Algebraic quantum mechanics

Algebraic quantum mechanics is an abstraction and generalization of the Hilbert space formulation of quantum mechanics due to von Neumann [5]. In fact, von Neumann himself played a major role in developing the algebraic approach. Firstly, his joint paper [3] with Jordan and Wigner was one of the first attempts to go beyond Hilbert space (though it is now mainly of historical value). Secondly, he founded the mathematical theory of operator algebras in a magnificent series of papers [4, 6]. Although his own attempts to apply this theory to quantum mechanics were unsuccessful [18], the operator algebras that he introduced (which are now aptly called von Neumann algebras) still play a central role in the algebraic approach to quantum theory. Another class of operator algebras, now called C^*-algebras, introduced by Gelfand and Naimark [1], is of similar importance in algebraic quantum mechanics and quantum field theory. Authoritative references for the theory of C^*-algebras and von Neumann algebras are [14] and [21]. Major contributions to algebraic quantum theory were also made by Segal [7, 8] and Haag and his collaborators [2, 13].

The need to go beyond Hilbert space initially arose in attempts at a mathematically rigorous theory of systems with an infinite number of degrees of freedom, both in quantum statistical mechanics [9, 12, 13, 19, 20, 22] and in quantum field theory [2, 13, 20]. These remain active fields of study. More recently, the algebraic approach has also been applied to quantum chemistry [17], to the → quantization and → quasi-classical limit of finite-dimensional systems [15, 16], and to the philosophy of physics [10, 11, 16].

Besides its mathematical rigour, an important advantage of the algebraic approach is that it enables one to incorporate → Superselection rules. Indeed, it was a fundamental insight of Haag that the superselection sectors of a quantum system correspond to (unitarily) inequivalent representations of its algebra of observables (see below). As shown in the references just cited, in quantum field theory such representations (and hence the corresponding superselection sectors) are typically labeled by charges, whereas in quantum statistical mechanics they describe different thermodynamic phases of the system. In chemistry, the chirality of certain molecules can be understood as a superselection rule. The algebraic approach also leads to a transparent description of situations where locality and/or entanglement play a role [11, 13].

The notion of a C^*-algebra is basic in algebraic quantum theory. This is a complex algebra A that is complete in a norm $\|\cdot\|$ satisfying $\|ab\| \leq \|a\|\,\|b\|$ for all $a, b \in A$, and has an involution $a \mapsto a^*$ such that $\|a^*a\| = \|a\|^2$. A quantum system is then supposed to be modeled by a C^*-algebra whose self-adjoint elements (i.e. $a^* = a$) form the observables of the system. Of course, further structure than the C^*-algebraic one alone is needed to describe the system completely, such as a time-evolution or (in the case of quantum field theory) a description of the localization of each observable [13].

A basic example of a C^*-algebra is the algebra M_n of all complex $n \times n$ matrices, which describes an n-level system. Also, one may take $A = B(H)$, the algebra of all bounded operators on an infinite-dimensional Hilbert space H, equipped with the usual operator norm and adjoint. By the Gelfand–Naimark theorem [1], any C^*-algebra is isomorphic to a norm-closed self-adjoint subalgebra of $B(H)$, for some Hilbert space H. Another key example is $A = C_0(X)$, the space of all continuous complex-valued functions on a (locally compact Hausdorff) space X that vanish at infinity (in the sense that for every $\varepsilon > 0$ there is a compact subset $K \subset X$ such that $|f(x)| < \varepsilon$ for all $x \notin K$), equipped with the supremum norm $\|f\|_\infty := \sup_{x\in X} |f(x)|$, and involution given by (pointwise) complex conjugation. By the Gelfand–Naimark lemma [1], any commutative C^*-algebra is isomorphic to $C_0(X)$ for some locally compact Hausdorff space X. The algebra of observables of a classical system can often be modeled as a commutative C^*-algebra.

