Chapter 2

Theory and Background

Since its inception in the beginning of the 20th century, quantum mechanics has been subject to continuous discussion and controversy. In this chapter, we will give both a historical and technical overview of some particular aspect of this controversy, namely, the possibility of *completing* quantum mechanics with so-called hidden variables. In particular, we will focus on 'no-go' theorems, which may be used to put empirical limits on any possible completions. We will gradually work our way towards the Kochen-Specker theorem and examine the question of its experimental testability.

2.1 The Completeness of Quantum Theory

In contrast to classical theories, quantum mechanics provides fundamentally probabilistic predictions. Thus, the question of the *completeness* of quantum theory arises: in analogy to classical theories, one might suppose that probabilities only enter into the theory because of our ignorance of the true, fundamental kinematics and/or dynamics. This may be called the *ignorance interpretation* of quantum probability. In order to yield a complete description of reality, quantum mechanics would then have to be supplemented by additional parameters, so-called *hidden variables*.

This question has been raised most famously by Einstein, Podolsky and Rosen (abbreviated EPR) in 1935 [2] (brought into the form most familiar today, referring to spin-entangled electrons, by Bohm

J. Szangolies, *Testing Quantum Contextuality,* BestMasters,
DOI 10.1007/978-3-658-09200-9_2, © Springer Fachmedien Wiesbaden 2015

and Aharonov in 1957 [3]). EPR define the following *condition of completeness*:

> Every element of the physical reality must have a counterpart in the physical theory. ([2], p. 777)

Thus, their conception of completeness rests on the notion of *elements of reality.* On these, they say the following:

> If, without in any way disturbing a system, we can predict with certainty [...] the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity. (*Ibid.*)

Their argument then is simple, yet striking: according to Heisenberg's uncertainty principle, if the observables corresponding to two physical quantities A and B do not commute, i.e. $[A, B] \neq 0$, both quantities cannot simultaneously be measured to arbitrary accuracy. However, they set up an example of two physical systems which, having interacted in the past, must be described by a simultaneous, entangled wave function. They then explain that by measurements on one of the systems, I, the other, II, may be left in an eigenstate of either of two observables, even if they fail to commute. Hence, by their criterion, since system II is not disturbed during the measurement, *both* observables must correspond to an element of physical reality—while naively, the uncertainty principle seems to allow definite reality for at most one of the observables. Thus, they conclude, quantum mechanics must be incomplete[1]. EPR end their discussion with the words:

> While we have thus shown that the wave function does not provide a complete description of the physical reality, we left

[1] Actually, they discuss another option: assigning simultaneous reality to two quantities only when both can be simultaneously measured or predicted. However, this would make the reality of a quantity dependent on the measurement, which they discard on the basis that this could not be permitted by any 'reasonable' definition of reality.

> open the question of whether or not such a description exists. We believe, however, that such a theory is possible. (*Ibid.*, p. 780)

This further question had, in fact, already been tackled by von Neumann in 1932 [4], in his seminal work on the mathematical foundations of quantum mechanics. In it von Neumann purported to answer this question in general, and in the negative: no completion of quantum mechanics through the introduction of hidden variables is possible. However, in 1966, Bell pointed to a critical shortcoming of the argument [5]. It is instructive to briefly review his version of von Neumann's theorem in order to build a foundation for different 'no-go'-theorems to be discussed later.

Consider two observables A and B of a system, represented in QM by self-adjoint operators (which we will not notationally distinguish from the observables themselves). Then, there exists an observable C such that $C = \alpha A + \beta B$, and if $\langle A \rangle$ and $\langle B \rangle$ denote the expectation values of A and B respectively, then $\langle C \rangle = \alpha \langle A \rangle + \beta \langle B \rangle$ is the expectation value of C. A hidden-variable theory now is committed to the simultaneous existence of definite values $v(A)$, $v(B)$ and $v(C)$ for all three observables (an assumption often referred to as *value definiteness*). Then, one would expect (and von Neumann requires) that $v(C) = \alpha v(A) + \beta v(B)$. But this is generally impossible: let $A = \sigma_x$, $B = \sigma_y$, and $C = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_y)$, with σ_i denoting the familiar Pauli matrices. Then, $v(A)$, $v(B)$ and $v(C)$ may all be either of ± 1. But $\pm 1 \neq \frac{1}{\sqrt{2}}(\pm 1 + \pm 1)$.

