Why are complex numbers needed in quantum mechanics? Some answers for the introductory level

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Abstract

Complex numbers are broadly used in physics, normally as a calculation tool that makes things easier due to Euler's formula. In the end, it is only the real component that has physical meaning or the two parts (real and imaginary) are treated separately as real quantities. However, the situation seems to be different in quantum mechanics, since the imaginary unit i appears explicitly in its fundamental equations. From a learning perspective, this can create some challenges to newcomers. In this article, four conceptually different justifications for the use/need of complex numbers in quantum mechanics are presented and some pedagogical implications are discussed.

I. INTRODUCTION

Complex numbers were invented (or discovered?) in 16^{th}-century Italy as a calculation tool to solve cubic equations. In the beginning, not much attention was paid to their meaning, since the imaginary terms should cancel out during the calculations and only (real) roots were considered. Around 250 years later, complex numbers were given a geometrical interpretation and, since then, they became quite a useful tool to physics.[1] One reason is that complex numbers represent direction algebraically (2D vectors) and many of their operations have a direct geometrical meaning (e.g., the product rule: multiply the norms and add the angles).

It is particularly helpful to use complex numbers to model periodic phenomena, especially to operate with phase differences. Mathematically, one can treat a physical quantity as being complex, but address physical meaning only to its real part. Another possibility is to treat the real and imaginary parts of a complex number as two related (real) physical quantities. In both cases, the structure of complex numbers is useful to make calculations more easily, but no physical meaning is actually attached to complex variables.

Quantum mechanics seems to use complex numbers in a more fundamental way. It suffices to look at some of the most basic equations, both in the matrix ($[\hat{p}, \hat{x}] = -i\hbar$) and wave ($i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$) formulations, to wonder about the presence of the imaginary unit. What is essentially different in quantum mechanics is that it deals with complex quantities (e.g. wave functions and quantum state vectors) of a special kind, which *cannot* be split up into pure real and imaginary parts that can be treated independently. Furthermore, physical meaning is not attached directly to the complex quantities themselves, but to some other operation that produces real numbers (e.g. the square modulus of the wave function or of the inner product between state vectors).

This complex nature of quantum mechanical quantities puzzled some of the very founders of the theory. Schrödinger, for instance, was bothered by the fact that his wave function was complex and tried for quite some time to find physical interpretations for its (real) component.[2,3] It was probably not until Dirac formulated his bra-ket notation that it became clearer that the complex quantities of quantum mechanics were of a different kind than the ones commonly used in classical physics.[4]

It is therefore very reasonable to expect that introductory level students will face consid-

erable difficulties with the peculiar use of complex numbers in quantum mechanics. However, it is not uncommon to find textbooks that postulate, from the get-go, that wave functions and quantum state vectors are complex valued, without providing any sort of explanation for why this is the case. It is not only natural, but even desirable, that students inquire about the reasons why certain mathematical structures are useful to describe physical properties. Thus, for newcomers to the field, one can say that it is perfectly legitimate to ask: "Why do we need complex numbers in quantum mechanics?".

There is certainly no unique straight answer to this question[5–8]; constructing plausible arguments to address it is a matter of pedagogical creativity. The aim of this paper is to present synthetic (and slightly modified) versions of four different justifications found in the literature[9] and discuss some of their pedagogical implications. The first two justifications (IIA and IIB) align best with a position first approach, whereas the last two (IIC and IID) with a spin first approach. The main selection criteria that guided this choice were the plausibility of the arguments and their applicability for the very first lessons of an introductory quantum mechanics course.

II. WHY ARE COMPLEX NUMBERS NEEDED IN QUANTUM MECHANICS?

A. No information on position when momentum is known exactly

This argument is found in R. Shankar's textbook[10] for the introductory level and goes as follows. Consider one particle in one dimension and assume de Broglie's matter waves relation ($\lambda = \frac{2\pi\hbar}{p}$), which is previously justified by empirical evidence from the double-slit experiment with electrons. Since there appears to be a wave associated with the electron, it is reasonable to assume that there is a wave function $\psi(x)$ describing it (ignore time dependence). Postulate that the absolute square of this function ($|\psi(x)|^2$) gives the probability density, i.e., the likelihood to find the particle between the positions x and $x + dx$.

The last piece needed for the argument is inspired by Heisenberg's uncertainty principle. It is presented qualitatively in Shankar's textbook by thought experiments like the gamma-ray microscope. One way to state the principle is to say that "it is impossible to prepare a particle in a state in which its momentum and position (along one axis) are *exactly* known."

