Are There Quantum Operators and Wave Functions in Standard Probability Theory

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Abstract The methods of quantum probability theory are radically different from standard probability as developed over the last 300 years. While the results of quantum probability, such as expectation values, are the same as standard probability theory, the methods used are strange, as they deal with operators and wave functions and use strange rules of manipulation. We ask whether there are operators and wave functions in standard probability theory. By generalizing a theorem of Khinchine on characteristic functions, we show that indeed the strange probabilistic methods of quantum mechanics follow from standard probability theory.

Keywords Probability theory • Operators • Quantum mechanics • Khinchine theorem

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1 Introduction

Quantum mechanics is the most successful theory ever devised, by far. It explains everything that we know about matter, atoms, stars, the universe, chemistry, and indeed all physical phenomena that it has been applied to. Moreover, quantum mechanics predicts bizarre phenomena, such as vacuum fluctuations, that have been experimentally observed.

Quantum mechanics is a probability theory. While the probabilistic "results" of quantum mechanics are of the same nature as standard probability theory, for example expectation values and probability densities, the method of calculation is radically different from standard probability theory. Quantum mechanics uses wave

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functions, operators, and methods which are seemingly totally foreign to standard probability theory.

There have been numerous attempts to formulate quantum mechanics as a standard probability theory. It is fair to say that these attempts have not succeeded. We reverse the question and ask: Since quantum mechanics is certainly the most successful probability theory ever devised, we ask whether standard probability theory has the concepts of wave functions and operators. We emphasize that we are not trying to formulate quantum mechanics as a standard probability theory; quite the contrary, we are trying to see if standard probability theory contains the ideas and methods of quantum probability theory and if it could be formulated in quantum mechanical language [2, 3, 8].

Notation Operators will be denoted by bold-face letters and the corresponding random variables by lower case letters. When it is not obvious what random variable the characteristic function and corresponding probability density are referring to, we use the notation $M_a(\theta)$ and $P_a(a)$ where the subscript denotes the random variable. All integrals go from $-\infty$ to ∞ or the appropriate range of the variables. Also, it is assumed that eigenfunctions are normalized to one for the discrete case and to a delta function for the continuous case.

2 Characteristic Functions

For a probability density, $P(x)$, the characteristic function, $M(\theta)$, is the expectation value of $e^{i\theta x}$

$$M(\theta) = \langle e^{i\theta x} \rangle = \int e^{i\theta x} P(x)\, dx \tag{1}$$

and from the characteristic function, one may obtain the probability density by Fourier inversion,

$$P(x) = \frac{1}{2\pi} \int M(\theta) e^{-i\theta x} d\theta \tag{2}$$

The characteristic function is standard in probability theory for many reasons [4, 7]. It is often easier to manipulate probabilistic results by using the characteristic function compared to the probability density function itself. For example, the moments, defined by

$$\langle x^n \rangle = \int x^n P(x)\, dx \tag{3}$$

may be obtained from

$$\langle x^n \rangle = \frac{1}{i^n} \frac{d^n}{d\theta^n} M(\theta) \bigg|_{\theta=0} \tag{4}$$

Since differentiation is easier then integration, Eq. (4) is often easier to use than Eq. (3) if indeed we know $M(\theta)$. Furthermore the characteristic function is very useful for obtaining probability densities for new variables [5].

The characteristic function is generally complex, but not every complex function is a characteristic function since it has to be derivable from a positive density function. What are necessary and sufficient conditions for a function $M(\theta)$ to be a characteristic function? Khinchine solved this problem [6]. A function, $M(\theta)$, is a characteristic function if and only if there exists a function, $g(x)$, so that the characteristic function is expressed in the following form [6, 7]

$$M(\theta) = \int g^*(x) g(x + \theta) dx \tag{5}$$

If there is such a function, it should be normalized to one, which insures that the corresponding density will integrate to one. While this theorem is fundamental in probability theory, it appears that the significance and properties of the $g(x)$ functions have not been extensively studied. We will argue that they are the "wave functions" of quantum mechanics, and that the generalization of Khinchine's theorem that we present in Sect. 3 leads to the concept of operators in standard probability theory. We first present our idea for the Khinchine theorem as originally given, Eq. (5), before we give the general result in the next section.

