Unknown Quantum States:
The Quantum de Finetti Representation

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Abstract

We present an elementary proof of the *quantum de Finetti representation theorem*, a quantum analogue of de Finetti's classical theorem on exchangeable probability assignments. This contrasts with the original proof of Hudson and Moody [Z. Wahrschein. verw. Geb. **33**, 343 (1976)], which relies on advanced mathematics and does not share the same potential for generalization. The classical de Finetti theorem provides an operational definition of the concept of an unknown probability in Bayesian probability theory, where probabilities are taken to be degrees of belief instead of objective states of nature. The quantum de Finetti theorem, in a closely analogous fashion, deals with exchangeable density-operator assignments and provides an operational definition of the concept of an "unknown quantum state" in quantum-state tomography. This result is especially important for information-based interpretations of quantum mechanics, where quantum states, like probabilities, are taken to be states of knowledge rather than states of nature. We further demonstrate that the theorem fails for real Hilbert spaces and discuss the significance of this point.

I. INTRODUCTION

What is a quantum state? Since the earliest days of quantum theory, the predominant answer has been that the quantum state is a representation of the observer's knowledge of a system [1]. In and of itself, the quantum state has no objective reality [2]. The authors hold this information-based view quite firmly [3,4]. Despite its association with the founders of quantum theory, however, holding this view does not require a concomitant belief that there is nothing left to learn in quantum foundations. It is quite the opposite in fact: Only by pursuing a promising, but incomplete program can one hope to learn something of lasting value. Challenges to the information-based view arise regularly, and

dealing with these challenges builds an understanding and a problem-solving agility that reading and rereading the founders can never engender [5]. With each challenge successfully resolved, one walks away with a deeper sense of the physical content of quantum theory and a growing confidence for tackling questions of its interpretation and applicability. Questions as fundamental and distinct as "Will a nonlinear extension of quantum mechanics be needed to quantize gravity?" [6,7] and "Which physical resources actually make quantum computation efficient?" [8,9] start to feel tractable (and even connected) from this perspective.

In this paper, we tackle an understanding-building exercise very much in the spirit of these remarks. It is motivated by an apparent conundrum arising from our own specialization in physics, quantum information theory. The issue is that of the *unknown* quantum state.

There is hardly a paper in the field of quantum information that does not make use of the idea of an "unknown quantum state." Unknown quantum states are teleported [10,11], protected with quantum error correcting codes [12,13], and used to check for quantum eavesdropping [14,15]. The list of uses, already long, grows longer each day. Yet what can the term "unknown quantum state" mean? In an information-based interpretation of quantum mechanics, the term is an oxymoron: If quantum states, by their very definition, are states of knowledge and not states of nature [16], then the state is *known* by someone—at the very least, by the describer himself.

This message is the main point of our paper. Faced with a procedure that uses the idea of an unknown quantum state in its description, a consistent information-based interpretation of quantum mechanics offers only two alternatives:

- The owner of the unknown state—a further decision-making agent or observer—must be explicitly identified. In this case, the unknown state is merely a stand-in for the unknown *state of knowledge* of an essential player who went unrecognized in the original formulation.

- If there is clearly no further decision-making agent or observer on the scene, then a way must be found to reëxpress the procedure with the term "unknown state" banished from the formulation. In this case, the end-product of the effort is a single quantum state used for describing the entire procedure—namely, the state that captures the describer's state of knowledge.

Of course, those inclined to an objectivist interpretation of quantum mechanics [17]— that is, an interpretation where quantum states are more like states of nature than states of knowledge—might be tempted to believe that the scarcity of existing analyses of this kind is a hint that quantum states do indeed have some sort of objective status. Why would such currency be made of the unknown-state concept were it not absolutely necessary? As a rejoinder, we advise caution to the objectivist: Tempting though it is to grant objective status to all the mathematical objects in a physical theory, there is much to be gained by a careful delineation of the subjective and objective parts. A case in point is provided by E. T. Jaynes' [18–20] insistence that entropy is a subjective quantity, a measure of ignorance about a physical system. One of the many fruits of this point of view can be found in the definitive solution [21] to the long-standing Maxwell demon problem [22], where it was realized that the information collected by a demon and used by it to extract work from heat has a thermodynamic cost at least as large as the work extracted [23].
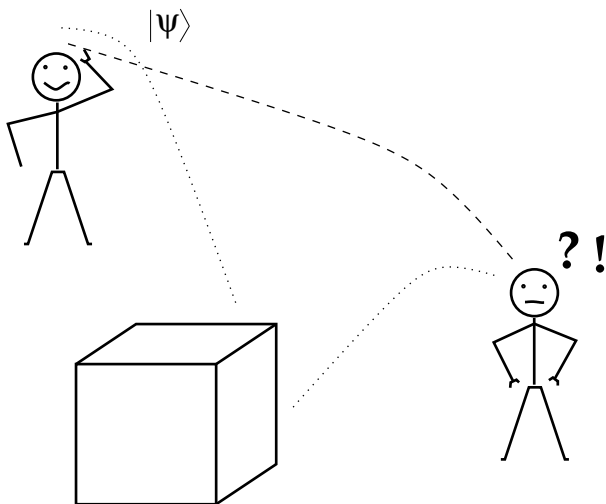
FIGURES

FIG. 1. What can the term "unknown state" mean if quantum states are taken exclusively to be states of knowledge rather than states of nature? When we say that a system has an unknown state, must we always imagine a further observer whose state of knowledge is symbolized by some $|\psi\rangle$, and it is the identity of the symbol that we are ignorant of?

The example analyzed in detail in this paper provides another case. Along the way, it brings to light a new and distinct point about why quantum mechanics makes use of complex Hilbert spaces rather than real or quaternionic ones [24–27]. Furthermore, the method we use to prove our main theorem employs a novel measurement technique that might be of use in the laboratory.

We analyze in depth a particular use of unknown states, which comes from the measurement technique known as *quantum-state tomography* [28–30]. The usual description of tomography is this. A device of some sort, say a nonlinear optical medium driven by a laser, repeatedly prepares many instances of a quantum system, say many temporally distinct modes of the electromagnetic field, in a fixed quantum state ρ, pure or mixed. An experimentalist who wishes to characterize the operation of the device or to calibrate it for future use might be able to perform measurements on the systems it prepares even if he cannot get at the device itself. This can be useful if the experimenter has some prior knowledge of the device's operation that can be translated into a probability distribution over states. Then learning about the state will also be learning about the device. Most importantly, though, this description of tomography assumes that the precise state ρ is unknown. The goal of the experimenter is to perform enough measurements, and enough kinds of measurements (on a large enough sample), to estimate the identity of ρ.

This is clearly an example where there is no further player on whom to pin the unknown state as a state of knowledge. Any attempt to find a player for the pin is entirely artificial: Where would the player be placed? On the inside of the device the tomographer is trying to characterize [31]? The only available course for an information-based interpretation of quantum-state tomography is the second strategy listed above—to banish completely the idea of the unknown state from the formulation of tomography.
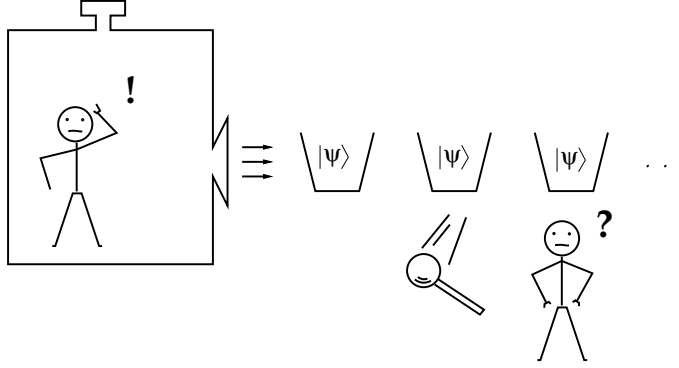
FIG. 2. To make sense of quantum tomography, must we go to the extreme of imagining a "man in the box" who has a better description of the systems than we do? How contrived our usage would be if that were so!

To do this, we take a cue from the field of Bayesian probability theory [32–34], prompted by the realization that Bayesian probability is to probability theory in general what an information-based interpretation is to quantum mechanics [3,35]. In Bayesian theory, probabilities are not objective states of nature, but rather are taken explicitly to be measures of credible belief, reflecting one's state of knowledge. The overarching Bayesian theme is to identify the conditions under which a set of decision-making agents can come to a common belief or probability assignment for a random variable even though their initial beliefs differ [34]. Following that theme is the key to understanding tomography from the informational point of view.

The offending classical concept is an "unknown probability," an oxymoron for the same reason as an unknown quantum state. The procedure analogous to quantum-state tomography is the estimation of an unknown probability from the results of repeated trials on "identically prepared systems," all of which are said to be described by the same, but unknown probability. The way to eliminate unknown probabilities from the discussion, introduced by Bruno de Finetti in the early 1930s [36,37], is to focus on the equivalence of repeated trials, which means the systems are indistinguishable as far as probabilistic predictions are concerned and thus that a probability assignment for multiple trials should be symmetric under permutation of the systems. With his *classical representation theorem*, de Finetti [36] showed that a multi-trial probability assignment that is permutation-symmetric for an arbitrarily large number of trials—de Finetti called such multi-trial probabilities *exchangeable*—is equivalent to a probability for the "unknown probabilities." Thus the unsatisfactory concept of an unknown probability vanishes from the description in favor of the fundamental idea of assigning an exchangeable probability distribution to multiple trials.