Now, suppose the electron is in a state of definite momentum. How would the wave

function for this state look like? According to de Broglie's relation, there is a wavelength associated with the electron. Therefore, it seems plausible to assume a classical/real oscillating wave function of the form

$$\psi_p(x) = A\cos\frac{2\pi x}{\lambda} = A\cos\frac{px}{\hbar}, \tag{1}$$

where $\psi_p(x)$ denotes a state of definite momentum. $\psi_p(x)$, as well as $|\psi_p(x)|^2$, are plotted in Fig. 1.

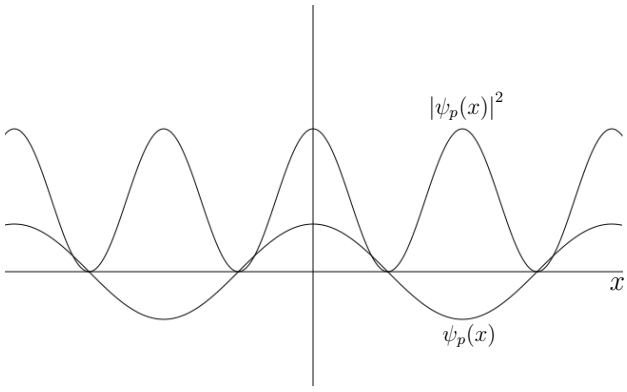

FIG. 1. Graphs of $\psi_p(x) = A\cos\frac{px}{\hbar}$ and $|\psi_p(x)|^2$. The graph of $|\psi_p(x)|^2$ (probability distribution) is inconsistent with the assertion that once momentum is exactly determined, one should have no information about the electron's position.

The graph of $|\psi_p(x)|^2$ (probability distribution) illustrates an apparent contradiction.[11] If you know the momentum of the electron *exactly*, you should have *no information* about its position. However, the graph of $|\psi_p(x)|^2$ is implying that there are regions where it is more likely to find the electron than others. If we should have no information about position, Shankar argues, the probability distribution should be "flat", meaning that it is equally likely to find it anywhere. Thus, one cannot accept the wave function as described in (1).

Is there a function that has a wavelength and, yet, a constant absolute value? The *complex exponential* has this property. Therefore, instead of (1), if the wave function looks like

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}}, \tag{2}$$

then its absolute square has a constant value $|\psi_p(x)|^2 = Ae^{\frac{ipx}{\hbar}} \cdot Ae^{\frac{-ipx}{\hbar}} = |A|^2$ (see Fig. 2). In sum, the wave function needs to be complex so that no information about the position is obtained for a state of definite momentum.

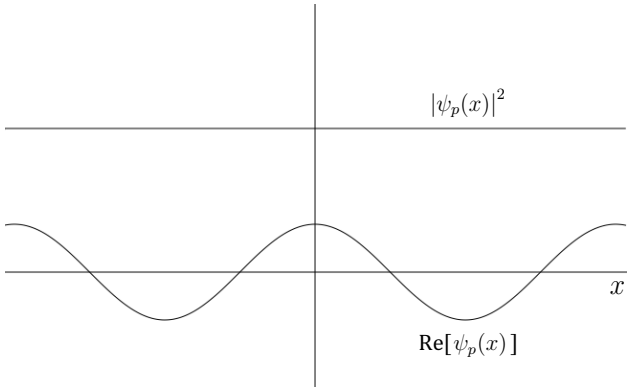

FIG. 2. Graphs of Re$[\psi_p(x)]$ and $|\psi_p(x)|^2$ for $\psi_p(x) = Ae^{\frac{ipx}{\hbar}}$. Now the contradiction is eliminated, since there is no information about the electron's position for a state of definite momentum.

One advantage of this argument is that it has the structure of a *reductio ad absurdum* proof, i.e., it starts by assuming a real wave function and reaches a contradiction, which can be psychologically more appealing to students. It also nicely stresses a formal difference between a cosine and a complex exponential, both are periodic functions but the latter has a constant absolute value, and therefore is more suitable to describe the intended physical properties. On the other hand, the argument relies on providing plausible reasons for why one cannot have full information about position and momentum simultaneously, and it postulates the square modulus of $\psi(x)$ as probability density, which can leave students wondering where this comes from.