Rewrite Khinchine's theorem in the following way

$$M(\theta) = \int g^*(x) e^{\theta \frac{d}{dx}} g(x) dx \tag{6}$$

where in going from Eqs. (5)–(6) we have used the fact that $e^{\theta \frac{d}{dx}}$ is the translation operator in that for any function $f(x)$ [10]

$$e^{\theta \frac{d}{dx}} f(x) = f(x + \theta) \tag{7}$$

We now insert i as indicated

$$M(\theta) = \int g^*(x) e^{i\theta \left(\frac{1}{i} \frac{d}{dx}\right)} g(x) dx \tag{8}$$

and write Eq. (6) as

$$M(\theta) = \int g^*(x) e^{i\theta \mathbf{p}} g(x) dx \tag{9}$$

where we have defined the operator, **p**, by

$$\mathbf{p} = \frac{1}{i}\frac{d}{dx} \tag{10}$$

We now calculate the expectation value by way of Eq. (4). In anticipation of the result we shall use the letter p for the random variables since it will turn out to be momentum and the letter p is standard for momentum. In particular,

$$\langle p \rangle = \frac{1}{i}\frac{d}{d\theta}M(\theta)\bigg|_{\theta=0} \tag{11}$$

$$= \frac{1}{i}\frac{d}{d\theta}\int g^*(x)e^{i\theta\mathbf{p}}g(x)dx\bigg|_{\theta=0} \tag{12}$$

$$= \int g^*(x)\left(\frac{1}{i}\frac{\partial}{\partial\theta}\right)e^{i\theta\mathbf{p}}g(x)dx\bigg|_{\theta=0} \tag{13}$$

$$= \int g^*(x)\mathbf{p}e^{i\theta\mathbf{p}}g(x)dx\bigg|_{\theta=0} \tag{14}$$

or

$$\langle p \rangle = \int g^*(x)\mathbf{p}\, g(x)dx = \int g^*(x)\left(\frac{1}{i}\frac{d}{dx}\right)g(x)dx \tag{15}$$

This is precisely how one calculates the average momentum in quantum mechanics when the system has the “wave function” $g(x)$ [1, 9]. Therefore we argue that for this case (momentum) the g’s of the Khinchine theorem are the wave functions of quantum mechanics. Note that the g’s are generally complex functions and that the operator **p** is self-adjoint, as indeed they should be. The reason for self-adjointness will be discussed in Sect. 3

The Probability Density What is the probability density that corresponds to the characteristic function given by Eq. (5)? Again, we use p for the random variable, which is an ordinary variable, and should not be confused with the operator **p**. Using Eq. (2) we have

$$P(p) = \frac{1}{2\pi}\int M(\theta)e^{-i\theta p}d\theta \tag{16}$$

$$= \frac{1}{2\pi}\iint g^*(x)\, g(x+\theta)e^{-i\theta p}d\theta dx \tag{17}$$

Making a change of variables

$$x' = x + \theta \qquad dx' = d\theta \tag{18}$$

we have

$$P(p) = \frac{1}{2\pi} \iint g^*(x)\, g(x') e^{-i(x'-x)p} dx' dx \tag{19}$$

$$= \frac{1}{2\pi} \left(\int g^*(x) e^{ixp} dx \right) \left(\int g(x') e^{-ix'p} dx' \right) \tag{20}$$

that is

$$P(p) = \frac{1}{2\pi} \left| \int g(x) e^{-ixp} dx \right|^2 \tag{21}$$

But this is precisely the probability density of "momentum" in quantum mechanics [1, 9].

Comment Notice that the random variable p is continuous, ranging from $-\infty$ to ∞. That is indeed the case in quantum mechanics, and we say that momentum is not quantized. How quantization for other physical quantities comes in will be clear when we discuss general operators and general random variables in the next section.