However, as Bell explicitly shows, it is possible after all to construct a hidden-variable description of a two-level quantum system. Thus, von Neumann's argument must be in error. In fact, the problem lies with the assumption of the additivity of expectation values for all observables. While this is a property of quantum mechanics, there is no reason to require it of the hidden-variable theory, and Bell's explicit model possesses it only for commuting observables. Bell levels the same criticism at a variant of von Neumann's theorem proposed by Jauch and Piron in [6].

The question of the possibility for a completion of quantum mechanics received its most famous (partial) answer in 1964 by, again, Bell [7]. He proved what today is known simply as *Bell's theorem*, to wit, that if such a more complete description exists, it cannot be local, i.e. dependent only on the events in a system's past lightcone, and agree with quantum mechanics in all instances. To this day, this result forms the paradigm example of a 'no-go' theorem.

Bell's argument proceeds from the Bohm-Aharonov version [3] of the EPR paradox. Consider two two-level quantum systems, for concreteness to be thought of as two spin-$\frac{1}{2}$ particles whose spin $\boldsymbol{\sigma}$ is measured along some direction $\mathbf{n}$. If the system is prepared in the singlet state $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|\uparrow_{\mathrm{I}}\downarrow_{\mathrm{II}}\rangle - |\downarrow_{\mathrm{I}}\uparrow_{\mathrm{II}}\rangle$, then, if the spin of particle I is measured along the direction $\mathbf{n}$, measurement of II along the same direction will yield the opposite value, i.e. measurement of $\boldsymbol{\sigma}_{\mathrm{I}} \cdot \mathbf{n}$ yielding 1 implies measurement of $\boldsymbol{\sigma}_{\mathrm{II}} \cdot \mathbf{n}$ yielding -1. This corresponds to the framework of EPR's original argument [2].

Any more complete description, provided by hidden variables collectively denoted $\lambda \in \Lambda$, must then match this behaviour. Take two observers, A and B, each in possession of one of the two particles comprising the EPR pair. Each measures the spin of their particle along some direction, denoted $\mathbf{a}$ and $\mathbf{b}$. Thus, the outcome of each experiment must then be determined by $\mathbf{a}$ and λ, respectively $\mathbf{b}$ and λ, i.e. $A = A(\mathbf{a}, \lambda) \in [-1, 1]$ and $B = B(\mathbf{b}, \lambda) \in [-1, 1]$. If now $p(\lambda)$ is the probability distribution of the hidden variables, we can write the expectation value of their product as

$$\langle AB \rangle \stackrel{HV}{=} \int_\Lambda d\lambda p(\lambda) A(\mathbf{a}, \lambda) B(\mathbf{b}, \lambda), \tag{2.1}$$

which must equal the quantum prediction

$$\langle AB \rangle \stackrel{QM}{=} -\mathbf{a} \cdot \mathbf{b}. \tag{2.2}$$

From these preliminary considerations, Bell then derives an inequality that all models of this kind (collectively denoted *local realistic*) have to obey. This original 'Bell inequality' is

$$1 + \langle BC \rangle \geq |\langle AB \rangle - \langle AC \rangle| \tag{2.3}$$

The great importance of Bell's theorem then derives from the fact that utilizing such an inequality, the question of the completion of quantum mechanics by (local) hidden variables becomes accessible to experiment: local realism necessitates a deviation from quantum mechanical predictions in certain situations.

However, Bell's original inequality is not well suited to experiment, since it does not apply in the presence of possible non-detections (i.e. measurements which yield neither $+1$ nor -1). To this end, Clauser, Horne, Shimony and Holt in 1969 proposed an alternative version, known after their initials as the CHSH-inequality [8]:

$$\langle\chi_{\mathrm{CHSH}}\rangle = \langle AB\rangle + \langle BC\rangle + \langle CD\rangle - \langle DA\rangle \leq 2 \tag{2.4}$$

This inequality, like Bell's original one, holds for all local realistic models. But if the EPR pair is in the state

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \tag{2.5}$$

then, choosing the observables $A = \sigma_x \otimes \mathbb{1}$, $B = -\frac{1}{\sqrt{2}}\mathbb{1} \otimes (\sigma_z + \sigma_x)$, $C = \sigma_z \otimes \mathbb{1}$ and $D = \frac{1}{\sqrt{2}}\mathbb{1} \otimes (\sigma_z - \sigma_x))$ (where $\mathbb{1}$ is the 2×2 unit matrix) yields $\langle\chi_{\mathrm{CHSH}}\rangle = 2\sqrt{2}$ (which value is indeed the maximum attainable for quantum mechanics, known as *Tsirelson's bound* [9]).