B. Because i appears explicitly in the Schrödinger equation

The second justification stems from the textbook "Quantum Theory" written by David Bohm[12] and is based on a structural difference between the classical wave equation and

Schrödinger's time-dependent equation. For simplicity reasons, let us first consider the wave equation in one dimension

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}. \tag{3}$$

Can we allow the solutions to this equation to be complex valued? In other words, what are the consequences of writing the solution as $y(x,t) = A(x,t) + iB(x,t)$? By substituting this complex function in (3), and setting the real and imaginary parts to be respectively equal, we get

$$\frac{\partial^2 A}{\partial t^2} = c^2 \frac{\partial^2 A}{\partial x^2} \quad \text{and} \quad \frac{\partial^2 B}{\partial t^2} = c^2 \frac{\partial^2 B}{\partial x^2}, \tag{4}$$

which means that the functions A and B can be *chosen freely*, as long as they both satisfy the wave equation. Due to its nice mathematical properties that make calculations easier, we often use the complex exponential $e^{i(kx-\omega t)}$ to represent oscillating travelling waves, but attach physical meaning only to its real part. As we can see from Euler's formula, both $A(x,t) = \cos(kx - \omega t)$ and $B(x,t) = \sin(kx - \omega t)$ are solutions to the wave equation, but given $A(x,t)$, $B(x,t)$ could be another function that satisfies the same equation.

Now let us try to do the same with the Schrödinger equation. Consider, for simplicity, the equation of a free particle in one dimension[13]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}. \tag{5}$$

Substituting $\psi(x,t) = A(x,t) + iB(x,t)$ in (5) and setting the real and imaginary parts to be respectively equal, we obtain the following conditions

$$\frac{\partial A}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 B}{\partial x^2} \quad \text{and} \quad \frac{\partial B}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2 A}{\partial x^2}. \tag{6}$$

Now we no longer have the freedom to choose the functions $A(x,t)$ and $B(x,t)$ arbitrarily since they are *coupled* by the relations (6). This implies that we need *two* functions to describe the physical situation and cannot assign meaning to just one of them, as it was the case with classical waves. This will generally happen when the imaginary unit appears explicitly in the differential equation, as in Schrödinger's. Another way to justify the need for *two* (real) functions is to see how they both appear in the definition of probability density $P = \psi^* \psi = A^2 + B^2$.

But then another question arises immediately: Why is there an i in the time-dependent Schrödinger equation? One answer can be found in Schrödinger's original derivation of his time-dependent equation, which consists in eliminating the energy parameter E from his time-independent equation[14]

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0. \tag{7}$$

The derivation involves assuming the Planck-Einstein relation $\omega = E/\hbar$ and using separation of variables to represent $\psi(x,t) = \Psi(x) \cdot e^{i\frac{E}{\hbar}t}$. In order to eliminate the energy parameter, we derive $\psi(x,t)$ with respect to time

$$\frac{\partial\psi}{\partial t} = i\frac{E}{\hbar}\psi, \tag{8}$$

and substitute in Eq. (7) to obtain

$$\frac{\partial^2\psi}{\partial x^2} - i\frac{2m}{\hbar}\frac{\partial\psi}{\partial t} - \frac{2m}{\hbar^2}V\psi = 0, \tag{9}$$

which, for a free particle, is exactly Eq. (5). Thus, one can say that the imaginary unit i appeared explicitly in the equation because a time periodic function was represented by a complex exponential. This enabled the isolation of the energy parameter already after the first time derivative.[16]

One nice thing about this justification is that it emphasizes formal differences between the classical wave equation and Schrödinger's equation, and is therefore closer to Schrödinger's original reasoning. For some people this can actually be a drawback, since it puts too much emphasis on the wave formalism, which can hinder a more authentic understanding of modern quantum mechanics. Another interesting aspect is that it highlights the relation between a complex function and two coupled real functions, implying that in quantum mechanics one needs two real functions to describe the dynamics of a system. As in the previous case, here we are also led to wonder about the implications of certain formal differences between a cosine and a complex exponential. One negative aspect of this justification is that if one truly wants to explore the consequences of a real wave function which is the solution of a fourth order differential equation (see note 16), then the explanation can become too demanding/distracting and not worth the trade-off from a pedagogical point of view.

C. S_x, S_y and S_z in sequential Stern-Gerlach experiments

This justification appears in some textbooks that adopt the so-called spin first approach (e.g. Ref. 18–20) and therefore differs fundamentally from the two previous ones. Sequential Stern-Gerlach (SG) experiments are presented to motivate the need for a departure from classical mechanics and to build the new formalism of quantum states. The situation illustrated in Fig. 3 is used to highlight some peculiarities of quantum mechanical systems, since it is rather counterintuitive that a component of S_z in the negative ($\downarrow$) direction "reappears" after the beam emerges from the third apparatus. The reason is that one cannot determine S_z and S_x simultaneously. In other words, they are *incompatible observables* and the selection of the component of S_x in the positive ($\uparrow$) direction by the second apparatus destroys any previous information about S_z.[18]

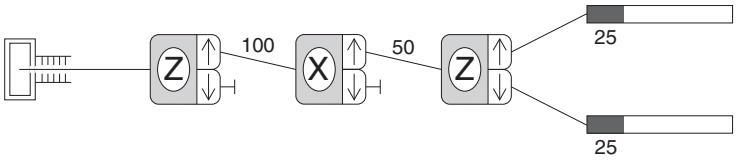

FIG. 3. Sequential SG experiments showing the counterintuitive result that particles with a negative S_z "reappear" after the beam emerges from the third apparatus, although they were previously "blocked" by the first apparatus. Figure in Ref. 19, p. 9.