3 Generalization of Khinchine's Theorem

We now generalize Khinchine's theorem to apply to arbitrary self adjoint operators. $M_a(\theta)$ is a characteristic function if and only if for a self adjoint operator $\mathbf{A}$ there exists the representation

$$M_a(\theta) = \int g^*(x) e^{i\theta \mathbf{A}} g(x) dx \tag{22}$$

We prove this in Appendix A, "Khinchine Theorem for Operators". For the expectation value we have, using Eq. (2), that

$$\langle a \rangle = \frac{1}{i} \frac{d}{d\theta} M_a(\theta) \bigg|_{\theta=0} \tag{23}$$

$$= \frac{1}{i} \frac{d}{d\theta} \int g^*(x) e^{i\theta \mathbf{A}} g(x) dx \bigg|_{\theta=0} \tag{24}$$

$$= \int g^*(x) \left(\frac{1}{i} \frac{\partial}{\partial \theta} \right) e^{i\theta \mathbf{A}} g(x) dx \bigg|_{\theta=0} \tag{25}$$

$$= \int g^*(x) \mathbf{A} e^{i\theta \mathbf{A}} g(x) dx \bigg|_{\theta=0} \tag{26}$$

giving

$$\langle a\rangle = \int g^*(x)\mathbf{A}\, g(x)\, dx \tag{27}$$

This is precisely the standard manner of calculating expectation values in quantum mechanics for a physical quantity associated with the self-adjoint operator **A** [1, 9].

3.1 Probability Density

We now discuss the probability density that corresponds to the characteristic function given by Eq. (22). Substitute Eq. (22) into Eq. (2) to obtain

$$P(a) = \frac{1}{2\pi}\int M_a(\theta)e^{-i\theta a}d = \frac{1}{2\pi}\iint g^*(x)e^{i\theta\mathbf{A}}\, g(x)e^{-i\theta a}dx\, d\theta \tag{28}$$

We evaluate Eq. (28) in Appendix B, "Probability Density". Here we state the result. There are two cases: namely, if we have discrete or continuous random variables. This follows naturally, as we show in the Appendix "Probability Density". In short, it is the spectrum of the operator **A** which determines whether the random variables are discrete or continuous. Moreover the random variables are the eigenvalues of the operator.

Continuous case If the spectrum of the operator has continuous eigenvalues we write

$$\mathbf{A}u_a(x) = au_a(x) \tag{29}$$

where a and $u_a(x)$ are the eigenvalues and corresponding eigenfunctions of the operator **A**. The probability density as evaluated by way of Eq. (28) is given by

$$P(a) = |c(a)|^2 \tag{30}$$

where

$$c(a) = \int g(x)u_a^*(x)dx \tag{31}$$

Hence, the random variables are the $a's$ (the eigenvalues) and their range is the range of the eigenvalues.

Discrete case If the spectrum of the operator is discrete, we write

$$\mathbf{A}u_n(x) = a_n u_n(x) \tag{32}$$

then the probability distribution is given by

$$P(a) = \sum_n |c_n|^2 \delta(a - a_n) \tag{33}$$

where

$$c_n = \int g(x) u_n^*(x) dx \tag{34}$$

Notice that the probability density is non-zero only when the random variable, a, is one of the discrete eigenvalues. In this case we have quantization. We may write Eq. (33) as

$$P(a_n) = |c_n|^2 \tag{35}$$

Discussion The probability densities derived above are called the Born rule. We have derived them from the generalization of the Khinchine theorem, Eq. (22). Also, we proved that the random variables are the eigenvalues of the operator **A**, which is usually just assumed in quantum mechanics.

