Investigating and improving student understanding of time dependence of expectation values in quantum mechanics using an interactive tutorial on Larmor precession

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We studied the challenges students face with time dependence in quantum mechanics, specifically in the context of Larmor precession of spin. This research informed the creation and evaluation of a learning tutorial aimed at helping students grasp these concepts using a two-state system. The tutorial utilizes visualization tools to enhance students' intuition and emphasizes the integration of qualitative and quantitative understanding. We also examine how students applied semi-classical or quantum mechanical reasoning in their answers and assess the improvement they showed after working with the tutorial.

I. INTRODUCTION

Quantum mechanics (QM) is a challenging subject even for upper-level undergraduate and graduate students and issues related to the time dependence of the quantum state vector has been found to be particularly challenging [1–5]. Singh and Marshman reviewed prior research on these difficulties emphasizing persistent challenges in learning foundational QM concepts [6]. The pedagogical methods include teaching QM via student engagement with laboratory experiments [7, 8], hands-on activities [9], tutorials [10, 11], visualization tools [13–17], and other interactive curricula [12]. Here we discuss the use of an interactive tutorial that incorporates scaffolding questions and visualization tools to help students learn about the time dependence of expectation values [18–20]. This work builds on the findings in Ref. [18], which were with graduate students answering multiple-choice questions, and includes revised questions in the open-ended format that ask students to explain their reasoning for each question. We expand upon Ref. [19] with a larger number of students and elaborate on students' quantum mechanical and classical reasoning while discussing the development and evaluation of a tutorial employing Larmor precession of spin as the physical system. The tutorial employs a guided learning approach to help upper-level undergraduate students learn about time dependence of expectation values using a two-state system. The supplementary materials provide the entire tutorial in packaged and unpackaged form and include instruction on how simulations can also be adapted from sources other than the source used in the tutorial.

Generally, the expectation value of some physical observable Q depends on time because the state of the system $|\psi(t)\rangle$ evolves in time (in the Schrödinger formalism). The expectation value of an observable Q in a given quantum state at time t can be written as $\langle Q(t)\rangle \equiv \langle\psi(t)|\hat{Q}|\psi(t)\rangle$. If the Hermitian operator $\hat{Q}$ corresponding to observable Q has no explicit time dependence (as is assumed throughout this work), Ehrenfest's theorem yields:

$$\frac{d}{dt}\langle Q(t)\rangle = -i\frac{\langle\psi(t)|[\hat{Q},\hat{H}]|\psi(t)\rangle}{\hbar}, \tag{1}$$

where $\hat{H}$ is the Hamiltonian operator for the system, and all other symbols have their usual meaning. Therefore, determining whether an expectation value is time-dependent is equivalent to examining if the right-hand side of Eqn. 1 equals zero. There are two distinct general conditions when the expectation value of a physical observable is time independent. One case is when the commutator $[\hat{Q}, \hat{H}]$ is zero. In this case, Q is a constant of the motion (corresponds to a conserved quantity). The other case is when the state vector $|\psi(t)\rangle$ is a stationary state, that is, an eigenstate of the Hamiltonian operator. All physical observables (that do not depend explicitly on time) have time independent expectation values in this case, as is seen in Eqn. 1.

The physical system used in the tutorial to help students with the time dependence of expectation values is Larmor precession of a spin-$1/2$ system. Working on the tutorial, students learn that a particle with a magnetic moment may exhibit Larmor precession if an external magnetic field is applied. In this case, spin operators in a given basis are 2×2 matrices, which are least likely to cause cognitive overload to students while learning about this challenging topic.