With this framework in hand, the first experimental test of a Bell inequality was carried out by Freedman and Clauser in 1972 [10]. Today, the quantum mechanical violation of Bell inequalities is widely accepted, thanks to experiments performed by Aspect and collaborators in 1981-82 [11, 12, 13], and to the 1998 experiment by the group of Zeilinger [14], thus establishing the consensus that local realistic completions of quantum mechanics are indeed ruled out.

2.2 The Kochen-Specker Theorem

It is instructive to inquire into the reason why quantum mechanics violates Bell inequalities. A necessary requirement for Bell-inequality violation is *entanglement*: only states that cannot be written as a tensor product of (pure) subsystem states, i.e. $|\psi_{\text{ent}}\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle$, may exceed classical bounds. But this is not sufficient: there exist entangled states[2] which nevertheless do not violate any Bell inequality [15, 16]. Thus, non-locality is a property of certain states only. But entanglement is a phenomenon seemingly remote from everyday existence, and therefore one might be tempted to 'shrug off' the implication of Bell's theorem, maintaining that it is of little consequence for most practical purposes. Hence, it would be interesting to investigate whether quantum mechanics as a whole, rather than just some quantum-mechanical states, deviates from classical predictions.

The first step towards just such a result was established by Gleason in 1957 [19]. He proved that on any Hilbert space of dimension greater than three, the only suitable probability measures are given by the density matrices, i.e. that if Π_i is some projector onto a subspace corresponding to the i-th eigenvalue of some observable O, $\mu_\rho(\Pi_i)$, the probability that measurement of O returns i for the state ρ, must be $\mathrm{Tr}(\Pi_i \rho)$, where Tr denotes the trace operation. This is of course nothing else but Born's rule. That in this work lies the germ of an exceptionally strong no-go theorem was first realized by Bell in 1966 [5], who proposed it as a stronger replacement of von Neumann's result consequent on his critique thereof. Earlier, in 1960, Specker had considered similar ideas [20].

As Bell argues, the important feature of Gleason's work with respect to the hidden-variable program is that, since the probability measure provided by density matrices is continuous, *any* assignment of probabilities to properties of some quantum system (represented by projection operators Π_i) must be continuous. However, in a hidden-variable description, only two distinct values, corresponding to the projectors' eigenvalues 0 and 1, which may be interpreted as truth values indicating whether a system possesses a certain property, can occur. Thus, the hidden-variable mapping necessarily contains discon-

[2] However, these states have to be mixed—all pure entangled states violate a Bell inequality [17, 18].

tinuities (cf. [21]), and as Bell showed, this entails that two states receiving different values cannot be arbitrarily close together. More explicitly, together with the nonexistence of dispersion-free states[3], Gleason's theorem may be used to demonstrate the nonexistence of a lattice homomorphism between $\mathcal{P}(H)$, the lattice of closed linear subspaces of Hilbert space, and the two-element Boolean algebra $\mathcal{B}_2$ [22]—that is, the nonexistence of a mapping that for every property a quantum system may have uniquely decides whether it does or does not have that property.

Bell then proceeds to subject his theorem to the same sort of criticism he had previously levelled at von Neumann's and Piron and Jauch's argument. His crucial conclusion:

> It was tacitly assumed that measurement of an observable must yield the same value independently of what other measurements may be made simultaneously. ([5], p. 451)

The same spirit is present in [20], where Specker considers 'non-simultaneously decidable propositions'. This assumption is nowadays generally referred to as *non-contextuality*: the requirement that the question of whether a system has a certain property can objectively be decided without taking into account what other questions are asked (i.e. measurements are performed) simultaneously. Like locality, which it supplants in the present formulation, this seems a sensible requirement, and it is certainly fulfilled for all familiar, macroscopic objects.