A von Neumann algebra M is a special kind of C^*-algebra, namely one that is concretely given on some Hilbert space, i.e. $M \subset B(H)$, and is equal to its own bicommutant: $(M')' = M$ (where M' consists of all bounded operators on H that commute with every element of M). For example, $B(H)$ is always a von Neumann algebra. Whereas C^*-algebras are usually considered in their norm-topology, a von Neumann algebra in addition carries a second interesting topology, called the σ-weak topology, in which its is complete as well. In this topology, one has convergence $a_n \rightarrow a$ if $\mathrm{Tr}\,\hat{\rho}(a_n - a) \rightarrow 0$ for each density matrix $\hat{\rho}$ on H. Unlike a general C^*-algebra (which may not have any nontrivial projections at all), a von Neumann algebra is generated by its projections (i.e. its elements p satisfying $p^2 = p^* = p$). It is often said, quite rightly, that C^*-algebras describe "non-commutative topology" whereas von Neumann algebra form the domain of "non-commutative measure theory".

In the algebraic framework the notion of a state is defined in a different way from what one is used to in quantum mechanics. An (algebraic) state on a C^*-algebra A is a linear functional $\rho : A \to \mathbb{C}$ that is positive in that $\rho(a^*a) \geq 0$ for all $a \in A$ and normalized in that $\rho(1) = 1$, where 1 is the unit element of A (provided A has a unit; if not, an equivalent requirement given positivity is $\|\rho\| = 1$). If A is a von Neumann algebra, the same definition applies, but one has the finer notion of a normal state, which by definition is continuous in the σ-weak topology (a state is automatically continuous in the norm topology). If $A = B(H)$, then a fundamental theorem of von Neumann [5] states that each normal state ρ on A is given by a density matrix $\hat{\rho}$ on H, so that $\rho(a) = \mathrm{Tr}\,\hat{\rho}a$ for each $a \in A$. (If H is infinite-dimensional, then $B(H)$ also possesses states that are not normal. For example, if $H = L^2(\mathbb{R})$ the Dirac eigenstates $|x\rangle$ of the position operator are well known not to exist as vectors in H, but it turns out that they do define non-normal states on $B(H)$.) On this basis, algebraic states are interpreted in the same way as states in the usual formalism, in that the number $\rho(a)$ is taken to be the expectation value of the observable a in the state ρ (this is essentially the $\to$ Born rule).

The notions of pure and mixed states can be defined in a general way now. Namely, a state $\rho : A \to \mathbb{C}$ is said to be pure when a decomposition $\rho = \lambda\omega + (1 - \lambda)\sigma$ for some $\lambda \in (0, 1)$ and two states ω and σ is possible only if $\omega = \sigma = \rho$. Otherwise, ρ is called mixed, in which case it evidently does have a nontrivial decomposition. It then turns out that a normal pure state on $B(H)$ is necessarily of the form $\psi(a) = (\Psi, a\Psi)$ for some unit vector $\Psi \in H$; of course, the state ρ defined by a density matrix $\hat{\rho}$ that is not a one-dimensional projection is mixed. Thus one recovers the usual notion of pure and mixed states from the algebraic formalism.

In the algebraic approach, however, states play a role that has no counterpart in the usual formalism of quantum mechanics. Namely, each state ρ on a C^*-algebra A defines a representation π_ρ of A on a Hilbert space H_ρ by means of the so-called GNS-construction (after Gelfand, Naimark and Segal [1, 7]). First, assume that ρ is faithful in that $\rho(a^*a) > 0$ for all nonzero $a \in A$. It follows that $(a, b) := \rho(a^*b)$ defines a positive definite sesquilinear form on A; the completion of A in the corresponding norm is a Hilbert space denoted by H_ρ. By construction, it contains A as a dense subspace. For each $a \in A$, define an operator $\pi_\rho(a)$ on A by $\pi_\rho(a)b := ab$, where $b \in A$. It easily follows that $\pi_\rho(a)$ is bounded, so that it may be extended by continuity to all of H_ρ. One then checks that $\pi_\rho : A \to B(H_\rho)$ is linear and satisfies $\pi_\rho(a_1a_2) = \pi_\rho(a_1)\pi_\rho(a_2)$ and $\pi_\rho(a^*) = \pi_\rho(a)^*$. This means that π_ρ is a representation of A on H_ρ. If ρ is not faithful, the same construction applies with one additional step: since the sesquilinear form is merely positive semidefinite, one has to take the quotient of A by the kernel N_ρ of the form (i.e. the collection of all $c \in A$ for which $\rho(c^*c) = 0$), and construct the Hilbert space H_ρ as the completion of A/N_ρ.

