

Modifying symbolic forms to study probability expressions in quantum mechanics

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As part of an effort to examine student understanding of expressions for probability in an upper-division spins-first quantum mechanics (QM) context, clinical think-aloud interviews were conducted with students following relevant instruction. Students were given various tasks to showcase their conceptual understanding of the mathematics and physics underpinning these expressions. The symbolic forms framework was used as an analytical lens. Various symbol templates and conceptual schemata were identified, in Dirac and function notations, with multiple schemata paired with different templates. The overlapping linking suggests that defining strict template-schema pairs may not be feasible or productive for studying student interpretations of expressions for probability in upper-division QM courses.

Keywords: Quantum mechanics, probability, notation, representation

Introduction and Background

Mathematics is used in physics for far more than simple computation. Physicists make use of mathematical expressions and relationships to help them understand and reason about the world (Uhden et al., 2012). This is more true than ever in quantum mechanics (QM), where physical intuition developed in everyday life has little application and one must rely on mathematical reasoning to help intuit, understand, and predict systems on the quantum scale. The level of abstraction and mathematical sophistication required in upper-division QM courses has been extensively shown to be difficult for students in many ways (Singh, 2001; Singh, 2008; Singh & Marshman, 2015; Emigh et al., 2015; Passante et al., 2020). Some of the reasons for this difficulty are the number of different notations on offer, the vast differences in how they each appear, and the variety of mathematics they each require (Gire & Price 2015).

In QM, particles and systems of particles are described as existing in “quantum states.” These states are defined as having some set associated, measurable quantity or quantities, such as specific energy values, positions, or momenta. Often, these quantities are incapable of being simultaneously determined together, and the most we can know about a particle with one definite quantity is the likelihood of measuring the various possible values of a separate quantity. Physicists primarily use linear algebra to express these probabilistic relationships, and use Dirac

notation to express these states as vectors: $|\psi\rangle = \sum_n c_n |n\rangle$. Here, $|\psi\rangle$ is a vector representation

(called a “ket”) of the state our particle is in, and the various $|n\rangle$ ’s are representative of the various states the particle could be measured in – an eigenbasis – each corresponding to a different value of whichever quantity we are measuring. The probability of measuring each of those $|n\rangle$ states is given by $|c_n|^2$, or by taking the complex square of the inner product of the initial state (vector) with the particular possible state (vector) that we’re interested in. In Dirac notation, this is written as: $P_n = |\langle n|\psi\rangle|^2$. This type of analysis is only applicable when the quantities in question are discretized, but is extended to include defining states with wave

functions: $|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)|x\rangle dx$. This can then be used to find probabilities for measuring that

quantity within a range of values: $P_{a \rightarrow b} = \int_a^b |\psi(x)|^2 dx$. The discrete probability written before

can also be written with these wave functions: $|\langle \psi \rangle|^2 = \int_{-\infty}^{\infty} \varphi_n^*(x) \psi(x) dx$, where

$\psi(x) = \sum_n c_n \varphi_n(x)$. The difference in appearance and the type of mathematics required for these different probabilities is one of the reasons for the aforementioned difficulties for students learning and using the requisite mathematics in QM.

One framework that has been used to explain student reasoning with mathematical expressions is that of symbolic forms (Sherin, 2001), which was proposed by Sherin to explain how students could generate symbolic expressions for different physical scenarios. Largely based on the knowledge-in-pieces model (diSessa, 1993), symbolic forms is predicated on the notion that students learn to develop a sort of grammar and syntax for different mathematical operations in physics, and subsequently apply that logic to make sense of physical relationships. Sherin found that there were some universal forms that expressions take that students grow to recognize, which he called symbol templates, and that students learn to associate these templates with a conceptual understanding known as a conceptual schema. Symbol templates, when combined with their associated conceptual schemata, become symbolic forms, which Sherin argues form the building blocks for student interpretations of mathematical expressions used in physics. For example, the *parts-of-a-whole* symbolic form has “[$\square + \square + \square + \dots$]” as its symbol template, and its conceptual schema contains the idea of multiple parts of a larger entity being summed together. This framework has since been extended to study the structure of expressions in more advanced topics in physics (Dreyfus et al., 2017; Schermerhorn & Thompson, 2019; Ryan & Schermerhorn, 2020) and has been looked at as a means to describe students' blending of conceptual and formal mathematical reasoning (Kuo et al., 2013).