Within this context, the notion of a *ket*, a quantum state vector, is introduced to express quantum states mathematically. By convention, the states with definite values of S_z (which we call S_z states) are denoted by $|+\rangle$ and $|-\rangle$, and are taken as basis vectors for other states with definite values of other spin observables. Thus, for the situation presented in Fig. 3, one can express the kets with definite values of S_x ($|+\rangle_x$ and $|-\rangle_x$, according to the notation used in Ref. 19) as a linear combination of the S_z basis vectors, i.e., $|+\rangle_x = a\,|+\rangle + b\,|-\rangle$ and $|-\rangle_x = c\,|+\rangle + d\,|-\rangle$.

The situation that leads to the need for complex numbers is described as follows. In Fig. 3, the beam is traveling in the y-direction. But the situation is symmetric, so the exact same result is to be expected if the beam travels in the x-direction and the SG_X apparatus is replaced by a SG_Y. However, it is important to distinguish between S_x and S_y states, e.g., $|+\rangle_y$ cannot have the same coefficients a and b. So how is that possible?

In his initial discussion of sequential SG experiments, Sakurai makes use of a formal analogy with light polarization to find a solution to this problem. He compares the decomposition of the S_x states with the mathematical expression of linearly polarized light in the xy-plane and inclined 45° with the x-direction. In order to represent the S_y states in a different way, Sakurai argues, one can refer to the mathematical expression of circularly polarized light, which is clearly a distinct physical situation. Because the perpendicular components of circularly polarized light are out of phase by 90°, complex numbers appear to represent this phase difference. Although the analogy is meaningful from a formal perspective, it seems confusing if one tries to make some kind of physical association between the two situations.

McIntyre[19] and Townsend[20] do not refer to the analogy with polarization, but introduce directly the formalism of quantum state vectors and the probabilistic interpretation of the square modulus of the inner product between two state vectors. This enables them to treat more formally the issue of distinguishing the S_x from the S_y states and to motivate the need for complex numbers. These states are first represented in the S_z basis as follows:

$$\begin{aligned} |+\rangle_x &= a\,|+\rangle + b\,|-\rangle \\ |-\rangle_x &= c\,|+\rangle + d\,|-\rangle \end{aligned} \quad \text{and} \quad \begin{aligned} |+\rangle_y &= e\,|+\rangle + f\,|-\rangle \\ |-\rangle_y &= g\,|+\rangle + h\,|-\rangle\,. \end{aligned} \tag{10}$$

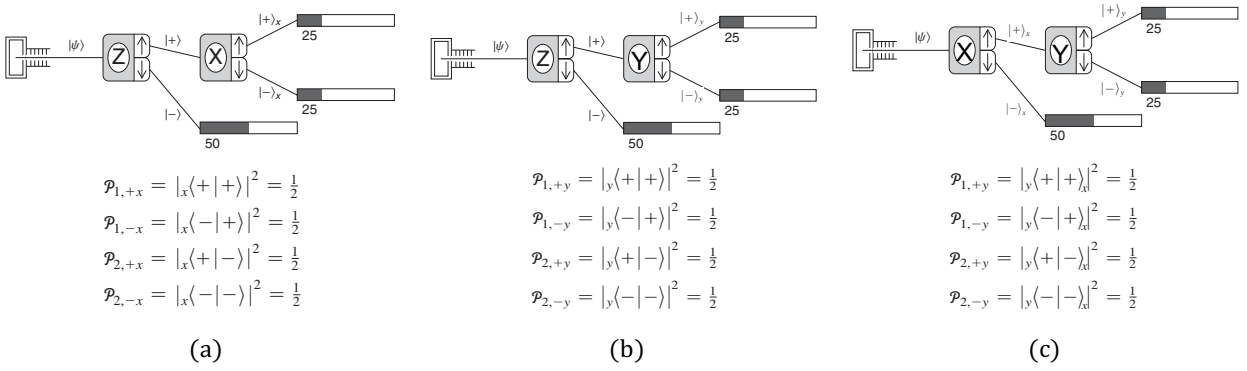

FIG. 4. Different configurations of sequential SG experiments are treated formally in order to motivate the need for complex numbers for the description of quantum state vectors. $|_x\langle +|+\rangle|^2 = \frac{1}{2}$ represents the probability that the output state is $|+\rangle_x$ when the input state is $|+\rangle$. Figures adapted from Ref. 19.