3.2 Two Ways of Calculating Expectation Values

We have shown, using Eq. (22) that one may calculate expectation values by

$$\langle a \rangle = \int g^*(x) \mathbf{A}\, g(x)\, dx \tag{36}$$

which is the standard quantum mechanical way. However in standard probability theory we calculate expectation values by

$$\langle a \rangle = \sum (\text{random variable}) \times (\text{probability}) \qquad (\text{discrete case}) \tag{37}$$

for the discrete case, and by

$$\langle a \rangle = \int (\text{random variable}) \times (\text{probability}) \qquad (\text{continuous case}) \tag{38}$$

for the continuous case. Substituting Eqs. (30) and (35) we have

$$\langle a \rangle = \sum a_n \left| \int g(x) u_n^*(x) dx \right|^2 \qquad (\text{discrete case}) \tag{39}$$

$$\langle a \rangle = \int a \left| \int g(x) u_a^*(x) dx \right|^2 da \qquad (\text{continuous case}) \tag{40}$$

It is well known in quantum mechanics that the two methods are the same, that is that

$$\int g^*(x)\mathbf{A}\, g(x)\, dx = \sum a_n \left| \int g(x) u_n^*(x) dx \right|^2 \qquad \text{(discrete case)} \tag{41}$$

$$\int g^*(x)\mathbf{A}\, g(x)\, dx = \int a \left| \int g(x) u_a^*(x) dx \right|^2 da \qquad \text{(continuous case)} \tag{42}$$

In Appendix C, "Standard vs. Quantum Manner of Calculating Expectation Values" we show the equivalence for the sake of readers that may not be familiar with the result.

4 Conclusion

We summarize the main results. We have generalized Khinchine's theorem for a self-adjoint operator **A** by showing that a function, $M_a(\theta)$, defined by

$$M_a(\theta) = \int g^*(x) e^{i\theta \mathbf{A}}\, g(x) dx \tag{43}$$

is a *proper* characteristic function. From Eq. (43) we have shown that the usual rules of quantum probabilities follow. In particular we have shown that:

1. The expected value is

$$\langle a \rangle = \int g^*(x)\mathbf{A}\, g(x)\, dx \tag{44}$$

2. The random variables are the eigenvalues of the operator **A**.
3. If the eigenvalues, a, are continuous, then the probability density associated with the characteristic function is

$$P(a) = \left| \int g(x) u_a^*(x) dx \right|^2 \tag{45}$$

   where $u_a(x)$ are the eigenfunctions.
4. If the eigenvalues, a_n, are discrete with corresponding eigenfunctions $u_n(x)$, the probability density is given by

$$P(a_n) = \left| \int g(x) u_n^*(x) dx \right|^2 \tag{46}$$

The above items are exactly how one obtains the random variables and probabilities in quantum mechanics. We have *derived* them from the characteristic function defined by Eq. (43).

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Appendix A: Khinchine Theorem for Operators

We prove that $M_a(\theta)$ is a characteristic function corresponding to the self-adjoint operator, $\mathbf{A}$, if and only if, there exists the representation

$$M_a(\theta) = \int g^*(x) e^{i\theta\mathbf{A}} g(x) dx \tag{47}$$

for some function $g(x)$. First, we show that $M_a(\theta)$ produces a proper probability density. Substituting Eq. (47) into Eq. (2) the probability density is then

$$P(a) = \frac{1}{2\pi} \int M(\theta) e^{-i\theta a} d\theta = \frac{1}{2\pi} \iint g^*(x) e^{i\theta\mathbf{A}} g(x) e^{-i\theta a} dx\, d\theta \tag{48}$$

We first consider the continuous case. Since the operator is self-adjoint, the solution to the eigenvalue problem

$$\mathbf{A} u_\alpha(x) = \alpha u_\alpha(x) \tag{49}$$

produces real eigenvalues, α, and complete and orthogonal eigenfunctions, $u_\alpha(x)$

$$\int u_\alpha^*(x) u_\beta(x) dx = \delta(\alpha - \beta) \tag{50}$$

$$\int u_\alpha^*(x) u_\alpha(x') d\alpha = \delta(x - x') \tag{51}$$

Since the eigenfunctions are complete and orthogonal, we can expand any function as

$$g(x) = \int u_\alpha(x) c(\alpha) d\alpha \tag{52}$$

and inversely

$$c(\alpha) = \int u_\alpha^*(x)\, g(x) dx \tag{53}$$

Substituting Eq. (52) into Eq. (48) we have

$$P(a) = \frac{1}{2\pi} \iiiint u_\beta^*(x) c^*(\beta) e^{i\theta \mathbf{A}} u_\alpha(x) c(\alpha) e^{-i\theta a} dx d\beta d\alpha d\theta \tag{54}$$