This cue in hand, it is easy to see how to reword the description of quantum-state tomography to meet our goals. What is relevant is simply a judgment on the part of the experimenter—notice the essential subjective character of this "judgment"—that there is no distinction between the systems the device is preparing. In operational terms, this is the judgment that *all the systems are and will be the same as far as observational predictions are concerned*. At first glance this statement might seem to be contentless, but the important point is this: To make this statement, one need never use the notion of an unknown state— a completely operational description is good enough. Putting it into technical terms, the statement is that if the experimenter judges a collection of N of the device's outputs to have

an overall quantum state $\rho^{(N)}$, he will also judge any permutation of those outputs to have the same quantum state $\rho^{(N)}$. Moreover, he will do this no matter how large the number N is. This, complemented only by the consistency condition that for any N the state $\rho^{(N)}$ be derivable from $\rho^{(N+1)}$, makes for the complete story.

The words "quantum state" appear in this formulation, just as in the original formulation of tomography, but there is no longer any mention of *unknown* quantum states. The state $\rho^{(N)}$ is known by the experimenter (if no one else), for it represents his state of knowledge. More importantly, the experimenter is in a position to make an unambiguous statement about the structure of the whole sequence of states $\rho^{(N)}$: Each of the states $\rho^{(N)}$ has a kind of permutation invariance over its factors. The content of the *quantum de Finetti representation theorem* [38,39]—a new proof of which is the main technical result of this paper—is that a sequence of states $\rho^{(N)}$ can have these properties, which are said to make it an *exchangeable* sequence, if and only if each term in it can also be written in the form

$$\rho^{(N)} = \int P(\rho)\, \rho^{\otimes N}\, d\rho \;, \tag{1.1}$$

where

$$\rho^{\otimes N} = \underbrace{\rho \otimes \rho \otimes \cdots \otimes \rho}_{\substack{N\text{-fold tensor} \\ \text{product}}} \tag{1.2}$$

and $P(\rho)$ is a fixed probability distribution over the density operators.

The interpretive import of this theorem is paramount. It alone gives a mandate to the term unknown state in the usual description of tomography. It says that the experimenter can act *as if* his state of knowledge $\rho^{(N)}$ comes about because he knows there is a "man in the box," hidden from view, repeatedly preparing the same state ρ. He does not know which such state, and the best he can say about the unknown state is captured in the probability distribution $P(\rho)$.

The quantum de Finetti theorem furthermore makes a connection to the overarching theme of Bayesianism stressed above. It guarantees for two independent observers—as long as they have a rather minimal agreement in their initial beliefs—that the outcomes of a sufficiently informative set of measurements will force a convergence in their state assignments for the remaining systems [40]. This "minimal" agreement is characterized by a judgment on the part of both parties that the sequence of systems is exchangeable, as described above, and a promise that the observers are not absolutely inflexible in their opinions. Quantitatively, the latter means that though $P(\rho)$ might be arbitrarily close to zero, it can never vanish.

This coming to agreement works because an exchangeable density operator sequence can be updated to reflect information gathered from measurements by a quantum version of Bayes's rule for updating probabilities. Specifically, if measurements on K systems yield results D_K, then the state of additional systems is constructed as in Eq. (1.1), but using an updated probability on density operators given by

$$P(\rho|D_K) = \frac{P(D_K|\rho)P(\rho)}{P(D_K)} \;. \tag{1.3}$$

Here $P(D_K|\rho)$ is the probability to obtain the measurement results D_K, given the state $\rho^{\otimes K}$ for the K measured systems, and $P(D_K) = \int P(D_K|\rho) P(\rho) \, d\rho$ is the unconditional probability for the measurement results. Equation (1.3) is a kind of *quantum Bayes rule* [40]. For a sufficiently informative set of measurements, as K becomes large, the updated probability $P(\rho|D_K)$ becomes highly peaked on a particular state ρ_{D_K} dictated by the measurement results, regardless of the prior probability $P(\rho)$, as long as $P(\rho)$ is nonzero in a neighborhood of ρ_{D_K}. Suppose the two observers have different initial beliefs, encapsulated in different priors $P_i(\rho)$, $i = 1, 2$. The measurement results force them to a common state of knowledge in which any number N of additional systems are assigned the product state $\rho_{D_K}^{\otimes N}$, i.e.,

$$\int P_i(\rho|D_K)\, \rho^{\otimes N}\, d\rho \quad \longrightarrow \quad \rho_{D_K}^{\otimes N}\,, \tag{1.4}$$

independent of i, for K sufficiently large.

This shifts the perspective on the purpose of quantum-state tomography: It is not about uncovering some "unknown state of nature," but rather about the various observers' coming to agreement over future probabilistic predictions [41]. In this connection, it is interesting to note that the quantum de Finetti theorem and the conclusions just drawn from it work only within the framework of complex vector-space quantum mechanics. For quantum mechanics based on real and quaternionic Hilbert spaces [24,25], the connection between exchangeable density operators and unknown quantum states does not hold.

The plan of the remainder of the paper is as follows. In Sec. II we discuss the classical de Finetti representation theorem [36,42] in the context of Bayesian probability theory. It was our familiarity with the classical theorem [43,44] that motivated our reconsideration of quantum-state tomography. In Sec. III we introduce the information-based formulation of tomography in terms of exchangeable multi-system density operators, accompanied by a critical discussion of objectivist formulations of tomography, and we state the quantum de Finetti representation theorem. Section IV presents an elementary proof of the quantum de Finetti theorem. There, also, we introduce a novel measurement technique for tomography based upon generalized quantum measurements. Finally, in Sec. V we return to the issue of number fields in quantum mechanics and mention possible extensions of the main theorem.

II. THE CLASSICAL DE FINETTI THEOREM

As a preliminary to the quantum problem, we turn our attention to classical probability theory. In doing so we follow a maxim of the late E. T. Jaynes [45]:

> We think it unlikely that the role of probability in quantum theory will be understood until it is generally understood in classical theory .... Indeed, our [seventy-five-year-old] bemusement over the notion of state reduction in [quantum theory] need not surprise us when we note that today, in all applications of probability theory, basically the same controversy rages over whether our probabilities represent real situations, or only incomplete human knowledge.

As Jaynes makes clear, the tension between the objectivist and informational points of view is not new with quantum mechanics. It arises already in classical probability the-

ory in the form of the war between "objective" and "subjective" interpretations [46]. According to the subjective or Bayesian interpretation, probabilities are measures of credible belief, reflecting an agent's potential states of knowledge. On the other hand, the objective interpretations—in all their varied forms, from frequency interpretations to propensity interpretations—attempt to view probabilities as real states of affairs or "states of nature." Following our discussion in Sec. I, it will come as no surprise to the reader that the authors wholeheartedly adopt the Bayesian approach. For us, the ultimate reason is simply our own experience with this question, part of which is an appreciation that objective interpretations inevitably run into insurmountable difficulties. We will not dwell upon these difficulties here; instead, the reader can find a sampling of criticisms in Refs. [20,32–34,47].

We will note briefly, however, that the game of roulette provides an illuminating example. In the European version of the game, the possible outcomes are the numbers $0, 1, \ldots, 36$. For a player without any privileged information, all 37 outcomes have the same probability $p = 1/37$. But suppose that shortly after the ball is launched by the croupier, another player obtains information about the ball's position and velocity relative to the wheel. Using the information obtained, this other player can make more accurate predictions than the first [48]. His probability is peaked around some group of numbers. The probabilities are thus different for two players with different states of knowledge.

Whose probability is the true probability? From the Bayesian viewpoint, this question is meaningless: There is no such thing as a true probability. All probability assignments are subjective assignments based specifically upon one's prior information.

For sufficiently precise data—including precise initial data on positions and velocities and probably also including other details such as surface properties of the wheel—Newtonian mechanics assures us that the outcome can be predicted with certainty. This is an important point: The determinism of classical physics provides a strong reason for adopting the subjectivist view of probabilities [49]. If the conditions of a trial are exactly specified, the outcomes are predictable with certainty, and all probabilities are 0 or 1. In a deterministic theory, all probabilities strictly greater than 0 and less than 1 arise as a consequence of incomplete information and depend upon their assigner's state of knowledge.

Of course, we should keep in mind that our ultimate goal is to consider the status of quantum states and, by way of them, quantum probabilities. One can ask, "Does this not change the flavor of these considerations?" Since quantum mechanics is avowedly *not* a theory of one's ignorance of a set of hidden variables [50,51], how can the probabilities be subjective? In Sec. III we argue that despite the intrinsic indeterminism of quantum mechanics, the essence of the point above carries over to the quantum setting intact. Furthermore, there are specifically quantum-motivated arguments for a Bayesian interpretation of quantum probabilities.