As in group theory, one has a notion of unitary (in)equivalence of representations of C^*-algebras. As already mentioned, this provides a mathematical explanation for the phenomenon of superselection rules, an insight that remains one of the most important achievements of algebraic quantum theory to date.

Literature

Primary

1. I.M. Gelfand & M.A. Naimark: On the imbedding of normed rings into the ring of operators in Hilbert space. Mat. Sbornik **12**, 197-213 (1943).

2. R. Haag & D. Kastler, An algebraic approach to quantum field theory. J. Math. Phys. **7**, 848-861 (1964).

3. P. Jordan, J. von Neumann & E. Wigner: On an algebraic generalization of the quantum mechanical formalism. Ann. Math. **35**, 29-64 (1934).

4. F.J. Murray & J. von Neumann: On rings of operators I, II, IV. Ann. Math. **37**, 116-229 (1936), Trans. Amer. Math. Soc. **41**, 208-248 (1937), Ann. Math. **44**, 716-808 (1943).

5. J. von Neumann: *Mathematische Grundlagen der Quantenmechanik* (Springer-Verlag, Berlin 1932). English translation: *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Berlin 1955).

6. J. von Neumann: On rings of operators III, V. Ann. Math. **41**, 94-161 (1940), ibid. **50**, 401-485 (1949).

7. I.E. Segal: Irreducible representations of operator algebras. Bull. Amer. Math. Soc. **61**, 69-105 (1947).

8. I.E. Segal: Postulates for general quantum mechanics. Ann. Math. **48**, 930-948 (1947).

Secondary

9. O. Bratteli & D.W. Robinson: *Operator Algebras and Quantum Statistical Mechanics. Vol 1: C* and W*-algebras, Symmetry Groups, Decomposition of States; Vol. 2: Equilibrium States, Models in Quantum Statistical Mechanics*, Second Edition ((Springer-Verlag, Heidelberg 1996, 2003).

10. J. Butterfield & J. Earman (ed.): *Handbook of the Philosophy of Science Vol. 2: Philosophy of Physics* (North-Holland, Elsevier, Amsterdam 2007).

11. R. Clifton, J. Butterfield & H. Halvorson: *Quantum Entanglements - Selected Papers* (Oxford University Press, Oxford 2004).

12. G.G. Emch: *Mathematical and Conceptual Foundations of 20th-Century Physics* (North-Holland, Amsterdam 1984).

13. R. Haag: *Local Quantum Physics: Fields, Particles, Algebras* (Springer-Verlag, Heidelberg 1992).

14. R.V. Kadison & J.R. Ringrose: *Fundamentals of the Theory of Operator Algebras. Vol. 1: Elementary Theory; Vol. 2: Advanced Theory* (Academic Press, New York 1983, 1986).

15. N.P. Landsman: *Mathematical Topics Between Classical and Quantum Mechanics* (Springer-Verlag, New York 1998).

16. N.P. Landsman: Between classical and quantum, in *Handbook of the Philosophy of Science Vol. 2: Philosophy of Physics*, ed. by J. Butterfield and J. Earman, pp. 417-554 (North-Holland, Elsevier, Amsterdam 2007).

17. H. Primas: *Chemistry, Quantum Mechanics and Reductionism*, Second Edition (Springer-Verlag, Berlin 1983).

18. M. Redei: Why John von Neumann did not like the Hilbert space formalism of quantum mechanics (and what he liked instead). Stud. Hist. Phil. Mod. Phys. **27**, 493-510 (1996).

19. G.L. Sewell: *Quantum Mechanics and its Emergent Macrophysics* (Princeton University Press, Princeton 2002).

20. F. Strocchi: *Elements of Quantum mechanics of Infinite Systems* (World Scientific, Singapore 1985).

21. M. Takesaki: *Theory of Operator Algebras. Vols. I-III.* (Springer-Verlag, New York 2003).

22. W. Thirring: *Quantum Mathematical Physics: Atoms, Molecules and Large Systems*, Second Edition (Springer-Verlag, New York 2002).

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