Using the fact that

$$e^{i\theta \mathbf{A}} u_\alpha(x) = e^{i\theta\alpha} u_\alpha(x) \tag{55}$$

we have

$$P(a) = \frac{1}{2\pi} \iiiint u_\beta^*(x) c^*(\beta) e^{i\theta\alpha} u_\alpha(x) c(\alpha) e^{-i\theta a} dx d\beta d\alpha d\theta \tag{56}$$

$$= \iint F^*(\beta) \delta(a-\alpha) \delta(\alpha-\beta) F(\alpha) d\beta d\alpha \tag{57}$$

The θ integration gives

$$\int e^{i\theta\alpha} e^{-i\theta a} d\theta = 2\pi \delta(\alpha - \beta) \tag{58}$$

and using Eq. (50) we have

$$P(a) = \iint c^*(\beta) \delta(a-\alpha) \delta(\alpha-\beta) c(\alpha) d\beta d\alpha \tag{59}$$

Therefore

$$P(a) = |c(a)|^2 \tag{60}$$

Equation (60) shows that we have a manifestly positive density, and that it will be normalized to one if the wave function is normalized to one because

$$\int |c(a)|^2 \, da = \int |\, g(x)|^2 \, dx \tag{61}$$

This proves the sufficiency of the form given by Eq. (47).

To prove the necessity, suppose we have the probability distribution $P(\alpha)$, and hence the characteristic function is given by

$$M(\theta) = \int e^{i\theta\alpha} P(\alpha) \, d\alpha \tag{62}$$

We expand, not the probability distribution but the square root of $P(\alpha)$

$$\sqrt{P(\alpha)} = \int u_\alpha(x) f(x) dx \tag{63}$$

Since $\sqrt{P(\alpha)}$ is real we also have

$$\sqrt{P(\alpha)} = \int u^*_\alpha(x) f^*(x) dx \tag{64}$$

Therefore

$$M(\theta) = \int e^{i\theta\alpha} \sqrt{P(\alpha)}\sqrt{P(\alpha)}\, d\alpha \tag{65}$$

$$= \iiint u^*_\alpha(x') f^*(x')\, u_\alpha(x) f(x) e^{i\theta\alpha} dx d\alpha dx' \tag{66}$$

$$= \iiint u^*_\alpha(x') f^*(x') \left\{ e^{i\theta\mathbf{A}} u_\alpha(x)\right\} f(x) dx dx' d\alpha \tag{67}$$

$$= \iint f^*(x') \left\{ e^{i\theta\mathbf{A}} \delta(x - x')\right\} f(x) dx dx' \tag{68}$$

or

$$M_a(\theta) = \int f^*(x) e^{i\theta\mathbf{A}} f(x) dx \tag{69}$$

which is of the form given by Eq. (47).

A similar proof follows for the discrete case.

Appendix B: Probability Density

We now derive the probability density corresponding to $M_a(\theta)$, where

$$M_a(\theta) = \int g^*(x) e^{i\theta\mathbf{A}} g(x)\, d\theta \tag{70}$$

Using Eq. (2) we have

$$P_a(a) = \frac{1}{2\pi} \iint g^*(x) e^{i\theta\mathbf{A}} g(x) e^{-i\theta a} dx\, d\theta \tag{71}$$

To evaluate Eq. (71) we consider two separate cases depending on whether the spectrum of the operator **A** is continuous or discrete. For a discrete spectrum we write

$$\mathbf{A}u_n(x) = a_n u_n(x) \tag{72}$$

where the eigenfunctions satisfy completeness and orthogonality properties

$$\int u_n^*(x)u_k(x)dx = \delta_{nk} \tag{73}$$

$$\sum_n u_n^*(x)u_n(x') = \delta(x - x') \tag{74}$$

We expand the wave function as

$$g(x) = \sum_n c_n u_n(x) \tag{75}$$

with

$$c_n = \int g(x)u_n^*(x)dx \tag{76}$$

Substituting Eq. (75) into Eq. (71) we have

$$P(a) = \frac{1}{2\pi}\iint \sum_{n,m} c_m^* u_m^*(x) e^{i\theta\mathbf{A}} c_n u_n(x) e^{-i\theta a} dx\, d\theta \tag{77}$$