In order to determine the coefficients, which are in principle assumed to be complex, the probabilities for the situations described in Fig. 4 are used. From the first line of Fig. 4(a),

we have

$$\begin{aligned} |_x\langle +|+\rangle|^2 &= \frac{1}{2} \\ |(a^*\langle +| + b^*\langle -|)|+\rangle|^2 &= \frac{1}{2} \\ |a|^2 &= \frac{1}{2}. \end{aligned} \tag{11}$$

Performing similar calculations for the other three lines of Fig. 4(a), we obtain the following relations between the coefficients of the S_x states

$$|a|^2 = |b|^2 = |c|^2 = |d|^2 = \frac{1}{2}. \tag{12}$$

Thus, we know the absolute square of each coefficient, but their phase is indeterminate. Since the absolute phase is not physically measurable, one coefficient of each vector of the S_x states can be chosen to be real without loss of generality[24], so that we can take $a = c = \frac{1}{\sqrt{2}}$.

Both state vectors ($|+\rangle_x$ and $|-\rangle_x$) are already normalized, but not necessarily orthogonal. Imposing the latter condition we obtain

$$\begin{aligned} |_x\langle -|+\rangle_x| &= 0 \\ \left[\frac{1}{\sqrt{2}}\langle +| + d^*\langle -|\right]\left[\frac{1}{\sqrt{2}}|+\rangle + b|-\rangle\right] &= 0 \\ d^*b &= -\frac{1}{2}. \end{aligned} \tag{13}$$

Since our goal is to try to use only real numbers, we are free to choose $b = \frac{1}{\sqrt{2}}$ and $d = -\frac{1}{\sqrt{2}}$, which enables us to represent the S_x states (in matrix notation)[25] as

$$|+\rangle_x \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad \text{and} \quad |-\rangle_x \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}, \tag{14}$$

showing that we managed to represent the S_x states in the S_z basis without using complex numbers. So far, so good.

Now let us try to do the same S_y states. From Fig. 4(b) we arrive at similar relations as (12), i.e., $|e|^2 = |f|^2 = |g|^2 = |h|^2 = \frac{1}{2}$, and make the same initial assumption that $e = g = \frac{1}{\sqrt{2}}$. Orthogonality of the S_y states gives us, just like in (13), $f^*h = -\frac{1}{2}$. In order to avoid complex numbers and to distinguish the S_y from the S_x states, we are tempted to choose $f = -\frac{1}{\sqrt{2}}$ and $h = \frac{1}{\sqrt{2}}$.

However, this would be in contradiction with the situation represented by Fig 4(c). Taking, for instance, the first line

$$\begin{aligned} |_y\langle +|+\rangle_x|^2 &= \frac{1}{2} \\ \left|(\frac{1}{\sqrt{2}}\langle +| + f^*\langle -|)\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)\right|^2 &= \frac{1}{2} \\ \left|\frac{1}{2} + \frac{f^*}{\sqrt{2}}\right|^2 &= \frac{1}{2}, \end{aligned} \tag{15}$$

we can see that $f = -\frac{1}{\sqrt{2}}$ cannot be a solution. Since f cannot be $\frac{1}{\sqrt{2}}$ either, in order to distinguish the S_y states from the S_x, this already suffices to demonstrate that we won't be able to represent the S_y states only with real numbers. In fact, by looking carefully at (15) we can already predict that f needs to be purely imaginary. To show this more formally, we write f as a general complex number with absolute square equal to $\frac{1}{2}$, i.e, $f = \frac{e^{i\alpha}}{\sqrt{2}}$, and substitute it in (15),

$$\begin{aligned} \left(\frac{1}{2} + \frac{e^{-i\alpha}}{2}\right)\left(\frac{1}{2} + \frac{e^{i\alpha}}{2}\right) &= \frac{1}{2} \\ \frac{1}{4} + \frac{1}{4}\left(e^{-i\alpha} + e^{i\alpha}\right) + \frac{1}{4} &= \frac{1}{2} \\ \cos\alpha &= 0 \\ \alpha &= \pm\frac{\pi}{2}. \end{aligned} \tag{16}$$

Choosing $\alpha = \frac{\pi}{2}$, $f = \frac{i}{\sqrt{2}}$ and $h = \frac{-i}{\sqrt{2}}$, since $f^*h = -\frac{1}{2}$. These coefficients also verify all the relations of Fig 4(c). Thus, we can represent the the S_y states in the S_z basis as

$$|+\rangle_y \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \quad \text{and} \quad |-\rangle_y \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}. \tag{17}$$

After arriving at this result, Townsend (Ref. 20, p. 17) concludes:

> The appearance of i's [in (17)] is one of the key ingredients of a description of nature by quantum mechanics. Whereas in classical physics we often use complex numbers as an aid to do calculations, there they are not essential. The straightforward Stern-Gerlach experiments we have outlined [...] *demand* complex numbers for their explanation.

