Student understanding of quantum mechanical expectation values in two different curricula

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As part of ongoing research to better understand how students relate Quantum Mechanics concepts to formalisms, we are studying student understanding of expectation values as well as the variety of mathematical representations they use for formalizing them in two different teaching paradigms. Analyzing students' written responses to a series of open-ended research questions has given us some insight into students' common interpretations of this concept, as well as the frequency of the various mathematical formalisms they use to represent expectation values. The results show some common patterns between students in Spin First (SF) and Position First (PF) curricular, as well as some differences.

I. INTRODUCTION

Quantum Mechanics (QM) is one of the most fascinating topics of the undergraduate physics curriculum, yet its abstract nature, complex mathematical formalisms, and less tangible concepts can hinder student sense-making ability [1-2]. Various aspects of teaching and learning QM have been studied with a growing physics education research literature on students' conceptual difficulties [3-8]. Successful sense-making and problem-solving in these courses demands a mental engagement that effectively relates QM concepts and formalisms, concurrently draws upon multiple conceptual and mathematical resources, and productively builds on classical ideas.

Despite considerable philosophical differences in interpretation of quantum measurement, measurement plays an important role in QM. While measurement in classical mechanics always has a degree of certainty and the outcome can be predicted according to the laws of classical physics, a quantum measurement is probabilistic in its nature. The formalism of QM provides probabilities for the different possible outcomes in an experiment, which allows us to calculate an *expectation value* (EV) using the weighted average of all possible observable eigenvalues.

Understanding and calculating the EV of physical observables is essential for understanding quantum measurement. Limited studies have been conducted about students' ideas about EV and some find that many students do not know the "weighted average" definition of the EV, have difficulty in interpreting the EV as an ensemble average [4] or are confused between the probability of a measurement outcome, measurement uncertainty, and the EV of position [7-9]. Previous studies are limited in scope, context, student population, and their findings. In this research study, we aim to better understand how students understand of the EV, how they relate this concept to its mathematical representations, and how often and in what ways they use different representations for formalizing them in two contexts of SF and PF curricular approaches [10]. We created a set of open-ended questionnaires to gauge students' ideas about EV and administered to three upper-division quantum classes at California State Polytechnic University Pomona (CPP) and Cal State Fullerton (CSUF). In this paper, we analyze students' written responses and discuss the frequency of different methods students present for calculating the EV of a physical observable with examples of common errors they make in their formalisms and calculation methods. We compare and contrast the frequency of the errors made by students in two different curricular.

II. EXPECTATION VALUE

The EV is a fundamental concept in all areas of quantum physics and can conceptually be thought of as a weighted average of all the possible outcomes of a large number of experimental measurements on identical systems. EV is not the expected value of any single experiment; rather, it is the expected mean value over many identical experiments. There are various formal ways to express and calculate EVs operationally; the expectation values of any function of the observable $\hat{A}$ can be expressed using Dirac notation $<\hat{A}> = <\psi|\hat{A}|\psi>$. For a discrete set of eigenvalues, this could be calculated by one of the following two methods.

1. *Summation:* sum of the products of each possible result (eigenvalues a_n) and its probability p_{a_n} :

$$<\hat{A}>=<\psi|\hat{A}|\psi> = \sum_n p_{a_n} a_n \; ;$$

2. *Matrix:* sandwiching the matrix elements of the operator between the state and its complex conjugate:

$$<\hat{A}>=<\psi|\hat{A}|\psi>= (a_1^* \, a_2^* \ldots a_n^*) \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ A_{n1} & n_{11} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

For observables with a continuous set of eigenvalues, it could be calculated by:

3. *Integral:* sandwiching the operator (e.g. position) between the state and its complex conjugate:

$$<\hat{x}> = <\psi|\hat{x}|\psi> = \int_{-\infty}^{+\infty} \psi^*(x) x \, \psi(x) dx$$

Part I- Please explain your answers to all the questions *clearly and in full sentences*.

Q1a. What does expectation-value of a physical observable (momentum, energy, position, spin, etc.) mean to you in words?

Q1b. How would you calculate the expectation-value of a physical observable?

Q1c. Are there any other ways to calculate the expectation-value of the physical observable? Please list all the different ways you know.

FIG. 1-Part I of the survey questions on EV.