For the present, though, let us consider in some detail the general problem of a repeated experiment—spinning a roulette wheel N times is an example. As discussed briefly in Sec. I, this allows us to make a conceptual connection to quantum-state tomography. Here the individual trials are described by discrete random variables $x_n \in \{1, 2, \ldots, k\}$, $n = 1, \ldots, N$; that is to say, there are N random variables, each of which can assume k discrete values. In an objectivist theory, such an experiment has a standard formulation in which the probability in the multi-trial hypothesis space is given by an independent, identically distributed (i.i.d.) distribution

$$p(x_1, x_2, \ldots, x_N) = p_{x_1} p_{x_2} \cdots p_{x_N} = p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k} \,. \tag{2.1}$$

The number p_j $(j = 1, \ldots, k)$ describes the objective, "true" probability that the result of a single experiment will be j $(j = 1, \ldots, k)$. The variable n_j, on the other hand, is the number of times outcome j is listed in the vector $(x_1, x_2, \ldots, x_N)$. This simple description—for the objectivist—only describes the situation from a kind of "God's eye" point of view. To the experimentalist, the "true" probabilities $p_1, \ldots, p_k$ will very often be *unknown* at the outset. Thus, his burden is to estimate the unknown probabilities by a statistical analysis of the experiment's outcomes.

In the Bayesian approach, it does not make sense to talk about estimating a true probability. Instead, a Bayesian assigns a prior probability distribution $p(x_1, x_2, \ldots, x_N)$ on the multi-trial hypothesis space, which is generally not an i.i.d., and then uses Bayes's theorem to update the distribution in the light of measurement results. A common criticism from the objectivist camp is that the choice of distribution $p(x_1, x_2, \ldots, x_N)$ with which to start the process seems overly arbitrary to them. On what can it be grounded, they would ask? From the Bayesian viewpoint, the subjectivity of the prior is a strength rather than a weakness, because assigning a prior amounts to laying bare the necessarily subjective assumptions behind *any* probabilistic argument, be it Bayesian or objectivist. Choosing a prior among all possible distributions on the multi-trial hypothesis space is, however, a daunting task. As we will now see, the de Finetti representation theorem makes this task tractable.

It is very often the case that one or more features of a problem stand out so clearly that there is no question about how to incorporate them into an initial assignment. In the present case, the key feature is contained in the assumption that an arbitrary number of repeated trials are equivalent. This means that one has no reason to believe there will be a difference between one trial and the next. In this case, the prior distribution is judged to have the sort of permutation symmetry discussed briefly in Sec. I, which de Finetti [37] called *exchangeability*. The rigorous definition of exchangeability proceeds in two stages.

A probability distribution $p(x_1, x_2, \ldots, x_N)$ is said to be *symmetric* (or finitely exchangeable) if it is invariant under permutations of its arguments, i.e., if

$$p(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(N)}) = p(x_1, x_2, \ldots, x_N) \tag{2.2}$$

for any permutation π of the set $\{1, \ldots, N\}$. The distribution $p(x_1, x_2, \ldots, x_N)$ is called *exchangeable* (or infinitely exchangeable) if it is symmetric and if for any integer $M > 0$, there is a symmetric distribution $p_{N+M}(x_1, x_2, \ldots, x_{N+M})$ such that

$$p(x_1, x_2, \ldots, x_N) = \sum_{x_{N+1}, \ldots, x_{N+M}} p_{N+M}(x_1, \ldots, x_N, x_{N+1}, \ldots, x_{N+M}) \,. \tag{2.3}$$

This last statement means the distribution p can be extended to a symmetric distribution of arbitrarily many random variables. Expressed informally, an exchangeable distribution can be thought of as arising from an infinite sequence of random variables whose order is irrelevant.

We now come to the main statement of this section: if a probability distribution $p(x_1, x_2, \ldots, x_N)$ is exchangeable, then it can be written uniquely in the form

$$p(x_1, x_2, \ldots, x_N) = \int_{\mathcal{S}_k} P(\mathbf{p}) \, p_{x_1} p_{x_2} \cdots p_{x_N} \, d\mathbf{p} = \int_{\mathcal{S}_k} P(\mathbf{p}) \, p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k} \, d\mathbf{p} \,, \tag{2.4}$$

where $\mathbf{p} = (p_1, p_2, \ldots, p_k)$, and the integral is taken over the probability simplex

$$\mathcal{S}_k = \left\{ \mathbf{p} : \ p_j \geq 0 \text{ for all } j \text{ and } \sum_{j=1}^{k} p_j = 1 \right\} . \tag{2.5}$$

Furthermore, the function $P(\mathbf{p}) \geq 0$ is required to be a probability density function on the simplex:

$$\int_{\mathcal{S}_k} P(\mathbf{p}) \, d\mathbf{p} = 1 . \tag{2.6}$$

Equation (2.4) comprises the classical de Finetti representation theorem for discrete random variables. For completeness and because it deserves to be more widely familiar in the physics community, we give a simple proof (due to Heath and Sudderth [42]) of the representation theorem for the binary random-variable case in an Appendix.

Let us reiterate the importance of this result for the present considerations. It says that an agent, making solely the judgment of exchangeability for a sequence of random variables x_j, can proceed *as if* his state of knowledge had instead come about through ignorance of an *unknown*, but objectively existent set of probabilities $\mathbf{p}$. His precise ignorance of $\mathbf{p}$ is captured by the "probability on probabilities" $P(\mathbf{p})$. This is in direct analogy to what we desire of a solution to the problem of the unknown quantum state in quantum-state tomography.

As a final note before finally addressing the quantum problem in Sec. III, we point out that both conditions in the definition of exchangeability are crucial for the proof of the de Finetti theorem. In particular, there are probability distributions $p(x_1, x_2, \ldots, x_N)$ that are symmetric, but not exchangeable. A simple example is the distribution $p(x_1, x_2)$ of two binary random variables $x_1, x_2 \in \{0, 1\}$,

$$p(0, 0) = p(1, 1) = 0 , \tag{2.7}$$

$$p(0, 1) = p(1, 0) = \frac{1}{2} . \tag{2.8}$$

One can easily check that $p(x_1, x_2)$ cannot be written as the marginal of a symmetric distribution of three variables, as in Eq. (2.3). Therefore it can have no representation along the lines of Eq. (2.4). (For an extended discussion of this, see Ref. [52].) Indeed, Eqs. (2.7) and (2.8) characterize a perfect "anticorrelation" of the two variables, in contrast to the positive correlation implied by distributions of de Finetti form. The content of this point is that both conditions in the definition of exchangeability (symmetry under interchange and infinite extendibility) are required to ensure, in colloquial terms, "that the future will appear much as the past" [53], rather than, say, the opposite of the past.

III. THE QUANTUM DE FINETTI REPRESENTATION

Let us now return to the problem of quantum-state tomography described in Sec. I. In the objectivist formulation of the problem, a device repeatedly prepares copies of a system in the same quantum state ρ. This is generally a mixed-state density operator on a Hilbert

space $\mathcal{H}_d$ of d dimensions. We call the totality of such density operators $\mathcal{D}_d$. The joint quantum state of the N systems prepared by the device is then given by

$$\rho^{\otimes N} = \rho \otimes \rho \otimes \cdots \otimes \rho \,, \tag{3.1}$$

the N-fold tensor product of ρ with itself. This, of course, is a very restricted example of a density operator on the tensor-product Hilbert space $\mathcal{H}_d^{\otimes N} \equiv \mathcal{H}_d \otimes \cdots \otimes \mathcal{H}_d$. The experimenter, who performs quantum-state tomography, tries to determine ρ as precisely as possible. Depending upon the version of the argument, ρ is interpreted as the "true" state of each of the systems or as a description of the "true" preparation procedure.

We have already articulated our dissatisfaction with this way of stating the problem, but we give here a further sense of why both interpretations above are untenable. Let us deal first with the version where ρ is regarded as the true, objective state of each of the systems. In this discussion it is useful to consider separately the cases of mixed and pure states ρ. The arguments against regarding mixed states as objective properties of a quantum system are essentially the same as those against regarding probabilities as objective. In analogy to the roulette example given in the previous section, we can say that, whenever an observer assigns a mixed state to a physical system, one can think of another observer who assigns a different state based on privileged information.

The quantum argument becomes yet more compelling if the apparently nonlocal nature of quantum states is taken into consideration. Consider two parties, A and B, who are far apart in space, say several light years apart. Each party possesses a spin-$\frac{1}{2}$ particle. Initially the joint state of the two particles is the maximally entangled pure state $\frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle)$. Consequently, A assigns the totally mixed state $\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ to her own particle. Now B makes a measurement on his particle, finds the result 0, and assigns to A's particle the pure state $|0\rangle$. Is this now the "true," objective state of A's particle? At what precise time does the objective state of A's particle change from totally mixed to pure? If the answer is "simultaneously with B's measurement," then what frame of reference should be used to determine simultaneity? These questions and potential paradoxes are avoided if states are interpreted as states of knowledge. In our example, A and B have different states of knowledge and therefore assign different states. For a detailed analysis of this example, see Ref. [54]; for an experimental investigation see Ref. [55].

