{\varphi}_\alpha(x)) \neq 0$;
8. There is a field $\hat{j}_0^a$ in A that generates the symmetry $\hat{\varphi}_\alpha \mapsto \delta^a \hat{\varphi}_\alpha$, in that:
   (a) The function $y \mapsto \omega([\hat{j}_0^a(y,0), \hat{\varphi}_\alpha(x,t)])$ is in $L^1(\mathbb{R}^d)$ for all $(x,t) \in \mathbb{R}^{d+1}$;
   (b) $\lim_{\Lambda \uparrow \mathbb{R}^d} \int_\Lambda d^d y\, \omega([\hat{j}_0^a(y,0), \hat{\varphi}_\alpha(x,t)]) = -i\omega(\delta^a \hat{\varphi}_\alpha(x,t))$ for all $(x,t) \in \mathbb{R}^{d+1}$;
9. For simplicity, assume $\hat{\varphi}_\alpha(x)^* = \hat{\varphi}_\alpha(x)$ and $\omega(\hat{\varphi}_\alpha(x)) = 0$ (neither is crucial).

Most of these use language we have seen before, with the difference that from now on A is merely a *-algebra instead of a C^*-algebra. We will be quite relaxed about this relaxation, as we will be about our treatment of quantum fields as if they were operators (whereas in a completely rigorous treatment, they should be operator-valued distributions—this simplification actually does not matter, cf. [44]).

To motivate assumption 8, recall from classical field theory that the *Noether current* is defined as $j_\mu^a = \sum_i \Pi_\mu^i \cdot \delta^a \varphi_i$, where we sum over all fields in the Lagrangian, $\Pi_\mu^i = \partial \mathcal{L} / \partial \partial_\mu \varphi_i$, and $\delta^a \varphi = (d/ds) \exp(sT^a)\varphi_{|s=0}$, for a basis (T^a) of the Lie algebra $\mathfrak{g}$ of the symmetry group G in question. Assuming the symmetry to be global, that is, $\partial_\mu \delta^a \varphi_i = \delta^a \partial_\mu \varphi_i$, the Euler–Lagrange equations $\partial_\mu \Pi_\mu^i = \partial \mathcal{L} / \partial \varphi_i$ then give $\partial_\mu j_\mu^a = \delta^a \mathcal{L}$, upon which G-invariance of $\mathcal{L}$ yields $\partial_\mu j_\mu^a = 0$. This is (Emmy) *Noether's First Theorem*, which implies that the *Noether charge* $Q^a(t) = \int_{\mathbb{R}^3} d^3 y\, j_0^a(y,t)$ is t-independent whenever it exists (which is the case if the fields fall off sufficiently rapidly at spatial infinity). In that case, from the canonical equal-time Poisson bracket $\{\Pi_0^i(y,t), \varphi_j(x,t)\} = \delta_j^i \delta(x-y)$, one has $\{Q^a, \varphi_i(x,t)\} = \delta^a \varphi_i(x,t)$. However, even if the spatial integral comprising Q^a does not exist, one nonetheless has the weaker property

$$\lim_{\Lambda \uparrow \mathbb{R}^3} \int_\Lambda d^3 y\, \{j_0^a(y,0), \varphi_i(x,t)\} = \delta^a \varphi_i(x,t). \tag{5.44}$$

We now turn classical fields into operators (indicated by a hat), and assume some sort of canonical quantization procedure according to which (5.44) remains valid upon the usual substitution of commutators (times i) for Poisson brackets (Dirac). Assumption 8 above, then, is a weak form of the operator relation thus obtained.

5.8 Goldstone Theorem in QFT: proof

Writing $\hat{\varphi}_\alpha(t) \equiv \alpha_t(\hat{\varphi}_\alpha)$ for $\varphi(x,t)$ for simplicity, we compute:

$$\frac{d}{dt}\omega(\delta^a\hat{\varphi}_\alpha(t)) = \frac{d}{dt}\frac{d}{ds}\,\omega(\gamma_{\exp(sT^a)} \circ \alpha_t(\hat{\varphi}_\alpha))_{|s=0} = \frac{d}{dt}\frac{d}{ds}\,\omega(\alpha_t \circ \gamma_{\exp(sT^a)}(\hat{\varphi}_\alpha))_{|s=0},$$