The theorem Bell considered in his 1966 paper was given an independent and more definite formulation in 1967 by Kochen and Specker [23]. Their presentation relies on the same crucial insight as Bell's: that rays in Hilbert space having different assignments of the truth values 0 and 1 for some property cannot be arbitrarily close to each other. However, the virtue of their argumentation lies in the explicit construction of a set of rays which, if arranged into a graph

[3] A dispersion-free state is a state ρ such that the dispersion $\sigma(O) = \langle O^2 \rangle - \langle O \rangle^2$ vanishes for all operators O.

such that vertexes corresponding to orthogonal rays are joined by an edge, is not true-false colorable, i.e. for which there does not exist a consistent simultaneous assignment of truth values. Basically, while Bell shows that the quantum-mechanical relation $S_x^2 + S_y^2 + S_z^2 = 2 \cdot \mathbb{1}$, where the S_i are the spin observables of a spin-1 particle and $\mathbb{1}$ is the identity operator, cannot always be satisfied using non-contextual hidden variables, Kochen and Specker exhibit an explicit—and most importantly, finite—set of vectors, such that not all of them can fulfill this relation simultaneously.

Before presenting the proof of the theorem, let us first briefly consider its relationship to Bell's 1964 one. Roughly, the Kochen-Specker theorem replaces Bell's assumption of locality with an assumption of non-contextuality. It is easy to show that in certain instances, non-contextuality implies locality [24]: if some observable A can be measured in conjunction with compatible observables $B, C, \ldots$ as well as $L, M, \ldots$, and this can be implemented in such a way that the system may be partinioned into subsystems such that only local manipulations are necessary to implement measurement of either context on either part of the system, then we have the notion of locality as used in Bell's theorem. Furthermore, any Bell inequality can be turned into a Kochen-Specker inequality [25]. Non-contextuality then may be viewed as being more general, and local realistic theories are a subset of non-contextual ones [26]. Also, as will be shown, proofs of the contextuality of quantum theory can be given that do not rely on any specific state being prepared, and thus, are said to be 'state-independent'. In particular, no entanglement is necessary to violate non-contextuality[4].

2.2.1 Kochen and Specker's Original Proof

We will begin by briefly discussing the original proof by Kochen and Specker of their eponymous theorem. This proof, while more involved than more recent examples, is instructive in the sense that it is the

[4] In fact, in their original paper [23], Kochen and Specker consider a single-particle realization of their argument.

original example of the 'coloring game' type of proof of the Kochen-Specker theorem. We will here mainly follow the presentation in [27].

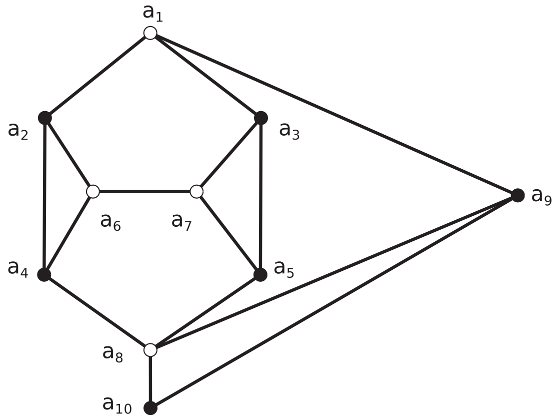

Figure 2.1: $\mathcal{G}_1$: Ten propositions a_i, where simultaneously nonsatisfiable ones are linked by an edge; the coloring shown is inconsistent with the orthogonality constraints, showing that they are incompatible with the requirements $g_1 = 1$ and $a_1 = 1$, but $a_{10} \neq 1$.