If one admits that mixed states cannot be objective properties, because another observer, possessing privileged information, can know which pure state underlies the mixed state, then it becomes very tempting to regard the pure states as giving the "true" state of a system. Probabilities that come from pure states would then be regarded as objective, and the probabilities for pure states within an ensemble decomposition of a mixed state would be regarded as subjective, expressing our ignorance of which pure state is the "true" state of the system. An immediate and, in our view, irremediable problem with this idea is that a mixed state has infinitely many ensemble decompositions into pure states [19,56,57], so the distinction between subjective and objective becomes hopelessly blurred.

This problem can be made concrete by the example of a spin-$\frac{1}{2}$ particle. Any pure state of the particle can be written in terms of the Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.2}$$

as

$$|\mathbf{n}\rangle\langle\mathbf{n}| = \frac{1}{2}(I + \mathbf{n}\cdot\boldsymbol{\sigma}) = \frac{1}{2}(I + n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3) , \tag{3.3}$$

where the unit vector $\mathbf{n} = n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3$ labels the pure state, and I denotes the unit operator. An arbitrary state ρ, mixed or pure, of the particle can be expressed as

$$\rho = \frac{1}{2}(I + \mathbf{S}\cdot\boldsymbol{\sigma}) , \tag{3.4}$$

where $0 \leq |\mathbf{S}| \leq 1$. This representation of the states of a spin-$\frac{1}{2}$ particle is called the *Bloch-sphere representation*. If $|\mathbf{S}| < 1$, there is an infinite number of ways in which $\mathbf{S}$ can be written in the form $\mathbf{S} = \sum_j p_j\mathbf{n}_j$, $|\mathbf{n}_j| = 1$, with the numbers p_j comprising a probability distribution, and hence an infinite number of ensemble decompositions of ρ:

$$\rho = \sum_j p_j\frac{1}{2}(I + \mathbf{n}_j\cdot\boldsymbol{\sigma}) = \sum_j p_j|\mathbf{n}_j\rangle\langle\mathbf{n}_j| . \tag{3.5}$$

Suppose for specificity that the particle's state is a mixed state with $\mathbf{S} = \frac{1}{2}\mathbf{e}_3$. Writing $\mathbf{S} = \frac{3}{4}\mathbf{e}_3 + \frac{1}{4}(-\mathbf{e}_3)$ gives the eigendecomposition,

$$\rho = \frac{3}{4}|\mathbf{e}_3\rangle\langle\mathbf{e}_3| + \frac{1}{4}|-\mathbf{e}_3\rangle\langle-\mathbf{e}_3| , \tag{3.6}$$

where we are to regard the probabilities 3/4 and 1/4 as subjective expressions of ignorance about which eigenstate is the "true" state of the particle. Writing $\mathbf{S} = \frac{1}{2}\mathbf{n}_+ + \frac{1}{2}\mathbf{n}_-$, where $\mathbf{n}_\pm = \frac{1}{2}\mathbf{e}_3 \pm \frac{\sqrt{3}}{2}\mathbf{e}_x$, gives another ensemble decomposition,

$$\rho = \frac{1}{2}|\mathbf{n}_+\rangle\langle\mathbf{n}_+| + \frac{1}{2}|\mathbf{n}_-\rangle\langle\mathbf{n}_-| , \tag{3.7}$$

where we are now to regard the two probabilities of 1/2 as expressing ignorance of whether the "true" state is $|\mathbf{n}_+\rangle$ or $|\mathbf{n}_-\rangle$.

The problem becomes acute when we ask for the probability that a measurement of the z component of spin yields spin up; this probability is given by $\langle\mathbf{e}_3|\rho|\mathbf{e}_3\rangle = \frac{1}{2}(1 + \frac{1}{2}\langle\mathbf{e}_3|\sigma_3|\mathbf{e}_3\rangle) = 3/4$. The eigendecomposition gets this probability by the route

$$\langle\mathbf{e}_3|\rho|\mathbf{e}_3\rangle = \frac{3}{4}\underbrace{|\langle\mathbf{e}_3|\mathbf{e}_3\rangle|^2}_{1} + \frac{1}{4}\underbrace{|\langle\mathbf{e}_3|-\mathbf{e}_3\rangle|^2}_{0} . \tag{3.8}$$

Here the "objective" quantum probabilities, calculated from the eigenstates, report that the particle definitely has spin up or definitely has spin down; the overall probability of 3/4 comes from mixing these objective probabilities with the subjective probabilities for the eigenstates. The decomposition (3.7) gets the same overall probability by a different route,

$$\langle\mathbf{e}_3|\rho|\mathbf{e}_3\rangle = \frac{1}{2}\underbrace{|\langle\mathbf{e}_3|\mathbf{n}_+\rangle|^2}_{3/4} + \frac{1}{2}\underbrace{|\langle\mathbf{e}_3|\mathbf{n}_-\rangle|^2}_{3/4} . \tag{3.9}$$

Now the quantum probabilities tell us that the "objective" probability for the particle to have spin up is 3/4. This simple example illustrates the folly of trying to have two kinds of probabilities in quantum mechanics. The lesson is that if a density operator is even partially a reflection of one's state of knowledge, the multiplicity of ensemble decomposition means that a pure state must also be a state of knowledge.

Return now to the second version of the objectivist formulation of tomography, in which the experimenter is said to be using quantum-state tomography to determine an unknown preparation procedure. Imagine that the tomographic reconstruction results in the mixed state ρ, rather than a pure state, as in fact all actual laboratory procedures do. Now there is a serious problem, because a mixed state does not correspond to a well-defined procedure, but is itself a probabilistic mixture of well-defined procedures, i.e., pure states. The experimenter is thus trying to determine an unknown procedure that has no unique decomposition into well defined procedures. Thus he cannot be said to be determining an unknown procedure at all. This problem does not arise in an information-based interpretation, according to which all quantum states, pure or mixed, are states of knowledge. In analogy to the classical case, the quantum de Finetti representation provides an operational definition for the idea of an unknown quantum state in this case.

Let us therefore turn to the information-based formulation of the quantum-state tomography problem. Before the tomographic measurements, the Bayesian experimenter assigns a prior quantum state to the joint system composed of the N systems, reflecting his prior state of knowledge. Just as in the classical case, this is a daunting task unless the assumption of exchangeability is justified.

The definition of the quantum version of exchangeability is closely analogous to the classical definition. Again, the definition proceeds in two stages. First, a joint state $\rho^{(N)}$ of N systems is said to be *symmetric* (or finitely exchangeable) if it is invariant under any permutation of the systems. To see what this means formally, first write out $\rho^{(N)}$ with respect to any orthonormal tensor-product basis on $\mathcal{H}_d^{\otimes N}$, say $|i_1\rangle|i_2\rangle \cdots |i_N\rangle$, where $i_k \in \{1, 2, \ldots, d\}$ for all k. The joint state takes the form

$$\rho^{(N)} = \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N} |i_1\rangle \cdots |i_N\rangle\langle j_1| \cdots \langle j_N| , \qquad (3.10)$$

where $R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N}$ is the density matrix in this representation. What we demand is that for any permutation π of the set $\{1, \ldots, N\}$,

$$\rho^{(N)} = \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N} |i_{\pi^{-1}(1)}\rangle \cdots |i_{\pi^{-1}(N)}\rangle\langle j_{\pi^{-1}(1)}| \cdots \langle j_{\pi^{-1}(N)}|$$

$$= \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} R^{(N)}_{i_{\pi(1)},\ldots,i_{\pi(N)};j_{\pi(1)},\ldots,j_{\pi(N)}} |i_1\rangle \cdots |i_N\rangle\langle j_1| \cdots \langle j_N| , \qquad (3.11)$$

which is equivalent to

$$R^{(N)}_{i_{\pi(1)},\ldots,i_{\pi(N)};j_{\pi(1)},\ldots,j_{\pi(N)}} = R^{(N)}_{i_1,\ldots,i_N;j_1,\ldots,j_N} . \qquad (3.12)$$

The state $\rho^{(N)}$ is said to be *exchangeable* (or infinitely exchangeable) if it is symmetric and if, for any $M > 0$, there is a symmetric state $\rho^{(N+M)}$ of $N + M$ systems such that the marginal density operator for N systems is $\rho^{(N)}$, i.e.,

$$\rho^{(N)} = \mathrm{tr}_M \, \rho^{(N+M)} \, , \tag{3.13}$$

where the trace is taken over the additional M systems. In explicit basis-dependent notation, this requirement is

$$\rho^{(N)} = \sum_{i_1,\ldots,i_N;j_1,\ldots,j_N} \left(\sum_{i_{N+1},\ldots,i_{N+M}} R^{(N+M)}_{i_1,\ldots,i_N,i_{N+1},\ldots,i_{N+M};j_1,\ldots,j_N,i_{N+1},\ldots,i_{N+M}} \right) |i_1\rangle \cdots |i_N\rangle \langle j_1| \cdots \langle j_N| \, . \tag{3.14}$$

In analogy to the classical case, an exchangeable density operator can be thought of informally as the description of a subsystem of an infinite sequence of systems whose order is irrelevant.