Previous work has also looked at the affordances and limitations of the different notations used in QM (Gire & Price, 2015; Schermerhorn et al., 2019; Wawro et al., 2020). Dreyfus et al. (2017) posited a number of potential symbolic forms within Dirac notation that they suspect students likely develop through the course of an upper-division QM course, though little work has been done to address how students interpret and work with expressions across and within the different representations that are commonly used in upper-division QM.

As part of a study on how students reason about expressions in the various notations used in QM and the ways in which they translate between them, we conducted clinical think-aloud interviews with a number of students following a one-semester, spins-first, upper-division QM course. In a spins-first course, students begin working with Dirac notation immediately in the context of spin-1/2 systems, before eventually including wave function notation when position is introduced as a continuous observable. The mathematical connections between Dirac state vectors and wave functions are shown in an effort to help deepen students' understanding of Dirac notation, as well as to make the transition to wave functions as smooth as possible. We asked the students to both generate and relate different expressions in both Dirac notation and wave function notation. Due to our focus on student understanding and interpretation of symbolic expressions, Sherin's symbolic forms framework (Sherin, 2001) was used as a starting point for analysis. Our analysis suggests a modest expansion of the symbolic forms framework to address multiple overlapping sets of templates and schemata. This paper describes our analysis

of student interpretations of expressions for probability in both Dirac and wave function notations, as well as the ways in which students translate between the two.

Study Design and Methodology

In order to elicit students' understanding of expressions commonly used to represent probability in QM, both in-person (paired, N=2) and virtual (individual, N=2) clinical think-aloud interviews were conducted following a one-semester upper-division QM course in two separate academic years. Students in both interview formats were asked to generate expressions for probabilities and to reason about both the expressions they generated as well as the processes by which they were generated. The virtual interviewees were provided with a number of symbolic building blocks with which to construct their expressions (see Figure 1), while the in-person interviewees were given a whiteboard and markers. In both cases, subjects were asked to generate expressions for probabilities based on scenarios similar to those studied in class. Some in-person interview questions gave the participants an expression describing a state and asked them to use it to find specific probabilities. The virtual interviewees were also given a card-sorting task where they were asked to sort a variety of expressions commonly seen in QM coursework, as well as generic vector expressions such as $\vec{v}$, $\hat{j}$, and $\vec{u} \cdot \vec{v}$.

The students' responses were transcribed and analyzed to determine which expressions they either grouped or generated, any intermediary expressions they used, and the language they used to explain their expressions. Excerpts of interest contained episodes of students interpreting specific expressions, explicitly connecting templates and schemata.

Figure 1. The symbolic building blocks of expressions that virtual participants had to work with when constructing their expressions.

Results and Discussion

Our analysis has revealed several different conceptual schemata, as well as a number of symbol templates with which students tended to associate them (Table 1). Despite differences in the tasks given between the two interview formats, our analysis did not suggest any modality-based distinctions. We propose that the focus on template-schema pairs common to symbolic form analysis is limiting when multiple symbol templates share the same conceptual schema.

Table 1. Identified conceptual schemata with their associated symbol templates. Some schemata are associated with multiple templates and vice versa.

Conceptual Schema	Symbol Templates
Vector in a space	$ \rangle, \langle , c_1 1\rangle + c_2 2\rangle + \dots$
Function in a space	$c_1 f_1(a) + c_2 f_2(a) + \dots$
Quantum state	$ \rangle, \langle , f(a), f^*(a), f_n(a), f_n^*(a)$
Projection/dot product	$\langle\rangle, \int f(a)g(a)da$

Probability density

$$\langle \rangle, |f(a)|^2$$

Probability

$$|c_n|^2, \langle \rangle, |\langle \rangle|^2, \int f(a)g(a)da, \int |f(a)|^2$$

Dirac notation paired with vector ideas

Students across all three interviews in this study (Aliyah and Bilbo in the virtual interviews and Castor and Delilah in-person) explicitly referred to both kets and bras as representing vector-like quantities, and Dirac brackets as being akin to dot products between them:

Bilbo (discussing sorted category containing $\vec{v}$, $\hat{j}$, $|\psi\rangle$, and $|E_n\rangle$): to me, all vectors. Unit vector $\hat{j}$, generic vector $\vec{v}$, state- ... wave vector $|\psi\rangle$, eigenstate vector $|E_n\rangle$

Bilbo (discussing operating $\hat{S}_z$ on $|\psi\rangle$): certainly changes the state ... if the state is purely in Z [meaning expressed as a superposition state in the $\hat{S}_z$ spin-1/2 basis], I believe it'll still change it, but I think by only lengthwise stretching ... rather than rotating.