This example shows that although it is possible to write the S_x states in the S_z basis without complex numbers, they are inevitable to describe the S_y states in the same basis. A more general way to put it is to say that complex numbers are indispensable to describe (two-state) systems with more than two incompatible observables.

This type of reason is analogous to other more mathematical arguments where complex numbers appear due to a necessity of some kind of generalization/expansion of our notion of number, e.g., in connection with the fundamental theorem of algebra. It is somehow also related with the first geometrical interpretation of complex numbers, where they appear as a necessity to fully represent direction in the plane.[21] One aspect that can be criticized in this approach is the fact that the coefficients of quantum state vectors are assumed to be complex numbers from the beginning, and no justification for that is usually offered.

D. To enable *continuous* transitions

The forth justification presented here is based on the last of Lucien Hardy's "five reasonable axioms" from which quantum theory can be deduced[22] and has been presented in an insightful paper written by Artur Eckert.[23] It starts with the possibility of building quantum mechanics entirely from classical probability in order to see where this leads. The initial assumption is that a quantum state is described by a column vector in which each term represents the probability of the system to be measured in a given configuration. For instance, in a two-state system like the spin 1/2 discussed in the previous section, such a vector could look like

$$\vec{p_0} = \begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix}, \tag{18}$$

meaning that it has 30% probability to be measured with its spin up and 70% down.

In such a formalism, transitions are represented by stochastic matrices, whose elements are positive real numbers and whose values in each column add up to 1. One random example of a transition (T_1) applied to $\vec{p_0}$ is

$$T_1\vec{p_0} = \begin{pmatrix} 0.2 & 0.4 \\ 0.8 & 0.6 \end{pmatrix} \begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix} = \begin{pmatrix} 0.34 \\ 0.66 \end{pmatrix}, \tag{19}$$

meaning that after this transition there is 34% probability for spin up and 66% for spin down. The elements of the stochastic matrices represent the probabilities for the system to either remain (main diagonal) or swap states (antidiagonal). Note that after the transition the probabilities still add up to 1.

When one thinks about time evolution, a physically desirable requirement is that these transitions are *continuous*. In other words, it should be possible to view any transition as a sequence of independent transitions over shorter periods of time. Among other things, this means that one should be able to extract square or cubic roots (in fact any n^{th} root) of any transition and the result should be another stochastic matrix. Let us take, for instance, one square root of T_1

$$(T_1)^{1/2} = \frac{1}{3}\begin{pmatrix} 1+\frac{2}{\sqrt{5}}i & 1-\frac{1}{\sqrt{5}}i \\ 2-\frac{2}{\sqrt{5}}i & 2+\frac{1}{\sqrt{5}}i \end{pmatrix},$$

which enables us to write T_1 as

$$T_1 = \frac{1}{3}\begin{pmatrix} 1+\frac{2}{\sqrt{5}}i & 1-\frac{1}{\sqrt{5}}i \\ 2-\frac{2}{\sqrt{5}}i & 2+\frac{1}{\sqrt{5}}i \end{pmatrix}\frac{1}{3}\begin{pmatrix} 1+\frac{2}{\sqrt{5}}i & 1-\frac{1}{\sqrt{5}}i \\ 2-\frac{2}{\sqrt{5}}i & 2+\frac{1}{\sqrt{5}}i \end{pmatrix}. \tag{20}$$

One can easily see that our initial goal was not achieved, i.e., it was not possible to write the stochastic matrix T_1 as the product of two (equal) stochastic matrices. The elements of $(T_1)^{1/2}$ are complex numbers with non-zero imaginary parts.[26]

This example is enough to show that if one requires continuity of transitions, real numbers are not sufficient. The attempt to describe quantum mechanical systems with classical probability failed and complex numbers appeared inevitably. As in the first justification, this one has also the *reductio ad absurdum* structure. Another advantage is that one counterexample is sufficient to show the need for a more general set of numbers. This justification can also lead to arguments related to the need for a unitary time evolution. A possible drawback is that this explanation can be too mathematical and wouldn't make much sense for newcomers who aren't used to a probabilistic description of the physical world. Another critical remark can be that although it shows that real numbers are not sufficient, it does not fully prove that complex numbers are enough for a complete quantum mechanical formalism.