The precise statement of the quantum de Finetti representation theorem [38,58] is that any exchangeable state of N systems can be written uniquely in the form

$$\rho^{(N)} = \int_{\mathcal{D}_d} P(\rho) \, \rho^{\otimes N} \, d\rho \, . \tag{3.15}$$

Here $P(\rho) \geq 0$ is normalized by

$$\int_{\mathcal{D}_d} P(\rho) \, d\rho = 1 \, , \tag{3.16}$$

with $d\rho$ being a suitable measure on density operator space $\mathcal{D}_d$ [e.g., one could choose the standard flat measure $d\rho = S^2 dS \, d\Omega$ in the parametrization (3.4) for a spin-$\frac{1}{2}$ particle]. The upshot of the theorem, as already advertised, is that it makes it possible to think of an exchangeable quantum-state assignment *as if* it were a probabilistic mixture characterized by a probability density $P(\rho)$ for the product states $\rho^{\otimes N}$.

Just as in the classical case, both components of the definition of exchangeability are crucial for arriving at the representation theorem of Eq. (3.15). The reason now, however, is much more interesting than it was previously. In the classical case, extendibility was used solely to exclude anticorrelated probability distributions. Here extendibility is necessary to exclude the possibility of Bell inequality violations for measurements on the separate systems. This is because the assumption of symmetry alone for an N-party quantum system does not exclude the possibility of quantum entanglement, and all states that can be written as a mixture of product states—of which Eq. (3.15) is an example—have no entanglement [59]. A very simple counterexample is the Greenberger-Horne-Zeilinger state of three spin-$\frac{1}{2}$ particles [60],

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}} \Big(|0\rangle|0\rangle|0\rangle + |1\rangle|1\rangle|1\rangle \Big) \, , \tag{3.17}$$

which is symmetric, but is not extendible to a symmetric state on four systems. This follows because the only states of four particles that marginalize to a three-particle pure state, like the GHZ state, are product states of the form $|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}| \otimes \rho$, where ρ is the state of the fourth particle; such states clearly cannot be symmetric. These considerations show that in order for the proposed theorem to be valid, it must be the case that as M increases in Eq. (3.13), the possibilities for entanglement in the separate systems compensatingly decrease [61].

IV. PROOF OF THE QUANTUM DE FINETTI THEOREM

To prove the quantum version of the de Finetti theorem, we rely on the classical theorem as much as possible. We start from an exchangeable density operator $\rho^{(N)}$ defined on N copies of a system. We bring the classical theorem to our aid by imagining a sequence of identical quantum measurements on the separate systems and considering the outcome probabilities they would produce. Because $\rho^{(N)}$ is assumed exchangeable, such identical measurements give rise to an exchangeable probability distribution for the outcomes. The trick is to recover enough information from the exchangeable statistics of these measurements to characterize the exchangeable density operators.

With this in mind, the proof is expedited by making use of the theory of generalized quantum measurements or positive operator-valued measures (POVMs) [62,63]. We give a brief introduction to that theory. The common textbook notion of a measurement— that is, a von Neumann measurement—is that any laboratory procedure counting as an observation can be identified with a Hermitian operator O on the Hilbert space $\mathcal{H}_d$ of the system. Depending upon the presentation, the measurement outcomes are identified either with the eigenvalues μ_i or with a complete set of normalized eigenvectors $|i\rangle$ for O. When the quantum state is ρ, the probabilities for the various outcomes are computed from the eigenprojectors $\Pi_i = |i\rangle\langle i|$ via the standard Born rule,

$$p_i = \mathrm{tr}(\rho \Pi_i) = \langle i|\rho|i\rangle \ . \tag{4.1}$$

This rule gives a consistent probability assignment because the eigenprojectors Π_i are positive-semidefinite operators, which makes the p_i nonnegative, and because the projectors form a resolution of the identity operator I,

$$\sum_{i=1}^{d} \Pi_i = I \ , \tag{4.2}$$

which guarantees that $\sum_i p_i = 1$.

POVMs generalize the textbook notion of measurement by distilling the essential properties that make the Born rule work. The generalized notion of measurement is this: *any* set $\mathcal{E} = \{E_\alpha\}$ of positive-semidefinite operators on $\mathcal{H}_d$ that forms a resolution of the identity, i.e., that satisfies

$$\langle\psi|E_\alpha|\psi\rangle \geq 0 \ , \quad \text{for all } |\psi\rangle \in \mathcal{H}_d \tag{4.3}$$

and

$$\sum_{\alpha} E_\alpha = I \ , \tag{4.4}$$

corresponds to at least one laboratory procedure counting as a measurement. The outcomes of the measurement are identified with the indices α, and the probabilities of those outcomes are computed according to the generalized Born rule,

$$p_\alpha = \mathrm{tr}(\rho E_\alpha) \ . \tag{4.5}$$

The set $\mathcal{E}$ is called a POVM, and the operators E_α are called POVM elements. Unlike von Neumann measurements, there is no limitation on the number of values α can take, the operators E_α need not be rank-1, and there is no requirement that the E_α be mutually orthogonal. This definition has important content because the older notion of measurement is simply too restrictive: there are laboratory procedures that clearly should be called "measurements," but that cannot be expressed in terms of the von Neumann measurement process alone.

One might wonder whether the existence of POVMs contradicts everything taught about standard measurements in the traditional graduate textbooks [64] and the well-known classics [65]. Fortunately it does not. The reason is that any POVM can be represented formally as a standard measurement on an ancillary system that has interacted in the past with the system of main interest. Thus, in a certain sense, von Neumann measurements capture everything that can be said about quantum measurements [63]. A way to think about this is that by learning something about the ancillary system through a standard measurement, one in turn learns something about the system of real interest. Indirect though this might seem, it can be a very powerful technique, sometimes revealing information that could not have been revealed otherwise [66].

For instance, by considering POVMs, one can consider measurements with an outcome cardinality that exceeds the dimensionality of the Hilbert space. What this means is that whereas the statistics of a von Neumann measurement can only reveal information about the d diagonal elements of a density operator ρ, through the probabilities $\mathrm{tr}(\rho\Pi_i)$, the statistics of a POVM generally can reveal things about the off-diagonal elements, too. It is precisely this property that we take advantage of in our proof of the quantum de Finetti theorem.

Our problem hinges on finding a special kind of POVM, one for which any set of outcome probabilities specifies a unique operator. This boils down to a problem in pure linear algebra. The space of operators on $\mathcal{H}_d$ is itself a linear vector space of dimension d^2. The quantity $\mathrm{tr}(A^\dagger B)$ serves as an inner product on that space. If the POVM elements E_α span the space of operators—there must be at least d^2 POVM elements in the set—the measurement probabilities $p_\alpha = \mathrm{tr}(\rho E_\alpha)$—now thought of as *projections* in the directions E_α—are sufficient to specify a unique operator ρ. Two distinct density operators ρ and σ must give rise to different measurement statistics. Such measurements, which might be called *informationally complete*, have been studied for some time [67].

For our proof we need a slightly refined notion—that of a *minimal* informationally complete measurement. If an informationally complete POVM has more than d^2 operators E_α, these operators form an overcomplete set. This means that given a set of outcome probabilities p_α, there is generally *no* operator A that generates them according to $p_\alpha = \mathrm{tr}(AE_\alpha)$. Our proof requires the existence of such an operator, so we need a POVM that has precisely d^2 linearly independent POVM elements E_α. Such a POVM has the minimal number of POVM elements to be informationally complete. Given a set of outcome probabilities p_α, there is a unique operator A such that $p_\alpha = \mathrm{tr}(AE_\alpha)$, even though, as we discuss below, A is not guaranteed to be a density operator.

Do minimal informationally complete POVMs exist? The answer is yes. We give here a simple way to produce one, though there are surely more elegant ways with greater symmetry. Start with a complete orthonormal basis $|e_j\rangle$ on $\mathcal{H}_d$, and let $\Gamma_{jk} = |e_j\rangle\langle e_k|$. It is easy to check that the following d^2 rank-1 projectors Π_α form a linearly independent set.

1. For $\alpha = 1, \ldots, d$, let

$$\Pi_\alpha \equiv \Gamma_{jj}, \tag{4.6}$$

where j, too, runs over the values $1, \ldots, d$.

2. For $\alpha = d + 1, \ldots, \frac{1}{2}d(d+1)$, let

$$\Pi_\alpha \equiv \Gamma_{jk}^{(1)} = \frac{1}{2}\big(|e_j\rangle + |e_k\rangle\big)\big(\langle e_j| + \langle e_k|\big) = \frac{1}{2}(\Gamma_{jj} + \Gamma_{kk} + \Gamma_{jk} + \Gamma_{kj}), \tag{4.7}$$

where $j < k$.

3. Finally, for $\alpha = \frac{1}{2}d(d+1) + 1, \ldots, d^2$, let

$$\Pi_\alpha \equiv \Gamma_{jk}^{(2)} = \frac{1}{2}\big(|e_j\rangle + i|e_k\rangle\big)\big(\langle e_j| - i\langle e_k|\big) = \frac{1}{2}(\Gamma_{jj} + \Gamma_{kk} - i\Gamma_{jk} + i\Gamma_{kj}), \tag{4.8}$$

where again $j < k$.