Aliyah (discussing $\langle\psi\rangle$): why would I do ψ of ψ ? Because physically like I'm thinking in terms of vectors it represents ψ along ψ

Aliyah (explaining what they mean by “__ along __”): it's a traditional way to think about vectors like because our dot product represents- like $\vec{a} \cdot \vec{b}$ represents, basically, the projection of $\vec{a}$ along $\vec{b}$ or projection of $\vec{b}$ along $\vec{a}$

Castor (explaining why for $n \neq m$, $\langle E_m | E_n \rangle = 0$): Because of like orthonormality, the eigenstates are perpendicular in a space

Castor (explaining why $\langle E_2 | E_2 \rangle = 1$): Because, like 100% of E_2 [gestures at the bra] is in the direction of E_2 [gestures at the ket]

These responses largely match up with what one would expect, as a large focus of a spins-first QM course is to help students reason geometrically with Dirac notation.

Through the lens of symbolic forms, two conceptual schemata appear to be expressed here: a “vector in a space” and the “projection” idea that often arises with dot products. The former conceptual schema is linked to “|)” and “(|”, while the latter is linked to “<)”.

Dirac bras and kets paired with “quantum state”

While interesting in its own right, a vector-like understanding is not the only way that students worked with and thought about these Dirac expressions. All four students described bras and kets as stand-ins for quantum states as well:

Aliyah: This $|E_n\rangle$ represents a ket energy eigenstate, and this $\langle E_n |$ represents a bra energy eigenstate. So these $|\psi\rangle$ and $\langle\psi|$ are general ones, these $|E_n\rangle$ and $\langle E_n |$ are specific energy eigenstates

Bilbo (discussing $|x\rangle$): You could make x an eigenstate, you could make it a spin state ... put anything in there ... I just need it to be a ket

Castor: So typically when I write $|\psi\rangle$ in terms of the energy eigenstates [points to $|E_2\rangle$]...

Delilah (discussing a superposition state written $|\psi\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|E_1\rangle + |E_2\rangle + 2|E_3\rangle)$): We just represent it as the probab- the square root of the probability times the first state [points to $|E_1\rangle$] plus the square root of probability times the second state [points to $|E_2\rangle$] plus the square root of the probability times the third state [points to $|E_3\rangle$]

These students appear to be using some of the same symbol templates as in the previous section (“|”) and “⟨|”), but with a “quantum state” conceptual schema. This is unsurprising, as the first half of a spins-first course uses bras and kets as representations for a quantum state.

Other Dirac pairings

An additional common use of Dirac brackets was as a means of describing and calculating probabilities or probability amplitudes:

Aliyah: This [$\langle\psi\rangle$] will also represent the probability of finding x - sorry, the probability of finding the general state ψ in the eigenstate x

Bilbo: That [$\langle\psi\rangle$] is just an inner product, though, I had been saying the inner product squared is a probability and that this [$\langle\psi\rangle$] is... just a density

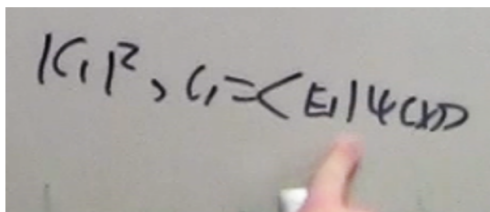
Again we see a symbol template from before (“⟨|”) being associated with a different conceptual schema: in this case, that of a probability-like concept. We note that “probability,” “probability amplitude,” and “probability density” are used somewhat interchangeably by the students throughout these interviews. Every student also eventually squares many of these Dirac brackets, which suggests yet another symbol template, “ $|\langle\rangle|^2$,” also with an associated “probability” conceptual schema.

While Castor and Delilah also related Dirac brackets to probability concepts, they almost exclusively did so by first claiming that the Dirac bracket gives “the coefficient,” and that “the coefficient squared” then gives the probability:

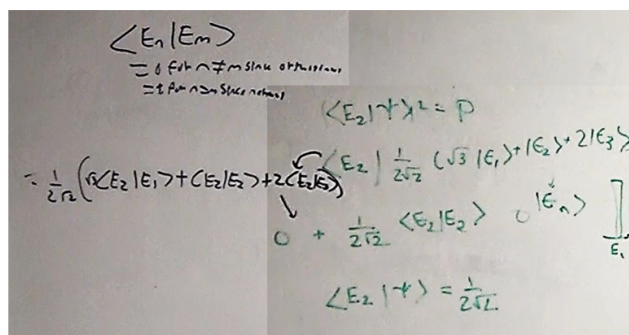
Castor (explaining why a number they found was a probability): Because it’s the coefficient for the first energy state. ... because we do, we do the same thing as... [writes $\langle\psi(x)\rangle$]

Delilah: Our probability for energy is the coefficient squared. And the coefficient is, E sub one times psi [writes $|c_1|^2$, $c_1 = \langle\psi(x)\rangle$] (see Figure 2a).