III. CONCLUSIONS

Complex numbers seem to be fundamental for the description of the world proposed by quantum mechanics. In principle, this can be a source of puzzlement: Why do we need such abstract entities to describe real things?

One way to refute this bewilderment is to stress that what we can measure is essentially real, so complex numbers are not directly related to observable quantities. A more philosophical argument is to say that real numbers are no less abstract than complex ones, the actual question is why mathematics is so effective for the description of the physical world.[28]

Regardless of philosophical discussions, a newcomer to quantum mechanics will encounter complex variables and it is legitimate for her/him to ask why do we need them. A brief search on the internet also shows numerous forums discussing the topic. As mentioned in the introduction, some of the very founders of theory were puzzled by this issue. So the question posed in the title is clearly perceived as relevant and it is worthwhile to dedicate some didactic effort to come up with plausible justifications.

When comparing the answers presented here, it is quite interesting to see how they differ from one another. Four apparently different physical principles/properties are used to justify the need for complex numbers, namely (II.A): the impossibility of having information on position when momentum is exactly known; (II.B): the fact that i appears explicitly in the Schrödinger equation; (II.C): the descriptions of S_x, S_y and S_z in sequential Stern-Gerlach experiments; and (II.D): the demand for continuous transitions. For courses adopting a position first framework, A and B should be more appropriate, whereas C and D are more suitable for the ones that chose a spin first. This diversity of explanations reflects a historical (and actual) characteristic trait of quantum mechanics, which is the possibility of multiple theoretical approaches.

It is reasonable to assume that people with different backgrounds will have different preferences. But perhaps the question "Which is THE best justification?" is not the most appropriate. One learns something from each justification and a deep understanding of the matter is probably related to the establishment of different connections. For a physics instructor, one can conjecture that "the more the better", as it seems plausible to assume that one important teaching competence is to possess a broad repertoire of explanations.

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[1] Salomon Bochner, "The significance of some basic mathematical conceptions for physics," *Isis* **54**(2), 179-205 (1963).

[2] This struggle is well documented in Schrödinger's letters and papers. Here we give two examples. In a letter to Lorentz on June 6, 1926, Schrödinger wrote: "What is unpleasant here, and indeed directly to be objected to, is the use of complex numbers. ψ is surely fundamentally a real function". The last paragraph of his forth communication to the *Annalen der Physik* also illustrates this feeling of puzzlement and frustration: "Meantime, there is no doubt a certain crudeness in the use of a complex wave function."

[3] C.N. Yang, "Square root of minus one, complex phases and Erwin Schrödinger," in Schrödinger: Centenary celebration of a polymath, edited by C.W. Kilmister (Cambridge University Press, Cambridge, 1987), pp. 53-64.

[4] In fact, Dirac is quite explicit about that in the forth edition of his celebrated book *The Principles of Quantum Mechanics* (p. 20, our emphasis): "Our bra and ket vectors are complex quantities, since they can be multiplied by complex numbers and are then of the same nature as before, but they are *complex quantities of a special kind which cannot be split up into real and pure imaginary parts*. The usual method of getting the real part of a complex quantity, by taking half the sum of the quantity itself and its conjugate, cannot be applied since a bra and a ket vector are of different natures and cannot be added."

[5] It is worth mentioning that we are scratching the surface of a much deeper question that has been

addressed by many serious researchers on mathematical foundations of quantum mechanics (e.g. Ref. 6). Among them, the work of Stueckelberg (Ref. 7) stands out as a plausible formulation of quantum mechanics in *real* Hilbert space (see Ref. 8 for a pedagogical introduction). The interested reader will also find numerous discussions about the topic in internet forums, such as `https://physics.stackexchange.com/questions/32422/qm-without-complex-numbers`.

[6] Felix M. Lev, "Why is quantum physics based on complex numbers?" *Finite Fields and Their Applications*, 12, 336 (2006).

[7] Ernst C. G. Stueckelberg, "Quantum Theory in Real Hilbert Space." *Helv. Phys. Acta* 33, 727 (1960).

[8] Jan Myrheim, "Quantum Mechanics on a Real Hilbert Space." arXiv:quant-ph/9905037.