Part III. Consider a spin operator $S_Z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ with two eigenvalues of $\pm\frac{\hbar}{2}$. Suppose a particle is in the following normalized spin state:

$$|\chi\rangle = \frac{1}{\sqrt{10}}\left(3|\uparrow\rangle + i|\downarrow\rangle\right) = \frac{1}{\sqrt{10}}\begin{pmatrix} 3 \\ i \end{pmatrix}$$

Q3. What is the expectation value of the Sz? Show your work.

FIG. 3- Part III of the survey questions on EV.

III. BACKGROUND & METHODOLOGY

This study is part of a larger research program focused on investigation of student learning in various quantum mechanical topics in two different curricular paradigms: Spin First (SF) vs. Position First (PF) [11,12]. The SF approach uses the sequential Stern-Gerlach experiments [13] with discrete bases of spin-half objects as a context to introduce the postulates of quantum mechanics. The PF approach starts by utilizing the Schrödinger equation and the continuous basis of position probability functions to solve problems related to the energy and position of a particle in various potentials. Our data are collected from three upper-division quantum classes at CPP and CSUF. Both are Hispanic-serving institutions primarily focused on undergraduate education with similar student demographics and populations. CPP is on a quarter system while CSUF has semester-long courses. We study and compare students' responses in SF and PF paradigms.

The survey was administered to a total of 90 students in these two institutions. The survey was first given in Winter 2017 to students in in the second quarter of a senior quantum mechanics class ($N = 30$) that was lecture-based and taught using a PF approach in both quarters (PF1). A second round of data was collected in Fall 2017 from students who were taught using a SF curriculum utilizing various interactive engagement strategies including utilizing frequent concept questions, peer-instruction methods, concept worksheets, and whiteboard group problem-solving activities. We refer to these two classes as SF2 ($N = 39$) and SF3 ($N = 21$). For PF1 and SF2 classes, the survey was part of a class quiz (worth a small amount of extra credit.) For the SF3 students, the survey was given on the last day of class as an optional survey. All three classes had different instructors.

Part II. Analyze the three statements regarding the expectation-value for a quantum system (Circle the appropriate word for each and explain. Please explain your reasoning for each (briefly but clearly!).

Q2a. The expectation value of an observable is equal to the most probable measurement outcome.

Always **Sometimes** **Never**

Q2b. The expectation value of an observable is equal to one of the possible measurement outcomes.

Always **Sometimes** **Never**

Q2c. The expectation value of an observable could be … (Circle ALL that apply):

Positive **Zero** **Negative** **Imaginary**

FIG. 2- Part II of the survey questions on EV.

Calculating the EV can be an automated process for most mathematically advanced students, yet some may not fully grasp the meaning of this quantum-mechanical concept, be able to clearly analyze its characteristics, or make sense of the mathematical processes involved its calculation. To that end, we designed a survey to investigate student ideas about this concept. First, we asked students to describe the meaning of the EV of a physical observable in their own words and list all the different ways they know to calculate it (Fig. 1). Then we asked students to analyze three statements about the EV (Fig. 2) and calculate EV of spin measurements for a spin-half system (Fig. 3).

IV. RESULTS

Below, we discuss students' responses to the EV survey in two parts. First, we focus on student sense-making of the EV concept by analyzing their written descriptions of EV (Q1a) and its characteristics discussed in Part II. Then, we discuss students' choices of mathematical expressions for EV calculation as well as common errors in the applications of those equations (Q1b, Q1c, and Q3).

A. Students' conceptual understanding of EV

The first part of the survey is intended to probe students' conceptual understanding and their knowledge about various ways to calculate EV. An ideal response entails operational definitions of EV for an ensemble of identically prepared systems with a distinction between equations used for calculating EV for operators with a discrete versus a continuous set of eigenvalues. In this study, only one of the 90 students separately discussed the calculation methods for discrete and continuous eigenvalues. In addition, only three of the 90 students made any reference to ensemble interpretation of identical quantum systems. Thus, in analyzing students' written responses to Q1a we treated any statements that referred to EV as an "average," "weighted average," or "analogous to a classical average" as a correct response.