Consider first the graph $\mathcal{G}_1$ in Figure 2.1. For the moment, we will consider it as simply having at its vertices certain classical propositions a_i, which are linked by an edge $\{i, j\}$ if a_i and a_j are mutually exclusive, i.e. cannot be both true at the same time. Thus, every edge represents again a proposition:

$$b_{i,j} = \neg(a_i \wedge a_j), \tag{2.6}$$

where $\neg$ stands for negation, and the wedge $\wedge$ represents the logical `and`. Thus, this proposition is true exactly if at least one of a_i and a_j is false. Similarly, the three triangles in the graph again represent new propositions:

$$c_{ijk} = a_i \vee a_j \vee a_k, \tag{2.7}$$

where $\vee$ denotes the logical `or`. These propositions are evidently true whenever at least one of a_i, a_j, or a_k is true. Call $\mathcal{E}_1$ the set of all pairs $\{i,j\}$ such that a_i and a_j are linked by an edge, and similarly $\mathcal{T}_1$ the set of all triples $\{i,j,k\}$ such that a_i, a_j and a_k form a triangle in $\mathcal{G}_1$. Now observe that the whole graph represents the following proposition, which is merely the conjunction of all edge and triangle propositions:

$$\begin{aligned} g_1 =& b_{1,2} \wedge b_{1,3} \wedge b_{1,9} \wedge b_{2,4} \wedge b_{2,6} \wedge b_{3,5} \wedge b_{3,7} \wedge b_{4,6} \wedge b_{4,8} \wedge b_{5,7} \\ & \wedge b_{5,8} \wedge b_{6,7} \wedge b_{8,9} \wedge b_{8,10} \wedge b_{9,10} \wedge c_{2,4,6} \wedge c_{3,5,7} \wedge c_{8,9,10} \\ \equiv & \bigwedge_{\{i,j\}\in\mathcal{E}_1} b_{ij} \wedge \bigwedge_{\{i,j,k\}\in\mathcal{T}_1} c_{ijk} \end{aligned} \tag{2.8}$$

It is now not difficult to see that the truth of g_1, i.e. $g_1 = 1$, together with the truth of a_1, implies the truth of a_{10}: if we assume to the contrary that $g_1 = a_1 = 1$, but $a_{10} = 0$, the truth of $b_{1,2}$, $b_{1,3}$, $b_{1,9}$ and $b_{8,10}$ imply that $a_2 = a_3 = a_9 = 0$, and thus, $a_8 = 1$, since $c_{8,9,10} = 1$. But this implies $a_4 = a_5 = 0$ (because $b_{4,8} = b_{5,8} = 1$), and hence, $a_6 = a_7 = 1$, since $c_{2,4,6} = c_{3,5,7} = 1$ (and we have shown that $a_2 = a_3 = a_4 = a_5 = 0$). But this obviously contradicts $b_{6,7} = 1$; see also the coloring in Figure 2.1.

Consider now the graph $\mathcal{G}_2$ in Figure 2.2, composed of 15 copies of $\mathcal{G}_1$. From $\mathcal{G}_2$, we can construct a proposition g_2 analogous to the way g_1 was constructed from $\mathcal{G}_1$:

$$g_2 = \bigwedge_{\{i,j\}\in\mathcal{E}_2} b_{ij} \wedge \bigwedge_{\{i,j,k\}\in\mathcal{T}_2} c_{ijk}, \tag{2.9}$$

where $\mathcal{E}_2$ and $\mathcal{T}_2$ are respectively the edge- and triangle-set of $\mathcal{G}_2$. Using the prior result that $a_1 = 1$ implies $a_{10} = 1$ (and similarly, $a_{18} = 1$ and so on), it is not hard to show that g_2 is always false. Consider the triangle $\{a_1, a_9, a_{41}\}$ in Fig. 2.2. Since $c_{1,9,41} = 1$, at least one of them must be true. Suppose thus $a_1 = 1$. Then, $a_{10} = 1$, $a_{18} = 1$, $a_{26} = 1$, $a_{34} = 1$, and finally, $a_{41} = 1$. However, this contradicts $b_{1,41} = 1$. Thus, since we can perform the same construction starting from a_9 or a_{41}, the proposition g_2 is never satisfiable; alternatively, one says that the graph $\mathcal{G}_2$ is not true/false colorable, i.e. there is no consistent attribution of truth values to the vertices.

Springer

http://www.springer.com/978-3-658-09199-6

Testing Quantum Contextuality
The Problem of Compatibility
Szangolies, J.
2015, XVIII, 108 p. 25 illus., Softcover
ISBN: 978-3-658-09199-6