All that remains is to transform these (positive-semidefinite) linearly independent operators Π_α into a proper POVM. This can be done by considering the positive semidefinite operator G defined by

$$G = \sum_{\alpha=1}^{d^2} \Pi_\alpha . \tag{4.9}$$

It is straightforward to show that $\langle \psi | G | \psi \rangle > 0$ for all $|\psi\rangle \neq 0$, thus establishing that G is positive definite (i.e., Hermitian with positive eigenvalues) and hence invertible. Applying the (invertible) linear transformation $X \to G^{-1/2} X G^{-1/2}$ to Eq. (4.9), we find a valid decomposition of the identity,

$$I = \sum_{\alpha=1}^{d^2} G^{-1/2} \Pi_\alpha G^{-1/2} . \tag{4.10}$$

The operators

$$E_\alpha = G^{-1/2} \Pi_\alpha G^{-1/2} \tag{4.11}$$

satisfy the conditions of a POVM, Eqs. (4.3) and (4.4), and moreover, they retain the rank and linear independence of the original Π_α.

With this generalized measurement (or any other one like it), we can return to the main line of proof. Recall we assumed that we captured our state of knowledge by an exchangeable density operator $\rho^{(N)}$. Consequently, repeated application of the (imagined) measurement $\mathcal{E}$ must give rise to an exchangeable probability distribution over the N random variables $\alpha_n \in \{1, 2, \ldots, d^2\}$, $n = 1, \ldots, N$. We now analyze these probabilities.

Quantum mechanically, it is valid to think of the N repeated measurements of $\mathcal{E}$ as a single measurement on the Hilbert space $\mathcal{H}_d^{\otimes N} \equiv \mathcal{H}_d \otimes \cdots \otimes \mathcal{H}_d$. This measurement, which we denote $\mathcal{E}^{\otimes N}$, consists of d^{2N} POVM elements of the form $E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}$. The probability

of any particular outcome sequence of length N, namely $\boldsymbol{\alpha} \equiv (\alpha_1, \dots, \alpha_N)$, is given by the standard quantum rule,

$$p^{(N)}(\boldsymbol{\alpha}) = \mathrm{tr}(\,\rho^{(N)}\, E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N})\,. \tag{4.12}$$

Because the distribution $p^{(N)}(\boldsymbol{\alpha})$ is exchangeable, we have by the classical de Finetti theorem [see Eq. (2.4)] that there exists a unique probability density $P(\mathbf{p})$ on $\mathcal{S}_{d^2}$ such that

$$p^{(N)}(\boldsymbol{\alpha}) = \int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, p_{\alpha_1} p_{\alpha_2} \cdots p_{\alpha_N}\, d\mathbf{p}\,. \tag{4.13}$$

It should now begin to be apparent why we chose to imagine a measurement $\mathcal{E}$ consisting of precisely d^2 linearly independent elements. This allows us to assert the existence of a *unique* operator $A_{\mathbf{p}}$ on $\mathcal{H}_d$ corresponding to each point $\mathbf{p}$ in the domain of the integral. The ultimate goal here is to turn Eqs. (4.12) and (4.13) into a single operator equation.

With that in mind, let us define $A_{\mathbf{p}}$ as the unique operator satisfying the following d^2 linear equations:

$$\mathrm{tr}(A_{\mathbf{p}} E_\alpha) = p_\alpha\,, \qquad \alpha = 1, \dots, d^2\,. \tag{4.14}$$

Inserting this definition into Eq. (4.13) and manipulating it according to the algebraic rules of tensor products—namely $(A \otimes B)(C \otimes D) = AC \otimes BD$ and $\mathrm{tr}(A \otimes B) = (\mathrm{tr}A)(\mathrm{tr}B)$—we see that

$$\begin{aligned}
p^{(N)}(\boldsymbol{\alpha}) &= \int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, \mathrm{tr}(A_{\mathbf{p}} E_{\alpha_1}) \cdots \mathrm{tr}(A_{\mathbf{p}} E_{\alpha_N})\, d\mathbf{p} \\
&= \int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, \mathrm{tr}(A_{\mathbf{p}} E_{\alpha_1} \otimes \cdots \otimes A_{\mathbf{p}} E_{\alpha_N})\, d\mathbf{p} \\
&= \int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, \mathrm{tr}[A_{\mathbf{p}}^{\otimes N}\, (E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N})]\, d\mathbf{p}\,.
\end{aligned} \tag{4.15}$$

If we further use the linearity of the trace, we can write the same expression as

$$p^{(N)}(\boldsymbol{\alpha}) = \mathrm{tr}\left[\left(\int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, A_{\mathbf{p}}^{\otimes n}\, d\mathbf{p}\right) E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}\right]\,. \tag{4.16}$$

The identity between Eqs. (4.12) and (4.16) must hold for all sequences $\boldsymbol{\alpha}$. It follows that

$$\rho^{(N)} = \int_{\mathcal{S}_{d^2}} P(\mathbf{p})\, A_{\mathbf{p}}^{\otimes N}\, d\mathbf{p}\,. \tag{4.17}$$

This is because the operators $E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}$ form a complete basis for the vector space of operators on $\mathcal{H}_d^{\otimes N}$.

Equation (4.17) already looks very much like our sought after goal, but we are not there quite yet. At this stage one has no right to assert that the $A_{\mathbf{p}}$ are density operators. Indeed they generally are not: the integral (4.13) ranges over some points $\mathbf{p}$ in $\mathcal{S}_{d^2}$ that cannot be generated by applying the measurement $\mathcal{E}$ to *any* quantum state. Hence some of the $A_{\mathbf{p}}$ in the integral representation are ostensibly nonphysical. An example might be helpful. Consider any four spin-$\frac{1}{2}$ pure states $|\mathbf{n}_\alpha\rangle$ on $\mathcal{H}_2$ for which the vectors $\mathbf{n}_\alpha$ in the

Bloch-sphere representation (3.3) are the vertices of a regular tetrahedron. One can check that the elements $E_\alpha = \frac{1}{2}|\mathbf{n}_\alpha\rangle\langle\mathbf{n}_\alpha|$ comprise a minimal informationally complete POVM. For this POVM, because of the factor $\frac{1}{2}$ in front of each projector, it is always the case that $p_\alpha = \text{tr}(\rho E_\alpha) \leq \frac{1}{2}$. Therefore, this measurement simply cannot generate a probability distribution like $\mathbf{p} = (\frac{3}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{16})$, which is nevertheless in the domain of the integral in Eq. (4.13).

The solution to this conundrum is provided by the overall requirement that $\rho^{(N)}$ be a valid density operator. This requirement places a significantly more stringent constraint on the distribution $P(\mathbf{p})$ than was the case in the classical representation theorem. In particular, it must be the case that $P(\mathbf{p})$ vanishes whenever the corresponding $A_\mathbf{p}$ is not a proper density operator. Let us move toward showing that.

We first need to delineate two properties of the operators $A_\mathbf{p}$. One is that they are Hermitian. The argument is simply

$$\text{tr}(E_\alpha A_\mathbf{p}^\dagger) = \text{tr}\left[(A_\mathbf{p} E_\alpha)^\dagger\right] = [\text{tr}(A_\mathbf{p} E_\alpha)]^* = \text{tr}(A_\mathbf{p} E_\alpha) , \tag{4.18}$$

where the last step follows from Eq. (4.14). Because the E_α are a complete set of linearly independent operators, it follows that $A_\mathbf{p}^\dagger = A_\mathbf{p}$. The second property tells us something about the eigenvalues of $A_\mathbf{p}$:

$$1 = \sum_\alpha p_\alpha = \text{tr}\left(A_\mathbf{p} \sum_\alpha E_\alpha\right) = \text{tr}A_\mathbf{p} . \tag{4.19}$$

In other words the (real) eigenvalues of $A_\mathbf{p}$ must sum to unity.

We now show that these two facts go together to imply that if there are any nonphysical $A_\mathbf{p}$ with positive weight $P(\mathbf{p})$ in Eq. (4.17), then one can find a measurement for which $\rho^{(N)}$ produces illegal "probabilities" for sufficiently large N. For instance, take a particular $A_\mathbf{q}$ in Eq. (4.17) that has at least one negative eigenvalue $-\lambda < 0$. Let $|\psi\rangle$ be a normalized eigenvector corresponding to that eigenvalue and consider the binary-valued POVM consisting of the elements $\widetilde{\Pi} = |\psi\rangle\langle\psi|$ and $\Pi = I - \widetilde{\Pi}$. Since $\text{tr}(A_\mathbf{q}\widetilde{\Pi}) = -\lambda < 0$, it is true by Eq. (4.19) that $\text{tr}(A_\mathbf{q}\Pi) = 1 + \lambda > 1$. Consider repeating this measurement over and over. In particular, let us tabulate the probability of getting outcome Π for every single trial to the exclusion of all other outcomes.