1. Is EV the most probable measurement outcome?

A striking number (12) of students (40%) in PF1 used terms such as "*most probable outcome*" or "*probable value*" in Q1a. In comparison, a fewer number of students in SF2 (6) and SF3 (1) used the term "*most probable*" in Q1a. In Q2a of the survey, students were explicitly asked whether the EV of an observable is equal to the "*most probable measurement outcome*." Over 35% of students in PF1 choose the option "*always*" for Q2a (consistent with their responses to Q1a). Although a fewer number of students in SF classes described EV using the term "*most probable*" in their responses to Q1a, in answering Q2a about 30% chose "*always*" as their answers, suggesting that the incorrect idea that EV is always the most probable outcome is common across the two groups. Examples of incorrect explanations that accompanied the choice "*always*" for Q2a are:

"when we make the EV [measurement] there is only one outcome. That outcome is the most probable outcome."

"the EV gives us a mean average of the measured physical observable. As such, it will always give the most probable measurement outcome."

"if you calculate $\langle x \rangle = 0$, it means you would "expect" the value to be most probably be 0."

2. Is the EV a possible measurement outcome?

Q2b targets another statistical interpretation by asking students whether the EV of an observable is equal to one of the possible measurement outcomes. 60% of the students in PF1 and 62% of the students in SF3 answered this question correctly by selecting the option "*sometimes*" with correct explanations. However, 23% in PF1 and 19% in SF2 choose the option "*always,*" overlooking the fact that the EV of a measurement might not be equal to any of eigenvalues and thus may not be a possible measurement outcome [14]. Furthermore, even if the EV is an allowed (or possible) measurement outcome, it could have a zero probability of being measured.

3. Can EV be an imaginary or negative number?

Q2c asked students about the type of number (positive, zero, negative, or imaginary) they should expect for the EV of physical observables. Nearly 80% of the students in PF1 recognized that the EV cannot be an "*imaginary*" number. However, 50% stated that the EV also has to be "*positive.*" In SF3, 75% circled all the correct options (20% stated that EV cannot be negative). In SF3, 75% circled all the correct options (20% stated that EV cannot be negative).

TABLE I: Percent correct calculation methods offered in Q1b and 1c. Numbers are rounded to nearest 5%.

	1 method	2+ methods
PF1 ($N = 30$)	45%	10%
SF2 ($N = 39$)	20%	65%
SF3 ($N = 21$)	20%	50%

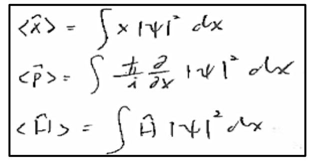

FIG. 4- Examples of students' integral setup.

B. Mathematical expressions for calculating the EV

For Q1b we considered students' responses correct if they had written down at least one correct equation for calculating the EV for either a discrete or continuous set of eigenvalues. In part Q1c we gave students credit if they expressed at least one additional method for calculating EV. A reasonable number of students were able to write down at least one correct mathematical expression for calculating EV in Q1b, (55% in Class PF1, 85%, in SF2, and 70% in SF3). Many students in PF1 made errors in the order of the integral setup.

1. Different methods & their frequency

There were some differences in the method students wrote for calculating EV among the three classes. A breakdown of percentages of students who expressed at least one or more than one method correctly is given in Table I. In PF1, approximately 45% (14) students wrote one method, from which 9 students used an integral and 5 merely wrote the bra-ket notation. Total of 8 students (25%) indicated they are aware of other methods and often used phrases such as: "do experimentally," "add probabilities," and "average measurements;" however, only 10% (3) were considered correct. In SF2, 20% (8) wrote at least one method and 65% (26) wrote more than one correct method. These numbers in SF3 were 20% (4) and 50% (10). In response to Q1b and Q1c, 5% of students in SF2 (2) and SF3 (1) presented all three EV calculation methods discussed above.

The integral method was attempted frequently among students in PF1; however, 9/20 students did not place the operator correctly between state vectors $\psi^*(x)$ and $\psi(x)$. Examples of students' responses are illustrated in Fig 4. Although the top row in Fig 4 is considered correct for calculating EV of the position operator, the same template would lead to an incorrect expression for momentum and Hamiltonian operators. The summation methods appeared much more often among the correct methods written down by students in the two classes that were taught using a SF approach (13/34 in SF2 and $11/15$ in SF3) and always in conjunction with bra-ket notation. In the two SF classes, fewer students attempted the integral method (7/39 in SF2 and $1/21$ in SF3) compared to PF1 (20/30). In contrast to

TABLE II: Attempts & accuracy of methods used in Q3. Numbers in parentheses are % correct of those attempted.