II. STUDENT DIFFICULTIES

Students at a large state research university in the US took part in the investigation (including written tests and interviews) following traditional lecture-based instruction on the topic in either an upper-level undergraduate or a graduate-level quantum mechanics course. After traditional lectures, these students answered questions that focused on the time dependence of expectation values related to Larmor precession. Previous study [18] used multiple-choice questions to probe graduate students' difficulties. In this study, we gave open-ended written tests in undergraduate classes to students and individually interviewed both undergraduate and graduate students with free-response questions that required students to explain their reasoning. We also raised follow-up questions if students' explanations were unclear and needed clarification. Fifteen upper-level undergraduate and graduate students from quantum mechanics courses were individually interviewed using semi-structured, think-aloud interviews to unravel the underlying cognitive mechanisms behind common difficulties. They were also asked to solve similar problems to those that were administered in written tests. Once the students completed the questions, they were prompted to clarify any points they had not fully explained earlier. The interviewers also had a list of related issues they wanted students to address. These issues were initially withheld to give students the opportunities to express their thought processes and develop their own responses. However, interviewers asked these questions to students if they had not already been answered in the course of solving the problems. Additional probing questions were created on-the-spot by the interviewer to gain deeper insight into each student's reasoning and thought process. As both undergraduate and graduate students showed similar difficulties, we will not further distinguish between the two groups. Below, we provide a summary of the difficulties which were consistent with those discussed in Refs. [18, 19] before discussing the tutorial and student performance on the pre-test and post-test and matched final exam questions using both quantum mechanical and classical reasonings:

(a) Difficulty recognizing the special properties of the energy eigenstates: When the magnetic field is aligned along the z-axis,, all expectation values are time independent if the initial state is an eigenstate of $\hat{S}_z$ because it is a stationary state. However, students frequently made the incorrect claim that $\langle S_x \rangle$ and $\langle S_y \rangle$ depend on time in this case even when the initial state is an eigenstate of $\hat{S}_z$. They reasoned that "since the system is not in an eigenstate of $\hat{S}_x$, the expectation value of S_x must be time dependent" or "since $\hat{S}_x$ does not commute with $\hat{H}$, its expectation value must be time-dependent," despite the system being in an energy eigenstate.

(b) Difficulty undestanding the importance of the commutation relation between $\hat{Q}$ and $\hat{H}$: Students often had difficulty with the consequence of the Ehrenfest's Theorem: if an operator $\hat{Q}$ commutes with the Hamiltonian, the time derivative of $\langle Q \rangle$ is zero, regardless of the quantum state.

(c) Difficulty understanding the difference between energy eigenstates and eigenstates of operators corresponding to observables other than energy: Any Hermitian operator has a corresponding set of eigenstates, but only the eigenstates of the Hamiltonian operator are stationary states. However, many students struggled to distinguish between these related concepts. For instance, in the case of Larmor precession with the magnetic field in the z direction, students often incorrectly assumed that if a system is initially in an eigenstate of $\hat{S}_x$ or $\hat{S}_y$, it will remain in that eigenstate. In interviews, students had difficulty differentiating between energy eigenstates and eigenstates of operators corresponding to other observables. Some students explicitly questioned how eigenstates of other observables could be different when they were eigenstates after all. A related common difficulty is exemplified by the following comment from a student: "if a system is initially in an eigenstate of $\hat{S}_x$, then only the expectation value of S_x will not depend on time."