Using

$$e^{i\theta\mathbf{A}} u_n(x) = e^{i\theta a_n} u_n(x) \tag{78}$$

gives

$$P(a) = \frac{1}{2\pi}\iint \sum_{n,m} c_m^* u_m^*(x) e^{i\theta a_n} c_n u_n(x) e^{-i\theta a} dx\, d\theta \tag{79}$$

$$= \frac{1}{2\pi}\int \sum_{n,m} c_m^* \delta_{nm}(x) e^{i\theta a_n} c_n e^{-i\theta a}\, d\theta \tag{80}$$

$$= \frac{1}{2\pi}\sum_n |c_n|^2 \int e^{i\theta a_n - i\theta a}\, d\theta \tag{81}$$

Therefore

$$P(a) = \sum_n |c_n|^2 \delta(a - a_n) \tag{82}$$

Equation (82) shows that the a_n are the random variables with corresponding probability $|c_n|^2$. This is exactly the quantum mechanical result. One can write Eq. (82) as

$$P(a_n) = |c_n|^2 \tag{83}$$

Note: Since **A** is self-adjoint the eigenvalues are real, as they should be, since they represent measurable quantities.

For the continuous case we write

$$\mathbf{A}u_\alpha(x) = au_\alpha(x) \tag{84}$$

and the eigenfunctions satisfy

$$\int u_\alpha^*(x)u_\beta(x)dx = \delta(\alpha - \beta) \tag{85}$$

$$\int u_\alpha^*(x)u_\alpha(x')d\alpha = \delta(x - x') \tag{86}$$

Expand $g(x)$ as

$$g(x) = \int c(\alpha)u_\alpha(x)d\alpha \tag{87}$$

with

$$c(\alpha) = \int g(x)u_\alpha^*(x)dx \tag{88}$$

and substitute Eq. (87) into (71) to obtain

$$P_a(a) = \frac{1}{2\pi} \iiiint c^*(\alpha)u_\alpha^*(x)e^{i\theta\mathbf{A}}c(\beta)u_\beta(x)e^{-i\theta a}dx\,d\theta d\alpha d\beta \tag{89}$$

$$= \frac{1}{2\pi} \iiiint c^*(\alpha)u_\alpha^*(x)e^{i\theta\beta}c(\beta)u_\beta(x)e^{-i\theta a}dx\,d\theta d\alpha d\beta \tag{90}$$

$$= \iint c^*(\alpha)c(\beta)\delta(\alpha - \beta)\delta(a - \beta)d\alpha d\beta \tag{91}$$

which evaluates to

$$P_a(a) = |c(a)|^2 \tag{92}$$

Appendix C: Standard vs. Quantum Manner of Calculating Expectation Values

We show Eq. (41) of the text, which we repeat here

$$\int g^*(x)\mathbf{A}\, g(x)\, dx = \sum a_n \left| \int g(x) u_n^*(x) dx \right|^2 \qquad \text{discrete case} \tag{93}$$

We expand $g(x)$

$$g(x) = \sum c_n u_n(x) \tag{94}$$

where

$$c_n = \int g(x) u_n^*(x) dx \tag{95}$$

Starting with the left hand side of Eq. (93) we have

$$\int g^*(x)\mathbf{A}\, g(x)\, dx \tag{96}$$

$$= \int \sum_{n,m} c_m^* u_m^*(x) \mathbf{A} c_n u_n(x)\, dx \tag{97}$$

$$= \int \sum_{n,m} c_m^* u_m^*(x) a_n c_n u_n(x)\, dx \tag{98}$$

$$= \sum_{n,m} c_m^* \delta_{nm} a_n c_n \tag{99}$$

$$= \sum_n a_n \left| \int g(x) u_n^*(x) dx \right|^2 \tag{100}$$

which is Eq. (93). The proof for the continuous case, Eq. (42), follows an analogous derivation.

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