The gist of the contradiction is most easily seen by *imagining* that Eq. (4.17) is really a discrete sum:

$$\rho^{(N)} = P(\mathbf{q}) A_\mathbf{q}^{\otimes N} + \sum_{\mathbf{p} \neq \mathbf{q}} P(\mathbf{p}) A_\mathbf{p}^{\otimes N} . \tag{4.20}$$

The probability of N occurrences of the outcome Π is thus

$$\begin{aligned}
\text{tr}(\rho^{(N)}\Pi^{\otimes N}) &= P(\mathbf{q})\,\text{tr}(A_\mathbf{q}^{\otimes N}\Pi^{\otimes N}) + \sum_{\mathbf{p} \neq \mathbf{q}} P(\mathbf{p})\,\text{tr}(A_\mathbf{p}^{\otimes N}\Pi^{\otimes N}) \\
&= P(\mathbf{q})\,[\text{tr}(A_\mathbf{q}\Pi)]^N + \sum_{\mathbf{p} \neq \mathbf{q}} P(\mathbf{p})\,[\text{tr}(A_\mathbf{p}\Pi)]^N \\
&= P(\mathbf{q})(1+\lambda)^N + \sum_{\mathbf{p} \neq \mathbf{q}} P(\mathbf{p})\,[\text{tr}(A_\mathbf{p}\Pi)]^N .
\end{aligned} \tag{4.21}$$

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There are no assurances in general that the rightmost term in Eq. (4.21) is positive, but if N is an even number it must be. It follows that if $P(\mathbf{q}) \geq 0$, for sufficiently large *even* N,

$$\text{tr}(\rho^{(N)}\Pi^{\otimes N}) > 1 \; , \tag{4.22}$$

contradicting the assumption that it should always be a probability.

All we need to do now is transcribe the argument leading to Eq. (4.22) to the general integral case of Eq. (4.17). Note that by Eq. (4.14), the quantity $\text{tr}(A_{\mathbf{p}}\Pi)$ is a (linear) continuous function of the parameter $\mathbf{p}$. Therefore, for any $\epsilon > 0$, there exists a $\delta > 0$ such that $|\text{tr}(A_{\mathbf{p}}\Pi) - \text{tr}(A_{\mathbf{q}}\Pi)| \leq \epsilon$ whenever $|\mathbf{p} - \mathbf{q}| \leq \delta$, i.e., whenever $\mathbf{p}$ is contained within an open ball $B_\delta(\mathbf{q})$ centered at $\mathbf{q}$. Choose $\epsilon < \lambda$, and define $\overline{B}_\delta$ to be the intersection of $B_\delta(\mathbf{q})$ with the probability simplex. For $\mathbf{p} \in \overline{B}_\delta$, it follows that

$$\text{tr}(A_{\mathbf{p}}\Pi) \geq 1 + \lambda - \epsilon > 1 \; . \tag{4.23}$$

If we consider an N that is even, $[\text{tr}(A_{\mathbf{p}}\Pi)]^N$ is nonnegative in all of $\mathcal{S}_{d^2}$, and we have that the probability of the outcome $\Pi^{\otimes N}$ satisfies

$$
\begin{aligned}
\text{tr}(\rho^{(N)}\Pi^{\otimes N}) &= \int_{\mathcal{S}_{d^2}} P(\mathbf{p}) \left[\text{tr}(A_{\mathbf{p}}\Pi)\right]^N d\mathbf{p} \\
&= \int_{\mathcal{S}_{d^2} - \overline{B}_\delta} P(\mathbf{p}) \left[\text{tr}(A_{\mathbf{p}}\Pi)\right]^N d\mathbf{p} \; + \int_{\overline{B}_\delta} P(\mathbf{p}) \left[\text{tr}(A_{\mathbf{p}}\Pi)\right]^N d\mathbf{p} \\
&\geq \int_{\overline{B}_\delta} P(\mathbf{p}) \left[\text{tr}(A_{\mathbf{p}}\Pi)\right]^N d\mathbf{p} \\
&\geq (1 + \lambda - \epsilon)^N \int_{\overline{B}_\delta} P(\mathbf{p}) \, d\mathbf{p} \; .
\end{aligned}
\tag{4.24}
$$

Unless

$$\int_{\overline{B}_\delta} P(\mathbf{p}) \, d\mathbf{p} = 0 \; , \tag{4.25}$$

the lower bound (4.24) for the probability of the outcome $\Pi^{\otimes N}$ becomes arbitrarily large as $N \to \infty$. Thus we conclude that the requirement that $\rho^{(N)}$ be a proper density operator constrains $P(\mathbf{p})$ to vanish almost everywhere in $\overline{B}_\delta$ and, consequently, to vanish almost everywhere that $A_{\mathbf{p}}$ is not a physical state.

Using Eq. (4.14), we can trivially transform the integral representation (4.17) to one directly over the convex set of density operators $\mathcal{D}_d$ and be left with the following statement. Under the sole assumption that the density operator $\rho^{(N)}$ is exchangeable, there exists a unique probability density $P(\rho)$ such that

$$\rho^{(N)} = \int_{\mathcal{D}_d} P(\rho) \, \rho^{\otimes N} \, d\rho \; . \tag{4.26}$$

This concludes the proof of the quantum de Finetti representation theorem.

V. OUTLOOK

Since the analysis in the previous sections concerned *only* the case of quantum-state tomography, we certainly have not written the last word on unknown quantum states in

the sense advocated in Sec. I. There are clearly other examples that need separate analyses. For instance, the use of unknown states in quantum teleportation [10]—where a *single* realization of an unknown state is "teleported" with the aid of previously distributed quantum entanglement and a classical side channel—has not been touched upon. The quantum de Finetti theorem, therefore, is not the end of the road for detailing implications of an information-based interpretation of quantum mechanics. What is important, we believe, is that taking the time to think carefully about the referents of various states in a problem can lead to insights into the structure of quantum mechanics that cannot be found by other means.

For instance, one might ask, "Was this theorem not inevitable?" After all, is it not already well established that quantum theory is, in some sense, just a noncommutative generalization of probability theory? Should not all the main theorems in classical probability theory carry over to the quantum case [68]? One can be skeptical in this way, of course, but then one will miss a large part of the point. There are any number of noncommutative generalizations to probability theory that one can concoct [70]. The deeper issue is, what is it in the natural world that forces quantum theory to the particular noncommutative structure it actually has [71]? It is not a foregone conclusion, for instance, that every theory has a de Finetti representation theorem within it.

Some insight in this regard can be gained by considering very simple modifications of quantum theory. To give a concrete example, let us take the case of real-Hilbert-space quantum mechanics. This theory is the same as ordinary quantum mechanics in all aspects *except* that the Hilbert spaces are defined over the field of real numbers rather than the complex numbers. It turns out that this is a case where the quantum de Finetti theorem fails. Let us start to explain why by first describing how the particular proof technique used above loses validity in the new context.

In order to specify uniquely a Hermitian operator $\rho^{(N)}$ in going from Eq. (4.16) to (4.17), the proof made central use of the fact that a complete basis $\{E_1, \ldots, E_{d^2}\}$ for the vector space of operators on $\mathcal{H}_d$ can be used to generate a complete basis for the operators on $\mathcal{H}_d^{\otimes N}$—one just need take the d^{2N} operators of the form $E_{\alpha_1} \otimes \cdots \otimes E_{\alpha_N}$, $1 \leq \alpha_j \leq d^2$. (All we actually needed was that a basis for the real vector space of Hermitian operators on $\mathcal{H}_d$ can be used to generate a basis for the real vector space of Hermitian operators on $\mathcal{H}_d^{\otimes N}$, but since the vector space of all operators is the complexification of the real vector space of Hermitian operators, this seemingly weaker requirement is, in fact, no different.) This technique works because the dimension of the space of $d^N \times d^N$ matrices is $(d^2)^N$, the Nth power of the dimension of the space of $d \times d$ matrices.

This technique does not carry over to real Hilbert spaces. In a real Hilbert space, states and POVM elements are represented by real symmetric matrices. The dimension of the vector space of real symmetric matrices acting on a d-dimensional real Hilbert space is $\frac{1}{2}d(d+1)$, this then being the number of elements in an minimal informationally complete POVM. The task in going from Eq. (4.16) to (4.17) would be to specify the real matrix $\rho^{(N)}$. When $N \geq 2$, however, the dimension of the space of $d^N \times d^N$ real symmetric matrices is strictly greater than the Nth power of the dimension of the space of $d \times d$ real symmetric matrices, i.e.,

$$\frac{1}{2}d^N(d^N + 1) > \left(\frac{1}{2}d(d+1)\right)^N . \tag{5.1}$$

Hence, specifying Eq. (4.16) for all outcome sequences $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)$ is not sufficient to specify a single operator $\rho^{(N)}$. This line of reasoning indicates that the particular *proof* of the quantum de Finetti theorem presented in Sec. IV fails for real Hilbert spaces, but it does not establish that the theorem itself fails. The main point of this discussion is that it draws attention to the crucial difference between real-Hilbert-space and complex-Hilbert-space quantum mechanics—a fact emphasized previously by Araki [26] and Wootters [27].