where we have consecutively used assumptions 4 and 5 in §5.7. Defining

$$f(t) = i \lim_{\Lambda\uparrow\mathbb{R}^d} \int_\Lambda d^d y\, \omega([\hat{j}^a_0(y,0), \hat{\varphi}_\alpha(x,t)]), \tag{5.45}$$

it then follows from assumptions 7 and 8 that $f(t)$ is well defined, nonzero, and independent of t. From assumption 9 and the GNS-construction, we then obtain

$$\omega([\hat{j}^a_0(y,0), \hat{\varphi}_\alpha(x,t)]) = 2\mathrm{Im}\,\omega(\hat{\varphi}_\alpha(x,t)\hat{j}^a_0(y,0)) = 2\mathrm{Im}\,(\Omega_\omega, \pi_\omega(\hat{\varphi}_\alpha(x,t))\pi_\omega(\hat{j}^a_0(y,0))\Omega_\omega).$$

- In physics style, we omit π_ω, write $|0\rangle$ for Ω_ω, and use the Fourier transform

$$\langle 0|\hat{\varphi}_\alpha(x,x_0)\hat{j}^a_0(y,y_0)|0\rangle = \int_{\mathbb{R}^{d+1}} dp_0\, d^dp\, e^{-ip_0\cdot(x_0-y_0)+ip\cdot(x-y)}\tilde{G}(p,p_0). \tag{5.46}$$

  This gives $G(t) = 2\cdot\lim_{p\to 0}\mathrm{Im}\int_{\mathbb{R}} dp_0\, \exp(-itp_0)\tilde{G}(p_0,p)$. Since this expression is nonzero by assumption, the only way for it to be independent of t is that $\tilde{G}(p_0,p) \sim \delta(p_0 - \varepsilon(p))$ for some dispersion relation that satisfies $\varepsilon(0) = 0$. For example, in the relativistic case we have $\varepsilon(p) = \sqrt{p^2+m^2}$, so that $m = 0$.

- Mathematically, by assumption 5, Theorem 4.4, and the SNAG-Theorem in representation theory, we have self-adjoint energy- and momentum operators $\hat{h}_\omega$ and $\hat{p}^i_\omega$ on H_ω, whose spectral projections commute, such that

$$\pi_\omega(a(x,t)) = e^{it\hat{h}_\omega - ix\cdot\hat{p}_\omega}\pi_\omega(a)e^{-it\hat{h}_\omega+itx\cdot\hat{p}_\omega}, \tag{5.47}$$

  and $e^{it\hat{h}_\omega - itx\cdot\hat{p}_\omega}\Omega_\omega = \Omega_\omega$. We now insert a resolution of the identity operator in H_ω over the joint spectrum of the $\hat{p}^i_\omega$, which leads to the same conclusion:

Theorem 5.2 *If the assumptions 1 to 9 in §5.7 are satisfied, then the two-point function* (5.46) *has a singularity* $\delta(p_0 - \varepsilon(p))$ *in which* $\varepsilon(0) = 0$.

In particular, the energy spectrum has no gap above the ground state.

The corresponding (quasi-) particles states, then, are the *Goldstone bosons*. If $|p\rangle$ is an improper momentum eigenstate of such a boson, then the proof shows that both $\langle 0|\varphi_\alpha(x)|p\rangle$ and $\langle 0|j^a_0(y)|p\rangle$ should be nonzero. For example, returning to §5.1 for notation, in the $SO(2)$ model discussed there, φ_2 is the present φ_α, with $\delta\varphi_\alpha = -\varphi_1$ as the order parameter. The Goldstone bosons $\theta = \varphi_2$ satisfies these conditions (check). For $SO(3)$, in order (sic) to obtain φ_1 as an order parameter, as in §5.1, one may take either $\alpha = 2, a = 3$ or *vice versa*. Either of the (quantized) Goldstone fields, viz. φ_2 or φ_3, will have the required properties in quantum field theory.

Thus the classical proof gives precise information about the choice of the Goldstone boson field(s), but one has to realize its lack of uniqueness: all that is required is that the field in question has the nonzero matrix elements just mentioned.

5.9 Higgs Mechanism in quantum field theory

It is fair to say that the Higgs Mechanism in quantum field theory—and more generally, the notion of SSB in gauge theories—is poorly understood. Indeed, the entire quantization of gauge theories is not well understood, except at the perturbative level or on a lattice. The problems already come out in the abelian case with $d = 3$.