[9] A broad literature review shows very few attempts to explain the need for complex numbers in quantum mechanics, both in introductory level textbooks or physics education journals. An exception is the paper "Why i?" (W. E. Baylis *et al.*, *Am J Phys* 60 (9), 788, 1992), which actually deals with the question of why complex numbers are useful for physics in general. This paper is based on the *geometric algebra* by David Hestenes, who proposes a new mathematical formalism for physics (*Am J Phys* 71 (2), 104, 2003). Because of its geometrical interpretation, the reasons for "Why i?" in quantum mechanics enabled by this formalism are very convincing and it is definitely worthwhile pursuing this project. However, here we are concerned with physics instructors who use more standard approaches.

[10] Ramamurti Shankar, *Fundamentals of Physics II: Electromagnetism, Optics, and Quantum Mechanics* (Yale University Press, New Haven, 2016).

[11] If one takes the precise definition of uncertainty in quantum theory, the cosine function does not violate the uncertainty principle, since its uncertainty is infinite (plane wave). Nevertheless, the general argument that this function does provide information about position still holds. I am indebted to two reviewers for pointing this out.

[12] David Bohm, *Quantum Theory* (Prentice-Hall, New York, 1951).

[13] The main argument would remain valid in the general case.

[14] From a pedagogical perspective it would be important to show where this equation comes from. Schrödinger derived it from Hamilton's optical-mechanical analogy (See Ref. 15). For our purpose here, it is worth stressing that one does *not* need to use the complex exponential in this derivation, i.e., the same expression is obtained if one assumes $\psi(x,t) = \Psi(x) \cdot \cos \frac{E}{\hbar} t$.

[15] Erwin Schrödinger, *Four lectures on wave mechanics*, delivered at the Royal institution, London, on 5th, 7th, 12th, and 14th March, 1928. (Blackie & son limited, London, Glasgow, 1928).

[16] If we had represented ψ as a purely real periodic function, e.g. $\psi(x,t) = \Psi(x) \cdot \cos \frac{E}{\hbar} t$, then we would need to derive it twice with respect to time to isolate the energy parameter ($\frac{\partial^2 \psi}{\partial t^2} = -\frac{E^2}{\hbar^2}\psi$). In order to substitute this in Eq. (7), we would also need to square the whole equation and would end up with a rather complicated fourth order equation that looks like $(\frac{\partial^2}{\partial x^2} - \frac{2m}{\hbar}V)^2\psi + \frac{4m^2}{\hbar^2}\frac{\partial^2 \psi}{\partial t^2} = 0$. Curiously, this fourth-order equation was the one Schrödinger initially claimed to be "*the uniform and general wave equation for the scalar field* ψ*"*, since apparently it would be possible to consider ψ as a real function. One can hypothesize that Schrödinger did this in order to avoid an explicit i in his fundamental equation. Dealing with this matter is beyond the scope of this article, but the interested reader can find deeper discussions about the implications of a real wave function in the continuation of Bohm's argument[12] and in Ref. 17.

[17] Robert L. W. Chen, "Derivation of the real form of Schrödinger's equation for a nonconservative system and the unique relation between Re(ψ) and Im(ψ)", *J. Math. Phys.*, 30 (1), 1988.

[18] Jun John Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Boston, 1967).

[19] D. H. McIntyre, C. A. Manogue, J. Tate, *Quantum Mechanics: A Paradigms Approach* (Pearson Addison-Wesley, Boston, 2012).

[20] John S. Townsend, *A Modern Approach to Quantum Mechanics, Second Edition* (University Science Books, Mill Valley, CA, 2013).

[21] Paul J. Nahin, *Imaginary Tale: The Story of* $\sqrt{-1}$ (Princeton University Press, Princeton, 1998).

[22] Lucien Hardy, "Quantum Physics From Five Reasonable Axioms," arXiv:quant-ph/0101012v4.

[23] Artur Ekert, "Complex and unpredictable Cardano," *Int J Theor Phys*,47, 2101 (2008).

[24] We will assume that a and c are real because we want to see if we can get away without complex numbers. A more general treatment of the situation is presented in Ref 20.

[25] The symbol $\doteq$ is used to indicate "is represented by". One cannot set the ket *equal* to the column vector, because the former is an abstract vector and the latter is its representation in a given basis.

[26] There is a great deal of gymnastics to calculate the square root of a square matrix. For this particular case, the fact that the determinant of T_1 is negative already guarantees that the components of its square roots are complex numbers with non-zero imaginary parts (see Ref. 27).

[27] Bernard W. Levinger, "The Square Root of a 2 x 2 Matrix", *Mathematics Magazine*, **53** (4), 222-224 (1980).

[28] See, for instance, Wigner's *Unreasonable Effectiveness* paper (Pure Appl. Math. 13, 114 , 1960) and the debates related to it.