Castor and Delilah’s focus on “the coefficient” as a sort of requisite step to allow a Dirac bracket to describe a probability was not seen in Aliyah or Bilbo’s virtual interviews. This may be a case of Aliyah and Bilbo glossing over a step that they have since automated, or it could be evidence of Castor and Delilah using the Dirac bracket’s “dot product” conceptual schema to reason about a larger process of “pulling out a coefficient” from an expression for a superposition state. This process was shown explicitly by Castor and Delilah, as can be seen in Figure 2b. This suggests that these students developed another symbol template during this course: “ $c_1|1\rangle + c_2|2\rangle + \dots$ ”. The associated conceptual schema appears to be that of a vector being described with components along various basis vectors, in which case it is likely a compound form as discussed by Dreyfus et al. (2017), potentially of the “parts-of-a-whole” and “magnitude direction” symbolic forms, the former from Sherin (2001) and the latter from Schermerhorn and Thompson (2019). It also seems clear that Castor and Delilah make use of another symbol template, that of one of these coefficients squared, “ $|c_n|^2$,” and that they associate with it the conceptual schema for a “probability” as well.



(a)



(b)

Figure 2. (a) Delilah expressing how the Dirac bracket gives the coefficient, which can then be squared to find a probability, and (b) Castor's (right) and Delilah's (left) work explaining how $\langle \psi \rangle$ yields the coefficient, which is then squared to find the probability. Delilah's work supplements Castor's by explicitly distributing the bra throughout the sum.

Functions paired with state ideas

Moving away from Dirac notation, students in all interviews also worked with functions, often describing them as representing quantum states:

Aliyah: Those $[\psi(x), \psi^*(x), \varphi_n(x), \text{ and } \varphi_n^*(x)]$ represent states ... some of them represent general states $[\psi(x) \text{ and } \psi^*(x)]$, some of them represent specific energy states $[\varphi_n(x), \text{ and } \varphi_n^*(x)]$, but they represent states

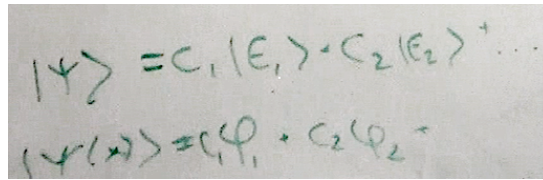
Bilbo: This $[\psi(x)]$ is just another function, so what I'm thinking of is like an eigenstate $[\varphi_n(x)]$ and just a generic state $[\psi(x)]$

Castor: These $[\varphi_1 \text{ and } \varphi_2 \text{ in } |\psi(x)\rangle = c_1\varphi_1 + c_2\varphi_2 + \dots]$ are the position eigenstates

Delilah: $\psi(x)$... is, like c_1 times $\varphi(x)$ [writes $\psi(x) = c_1\varphi_1(x) + \dots$] ... I think these [points to $\varphi_1(x)$] are the energy eigens- the energy eigenstates written in the position basis

Castor is being somewhat loose with their notation, mixing Dirac notation together with wave function notation in the same expression, but seems to have “translated” the kets they wrote previously into functions directly below them (see Figure 3). At this point the “quantum state” conceptual schema is being used to describe a very different-looking symbol template (that of a function, perhaps “ $f(a)$ ” or “ $f_n(a)$ ”). These excerpts potentially suggest a distinction between “ $f(a)$ ” and “ $f_n(a)$ ” as representing specifically “generic states” and “eigenstates,” respectively. Figure 3 also suggests another symbol template analogous to that discussed in the previous section, but in this case in wave function notation: “ $c_1f_1(a) + c_2f_2(a) + \dots$ ”. The paired schema is that of a “function in a space,” described as a sum of component functions—analogue to the compound form discussed above.

This shared schema is a reasonable instructional outcome as, once students begin working with wave function notation, they are often told that kets can be translated to functions and use $\psi(x)$ and $\varphi_n(x)$ to describe generic states and energy eigenstates, respectively.



$$|\psi\rangle = c_1|E_1\rangle + c_2|E_2\rangle + \dots$$

$$\psi(x) = c_1\phi_1 + c_2\phi_2 + \dots$$

Figure 3. Castor's expressions for a superposition state. They wrote the top line first, then the bottom beneath it.