	Summation (Correct)	Matrix (Correct)	Both (Correct)
PF1	35% (90%)	65% (10%)	0%
SF2	7.5 % (65%)	90% (70%)	13% (100%)
SF3	35% (90%)	65% (55%)	10% (100%)

the errors when writing the integral method from PF1 (Fig. 4), we found no such errors in the SF classes. We also noticed that a majority of students in PF1 described EV in the context of a position $\hat{x}$ or momentum $\hat{p}$ operators, while students in SF1 and SF3 classes more often used a general operator such as $\hat{Q}$ or $\hat{A}$ in their mathematical expression.

2. Common calculation methods

To calculate a discrete EV in Q3, we see some variations among the three classes. The breakdown of the methods and the accuracy for these classes are shown in Table II. Those students in the PF1 and SF3 who used a summation method had 90% accuracy. The remaining students used a matrix method, but due to various errors related to complex-numbers the accuracy was 10% in PF1 and 55% for SF3. 90% of students' first approach in SF2 was a matrix method with 70% accuracy. Only 3 students (~7.5%) initially attempted calculating EV with the summation method in this class, with two arriving at the correct answer.

The most common errors in Q3 involved complex numbers. Interestingly, students who used a summation method and only had to square the complex coefficient, rarely made any errors, compared to those who multiplied $-i$ and $-i$ in the context of matrix multiplications (Fig. 5). This error appeared in 15% of our entire sample data.

$$\langle S_z\rangle = \langle x|S_z|x\rangle = \frac{1}{\sqrt{10}}(3\;\; -i)\,\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\frac{1}{\sqrt{10}}\begin{pmatrix}3\\ i\end{pmatrix} = \frac{1}{10}\frac{\hbar}{2}(3\;\; -i)\begin{pmatrix}3\\ -i\end{pmatrix} = \frac{1}{10}\frac{\hbar}{2}(9+1) = \boxed{\frac{\hbar}{2}}$$

FIG. 5- Common student complex number calculation error in using matrix notation in Q3.

The meaning of EV as an ensemble average of a large number of measurements on identically prepared systems is of fundamental importance to interpreting quantum measurement and is useful experimentally. Our finding that the ensemble interpretation of quantum measurement does not seem to be emphasized or recalled by many students is consistent with previous research [7]. Only 3 students in our entire sample made any mention of the ensemble interpretation of quantum mechanics.

V. DISCUSSION

Our data suggest some common ideas about EV among students regardless of the teaching paradigm. For example, about one third of students at some point of the survey referred to EV as the "*most probable value.*" The EV is not generally the "*most probable*" value of a measurement and indeed, the expectation value may have zero probability of occurring. Overall, about 20% of all students incorrectly stated the EV of an observable is "*always*" equal to one of the possible measurement outcomes. It is possible that these students might generally think the average value is supposed to be at least one of the measurement outcomes in any statistical distributions (quantum and classical). Lastly, about one fourth of students thought the EV cannot be a negative number, perhaps due to the repeated emphasize on the positive nature of probability that primed some students to incorrectly associate this characteristic with EV.

Apart from errors in representing the order of states and operators, most students were able to write down at least one method of calculation for calculating EV of a physical observable. However, students in the SF classes more frequently offered more than one method (65% and 50% compared to 10% in PF1) and some used more than one method to calculate the EV in for the spin-half system to check the accuracy of their first method.

Students in PF1 often made errors writing the correct order of the operator and state vectors for the integral method. Most interestingly, no instances of such errors were present in the work of SF students. Lastly, students in SF classes often wrote the bra-ket notation in conjunction with other methods and offered a summation more often than an integral as a general method. These preliminary results show some differences in students' responses to the EV questionnaires. These variances could be due to differences in instructional emphasis in these courses. We plan to further investigate which results can be attributed to the curricular content and which can be attributed to (e.g.) different emphases around conceptual understanding and problem solving.

ACKNOWLEDGEMENTS

We thank all our respective PER groups, students, and colleagues for their invaluable help and support, particularly Benjamin Schermerhorn. This work was funded by NSF DUE-1626482, 1626280, and 1626594.

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