The main culprit is Gauss' Law $\nabla \cdot \vec{E} = j_0$. One would naively expect this constraint to remain valid in quantum field theory as an operator equation $\partial_i \hat{E}_i = \hat{j}_0$, and this is indeed the case in so-called physical gauges (like the Coulomb gauge $\partial_i \hat{A}_i = 0$). If we now look at condition 8(b) in §5.7, which for $G = U(1)$ reads

$$\lim_{\Lambda \uparrow \mathbb{R}^3} \int_\Lambda d^3y \, \omega([\hat{j}_0(y,0), \hat{\varphi}_\alpha(x,t)]) = -i\omega(\delta\hat{\varphi}_\alpha(x,t)), \text{[71]} \tag{5.48}$$

then it is clear that (5.48) can only hold if charged fields are nonlocal. For by Gauss' Law the commutator $[\hat{j}_0(y,0), \hat{\varphi}_\alpha(x,t)]$ equals $[\nabla \cdot \vec{E}(0,y), \hat{\varphi}_\alpha(x,t)]$, and by Gauss'(!) Theorem in vector calculus all contributions to the left-hand side of (5.48) come from terms $[E_i(0,y), \hat{\varphi}_\alpha(x,t)]$, with $y \in \partial\Lambda$ (i.e., the boundary of Λ). These must remain nonzero if $\Lambda \uparrow \mathbb{R}^3$, at least if (5.48) holds. On the other hand, such nonlocality must be enforced by massless fields, which idea leads to practically the only know rigorous result about the Higgs Mechanism (in the continuum) [45]:

Theorem 5.3 *In the Coulomb gauge the following conditions are equivalent:*

- *The electromagnetic field $\vec{A}$ is massless;*
- *Eq.* (5.48) *holds for any field $\hat{\varphi}_\alpha$;*
- *The charge operator $\hat{Q} = \lim_{\Lambda \uparrow \mathbb{R}^3} \int_\Lambda d^3y \, \hat{j}_0(y,0)$ exists,*[72] *and satisfies $\hat{Q}\Omega_\omega = 0$.*

Hence (contrapositively), SSB of $U(1)$ by the state ω is only possible if $\vec{A}$ is massive. In that case, the Fourier transform of the two-point function $\langle 0|\hat{\varphi}_\alpha(x,x_0)\hat{j}^a_0(y,y_0)|0\rangle$ (cf. the proof of the Goldstone Theorem in §5.8) has a pole at the mass of $\vec{A}$.

This theorem indeed yields the Higgs Mechanism for say the abelian Higgs model in a specific physical gauge: note that the idea that the would-be Goldstone boson is eaten by the gauge field is already suggested by Gauss' Law, through which (minus) the canonical momentum $\vec{E}$ to $\vec{A}$ acquires j_0 as its longitudinal component; that is, the very same field that creates the Goldstone boson from the ground state.

In covariant gauges, all fields remain local, but (5.48) is rescued by the gauge-fixing term added to the Lagrangian. For example, adding $\mathcal{L}_{gf} = -(1/2\xi)(\partial_\mu A^\mu)^2$ to (5.22) leads to an equation of motion $\partial_\mu F^\mu_\nu = j_\nu - \partial_\nu \partial_\mu A^\mu$, so that (discarding all surface terms by locality), $-i\omega(\delta\hat{\varphi}_\alpha(x,t)) = \int_{\mathbb{R}^3} d^3y \, \omega([\partial_0^2 \hat{A}_0(y,0), \hat{\varphi}_\alpha(x,t)])$. In the proof of the Goldstone Theorem, the massless Goldstone bosons do emerge, but they turn out to lie in some 'unphysical subspace' of H_ω (which, for local gauges, is not a Hilbert space but has zero- and negative norm states). This, however, would be a more appropriate topic for a course on the quantization of constrained systems!

[71] E.g., with $\delta\hat{\varphi}_1 = \hat{\varphi}_2$ and $\delta\hat{\varphi}_2 = -\hat{\varphi}_1$ for a charged field $\varphi = (\varphi_1 + i\varphi_2)/\sqrt{2}$, or $\delta\hat{\varphi} = i\hat{\varphi}$.

[72] That is, on some suitable domain in H_ω containing Ω_ω.

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