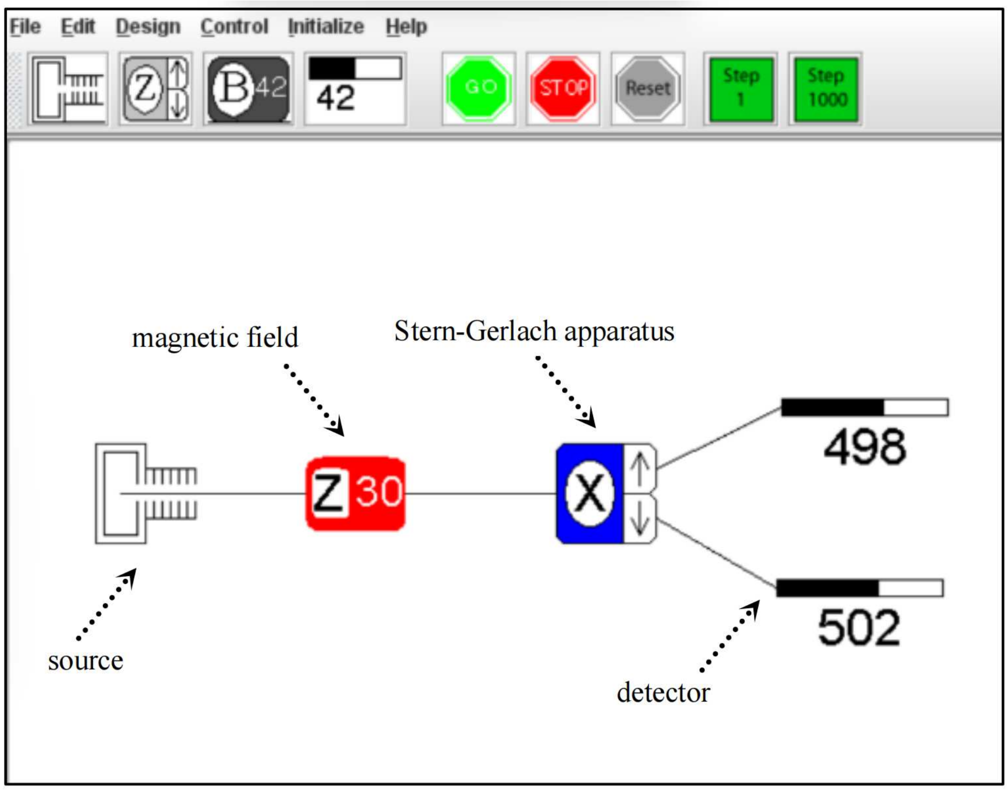
III. DESCRIPTION OF THE TUTORIAL

The details of the development of the tutorial and the corresponding pre-/post-tests can be found in the supplementary materials, along with the final form of the tutorial and the details about how to use the pre-packaged and unpackaged versions with simulations. In the tutorial, the spin-1/2 particle is in a uniform magnetic field in the z direction but prepared in three different initial states: (1) an eigenstate of $\hat{S}_z$, (2) a generic state $a\left|\uparrow\right\rangle_z + b\left|\downarrow\right\rangle_z$ and (3) an eigenstate of $\hat{S}_x$, e.g., $\left|\uparrow\right\rangle_x$. These three initial states serve to address difficulties (a), (b), and (c), respectively, and also to help students learn about the special properties of stationary states. In each case, the tutorial worksheet asks students to write the state after a certain time t and predict the probabilities of measuring different components of spin as well as their expectation values for each case. Then students check their predictions with outcomes of hypothetical experiments using computer simulations [15].

The tutorial adapts computer simulations developed by Christian and Belloni [15]. Students make predictions about whether probabilities of outcomes and expectation values of measurements depend on time in various situations and then use the simulations of Larmor precession to learn whether their predictions are correct. For each simulation in the tutorial, all particles leaving the oven are in a specific pure state. The screenshot of a particular situation students engage with is shown in Figure 1. Further details of the simulations can be found in the supplementary materials. For computer platforms that make it challenging to use the pre-packaged simulations relevant for the tutorial, the tutorial worksheet can be used with the Quvis spin-precession simulations [14].

After students have made each set of predictions and checked them via simulations, the tutorial provides guidance to help them reconcile any discrepancy between their prediction and observation. The tutorial uses questions after each simulation to address the difficulties we identified. Students are provided Ehrenfest's theorem and asked for its implications regarding the time dependence of expectation values in a stationary state (difficulty (a)). They are asked what happens if the operator corresponding to an observable commutes with the Hamiltonian in a generic state (difficulty (b)) or if the system is in an eigenstate of an operator that does not commute with the Hamiltonian (difficulty (c)). There are also activities in which students are presented with hypothetical student discussions and are asked to explain why they agree or disagree with each person. Additional questions focus on how the expectation value of $\vec{S}$ will precess about the z-axis in cases in which the initial state is not a stationary state. Such method of guiding students to reconcile inconsistencies between prediction and observation has been proven to be effective in improving students' understanding of quantum mechanical concepts [10, 21].