To show that the theorem fails, we need a counterexample. One such example is provided by the N-system state

$$\rho^{(N)} = \frac{1}{2}\,\rho_+^{\otimes N} + \frac{1}{2}\,\rho_-^{\otimes N}\ , \tag{5.2}$$

where

$$\rho_+ = \frac{1}{2}(I + \sigma_2) \qquad \text{and} \qquad \rho_- = \frac{1}{2}(I - \sigma_2)\ , \tag{5.3}$$

and where σ_2 was defined in Eq. (3.2). In complex-Hilbert-space quantum mechanics, this is clearly a valid density operator: It corresponds to an equally weighted mixture of N spin-up particles and N spin-down particles in the y direction. The state $\rho^{(N)}$ is clearly exchangeable, and the decomposition in Eq. (5.2) is unique according to the quantum de Finetti theorem.

Now consider $\rho^{(N)}$ as an operator in real-Hilbert-space quantum mechanics. Despite the apparent use of the imaginary number i in the σ_2 operator, $\rho^{(N)}$ remains a valid quantum state. This is because, upon expanding the right-hand side of Eq. (5.2), all the terms with an odd number of σ_2 operators cancel away. Yet, even though it is an exchangeable density operator, it cannot be written in de Finetti form of Eq. (3.15) using only real symmetric operators. This follows because Eq. (5.2), the unique de Finetti form, contains σ_2, which is an antisymmetric operator and cannot be written in terms of symmetric operators. Hence the de Finetti representation theorem does not hold in real-Hilbert-space quantum mechanics.

Similar considerations show that in quaternionic quantum mechanics (a theory again precisely the same as ordinary quantum mechanics except that it uses Hilbert spaces over the quaternionic field [25]), the connection between exchangeable density operators and decompositions of the de Finetti form (3.15) breaks down. The failure mode is, however, even more disturbing than for real Hilbert spaces. In quaternionic quantum mechanics, most operators of the de Finetti form (3.15) do not correspond to valid quaternionic quantum states, even though the states ρ in the integral are valid quaternionic states. The reason is that tensor products of quaternionic Hermitian operators are not necessarily Hermitian.

In classical probability theory, exchangeability characterizes those situations where the only data relevant for updating a probability distribution are frequency data, i.e., the numbers n_j in Eq. (2.4) which tell how often the result j occurred. The quantum de Finetti representation shows that the same is true in quantum mechanics: Frequency data (with respect to a sufficiently robust measurement) are sufficient for updating an exchangeable state to the point where nothing more can be learned from sequential measurements; that is, one obtains a convergence of the form (1.4), so that ultimately any further measurements on the individual systems are statistically independent. That there is no quantum de Finetti theorem in real Hilbert space means that there are fundamental differences between real and complex Hilbert spaces with respect to learning from measurement results. The ultimate

reason for this is that in ordinary, complex-Hilbert-space quantum mechanics, exchangeability implies separability, i.e., the absence of entanglement. This follows directly from the quantum de Finetti theorem, because states of the form Eq. (3.15) are not entangled. This implication does not carry over to real Hilbert spaces. By the same reasoning used to show that the de Finetti theorem itself fails, the state in Eq. (5.2) cannot be written as *any* mixture of real product states. Interpreted as a state in real Hilbert space, the state in Eq. (5.2) is thus not separable, but entangled [72]. In a real Hilbert space, exchangeable states can be entangled and local measurements cannot reveal that.

Beyond these conceptual points, we also believe that the technical methods exhibited here might be of interest in the practical arena. Recently there has been a large literature on which classes of measurements have various advantages for tomographic purposes [73,74]. To our knowledge, the present work is the only one to consider tomographic reconstruction based upon minimal informationally complete POVMs. One can imagine several advantages to this approach via the fact that such POVMs with rank-one elements are automatically extreme points in the convex set of all measurements [75].

Furthermore, the classical de Finetti theorem is only the tip of an iceberg with respect to general questions in statistics to do with exchangeability and various generalizations of the concept [76]. One should expect no less of quantum exchangeability studies. In particular here, we are thinking of things like the question of representation theorems for finitely exchangeable distributions [52,77]. Just as our method for proving the quantum de Finetti theorem was able to rely heavily on the the classical theorem, so one might expect similar benefits from the classical results in the case of quantum finite exchangeability— although there will certainly be new aspects to the quantum case due to the possibility of entanglement in finite exchangeable states. A practical application of such representation theorems could be their potential to contribute to the solution of some outstanding problems in constructing security proofs for various quantum key distribution schemes [78].

In general, our effort in the present paper forms part of a larger program to promote a consistent information-based interpretation of quantum mechanics and to delineate its consequences. We find it encouraging that the fruits of this effort may not be restricted solely to an improved understanding of quantum mechanics, but also possess the potential to contribute to practical applications.

ACKNOWLEDGMENTS

APPENDIX A: PROOF OF THE CLASSICAL DE FINETTI THEOREM

In this Appendix we reprise the admirably simple proof of the classical de Finetti representation theorem given by Heath and Sudderth [42] for the case of binary variables.

Suppose we have an exchangeable probability assignment for M binary random variables, $x_1, x_2, \ldots, x_M$, taking on the values 0 and 1. Let $p(n, N)$, $N \leq M$, be the probability for n 1s in N trials. Exchangeability guarantees that

$$p(n, N) = \binom{N}{n} p(x_1 = 1, \ldots, x_n = 1, x_{n+1} = 0, \ldots, x_N = 0) . \tag{A1}$$

We can condition the probability on the right on the occurrence of m 1s in all M trials:

$$p(n, N) = \binom{N}{n} \sum_{m=0}^{M} p(x_1 = 1, \ldots, x_n = 1, x_{n+1} = 0, \ldots, x_N = 0 \mid m, M) p(m, M) . \tag{A2}$$

Given m 1s in M trials, exchangeability guarantees that the $\binom{M}{m}$ sequences are equally likely. Thus the situation is identical to drawing from an urn with m 1s on M balls, and we have that

$$
\begin{aligned}
p(x_1 &= 1, \ldots, x_n = 1, x_{n+1} = 0, \ldots, x_N = 0 \mid m, M) \\
&= \frac{m}{M} \frac{m-1}{M-1} \cdots \frac{m-(n-1)}{M-(n-1)} \frac{M-m}{M-n} \frac{M-m-1}{M-n-1} \cdots \frac{M-m-(N-n-1)}{M-(N-1)} \\
&= \frac{(m)_n (M-m)_{N-n}}{(M)_N} ,
\end{aligned} \tag{A3}
$$

where

$$(r)_q \equiv \prod_{j=0}^{q-1} (r - j) = r(r-1) \cdots (r - q + 1) = \frac{r!}{(r-q)!} . \tag{A4}$$

The result is that

$$p(n, N) = \binom{N}{n} \sum_{m=0}^{M} \frac{(m)_n (M-m)_{N-n}}{(M)_N} p(m, M) . \tag{A5}$$

What remains is to take the limit $M \to \infty$, which we can do because of the extendibility property of exchangeable probabilities. We can write $p(n, N)$ as an integral

$$p(n, N) = \binom{N}{n} \int_0^1 \frac{(zM)_n ((1-z)M)_{N-n}}{(M)_N} P_M(z) \, dz , \tag{A6}$$

where

$$P_M(z) = \sum_{m=0}^{M} p(zM, M) \delta(z - m/M) \tag{A7}$$

is a distribution concentrated at the M-trial frequencies m/M. In the limit $M \to \infty$, $P_M(z)$ converges to a continuous distribution $P_\infty(z)$, and the other terms in the integrand go to $z^n(1-z)^{N-n}$, giving

$$p(n, N) = \binom{N}{n} \int_0^1 z^n(1-z)^{N-n} P_\infty(z)\, dz \ . \tag{A8}$$

We have demonstrated the classical de Finetti representation theorem for binary variables: If $p(n, N)$ is part of an infinite exchangeable sequence, then it has a de Finetti representation in terms of a "probability on probabilities" $P_\infty(z)$. The proof can readily be extended to nonbinary variables.

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> The state of a classical system is an objective property of the system and therefore changes only by dynamical laws. A quantum-mechanical state, being a summary of the observers' information about an individual physical system, changes both by dynamical laws and whenever the observer acquires new information about the system through the process of measurement. The existence of two laws for the evolution of the state vector by the Schrödinger equation on the one hand and by the process of measurement (sometimes described as the "reduction of the wave packet") on the other, is a classic subject for discussion in the quantum theory of measurement. The situation becomes problematical only if it is believed that the state vector is an objective property of the system. Then, the state vector must be required to change only by dynamical law, and the problem must be faced of justifying the second mode of evolution from the first. If, however, the state of a system is defined as a list of [*experimental*] propositions together with their [*probabilities of occurrence*], it is not surprising that after a measurement the state must be changed to be in accord with the new information .... The "reduction of the wave packet" does take place in the consciousness of the observer, not because of any unique physical process which takes place there, but only because the state is a construct of the observer and not an objective property of the physical system.

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> There was a young man who said, "God
> Must think it exceedingly odd
> If he finds that this tree
> Continues to be
> When there's no one about in the Quad."

REPLY

> Dear Sir:
> Your astonishment's odd:
> I am always about in the Quad.
> And that's why the tree
> Will continue to be,
> Since observed by
> > Yours faithfully,
> > God.

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