Other function pairings

Students would also often write integrals of these functions when asked to generate expressions for probabilities. Below is an example of Bilbo's response after being asked how they would find the probability of measuring a given energy:

Bilbo: in this case $[\int \phi_n^*(x)\psi(x)dx]$ here ... I'm thinking okay, you have this state [points to $\psi(x)$] ... and you want to ask the question of, you know, "what about that state [$\psi(x)$] being in this [$\phi_n^*(x)$] eigenstate." And, or what is- to me I'm looking at this thing I'm thinking, "what is the projection of this eigenstate onto this wave function," or maybe vice versa, but I don't think it should matter- dot products are ... commutative

Bilbo generated an integral when asked for a probability, and discussed it with very similar language as was used for Dirac brackets above—that of a "projection" of one state onto another, both being represented as different functions within the integral. This supports a potential symbol template of " $\int f(a)g(a)da$ " being paired with a conceptual schema encapsulating ideas of "projection" or "dot product," providing the functional analog to the Dirac inner product expression.

Castor and Delilah were asked to find the probability of measuring a particle to be in the left half of an infinite square well, and used very different language to discuss their work:

Delilah: [writes $\int_0^{\frac{L}{2}} \frac{1}{8} (\sqrt{3}\phi_{E_1} + \phi_{E_2} + 2\phi_{E_3})^2 dx$] So we're- at every position we're computing [points to integrand]- like every infinitesimally small position we're computing the probability [again points to integrand]-

Castor: You're taking the probability, kind of at like an instant, and taking that like, infinitely small sum to get your, like, probability distribution.

Delilah: [writes " $|\psi(x)|^2 = \text{Probability Density}$ "] So yeah, so it just yeah, every- every infinitesimally- ... dx , yeah, essentially. We're finding the probability of it being there ... [it's] just the summation of all the values in the left half of the well.

It is worth pointing out that Castor and Delilah are, on the surface, doing a very different problem than Bilbo was above. Bilbo was finding a probability for an energy value, while Castor and Delilah were finding the probability of a range of position measurements. While a mathematical equivalence can be shown between these two problems, they appear to be different problems to the students, as they reasoned about the two integrals very differently. First, even though Castor and Delilah generated an integral, the symbol template is very different. Rather than two different functions (representing two separate quantum states) as the integrand, they instead used $|f(a)|^2$ (which may perhaps be thought of as $f^*(a)f(a)$, or the complex conjugation of the same function with itself). Second, Bilbo used very similar "projection" reasoning as was paired with the Dirac brackets in all three interviews, even explicitly bringing

up dot products. Castor and Delilah instead reasoned with probability distributions and Riemann sums, invoking an “adding up pieces” model for integration (Hu & Rebello, 2013; Jones, 2015).

The difference in how these integrals are written and interpreted suggests Castor and Delilah are utilizing a different symbol template here: “ $\int |f(a)|^2 da$ ” or perhaps “ $\int f^*(a)f(a)$ ”. It also seems evident that there may be a further symbol template here: “ $|f(a)|^2$ ”, which Castor and Delilah associate with a schema of “probability density.”

Conclusions

The symbolic forms framework gives us a language with which to discuss student interpretations of symbolic mathematical expressions. In our study we have seen that, in a spins-first context, students develop a multitude of conceptual schemata and numerous symbol templates, each often associated with multiple of the other. While we could take each identified template/schema pair and declare them all as separate symbolic forms, the level of overlap between many of them suggests it may be more productive to instead treat them as laid out in Table 1: as conceptual schemata that can be expressed in various ways by using various symbol templates, depending on context. This could be seen as a complication of an otherwise simple framework, but we believe that it is a more accurate description of the reasoning needed in upper-division QM coursework. Students need to be able to start from either a Dirac state vector expressed as a ket or a wave function and work their way to an expression for a probability, sometimes expressed in Dirac notation and sometimes in wave function notation. We posit that it is these shared conceptual schemata among different symbol templates that allow for students to understand how and where to make mathematical decisions to arrive at an answer—and that they may even partially explain how students reason and translate across notations. Developing this interwoven mathematical vocabulary is one challenging aspect of learning quantum mechanics.

Acknowledgements

This work is supported in part by the National Science Foundation under Grant No. PHY-1912087.

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