FIG. 1. Screen shot of a simulation used in the tutorial showing one possible outcome after 1000 particles have been emitted. The red block is the strong uniform magnetic field that may cause Larmor precession. The number "30" in the red block means that the particle stays in the magnetic field for time t_0 satisfying $-\gamma B_0 t_0/2 = \pi/6 = 30°$. The blue block is the Stern-Gerlach apparatus that is used to detect the spin state of the system.



IV. EVALUATING THE EFFECTIVENESS OF TUTORIAL

Once we determined that the tutorial was effective if administered to students individually, then we tested it in four 3rd-4th year undergraduate quantum mechanics courses totaling 95 students over a several year period, involving two different instructors who used books by Griffiths [22] and Liboff [23]. Students completed the pre-test after

TABLE I. Average scores (with standard error) on the pre-test, post-test, and final exam. One class with 18 students was given four matched questions (items 1,2,3,5) on their final exam. Their performance on these four matched questions are listed separately as "matched pre-/post-test".

	Students	Strict	Partial
Pre-Test	95	41 ± 3 %	46 ± 3 %
Post-test	95	72 ± 3 %	75 ± 3 %
Matched Pre-Test	18	32 ± 9%	42 ± 8%
Matched Post-test	18	78 ± 7%	82 ± 6%
Matched Final Exam	18	83 ± 6%	86 ± 5%

traditional instruction, and then worked through the tutorial in small groups in one class period with the guidance of the instructor. Students could usually finish about half of the tutorial in a 50-minute class period and they were asked to complete the rest as homework. Then, the post-test, which had analogous questions to the pre-test (except that S_x and S_y are swapped in various questions) was administered in the subsequent class. Additionally, one class of 18 students (part of the total 95 students) received four matching questions on their final exam (which are the same as four of the questions on the pre-test/post-test) on time dependence of expectation values to assess retention of these concepts over two months later. The pre/post tests, which can be found in the Appendix, have six questions. Item 5 probes difficulty (a) and item 3 probes difficulty (b). Items 1, 2, 4, and 6 mainly probe difficulty (c) but we note that difficulties (a) and (b) are also reflected in these items.

A. Reasoning-based Rubric

To evaluate student learning, both the pre-test and post-test were scored based on two rubrics collaboratively developed by the researchers. The "strict" rubric only gives credit if the student provides a completely correct answer, in which the correct answer is given and also supported with correct reasoning. The correct reasoning can be either quantum mechanical or semi-classical (called classical from now on). High scores on this strict rubric likely indicate expert-like performance. The "partial" rubric award half credit for a correct answer regardless of the reasoning and half credit for correct quantum mechanical or classical reasoning. More than 20% of the sample was scored by two raters independently for inter-rater agreement. The two raters' scores for each student were compared and the average differences between the raters were less than 10%. To evaluate retention of the concepts related to the time dependence of expectation values, the same rubrics were used to score the matched questions on the final exam that was given approximately two months later.

B. Performance on Pre-test, Post-test and Final Exam

The average scores on the pre-test, post-test, and final exam are shared in Table 1. We note that not only did students perform much better on the post-test than on the pre-test, but the performance rose further on the final exam, which is encouraging. This improvement on the final exam could have been because students prepared carefully for the exam or due to the known positive effect of repeated testing on learning, but, either way, it shows that students' memories did not degrade. The supplementary material includes further statistics, including the statistical data for each item, t-test, p-value, and effect size results.

C. Determination of Quantum vs. Classical Reasoning

Most questions posed in the pre-/post-tests about the time dependence of expectation values can be answered using either a quantum mechanical or a classical explanation. This situation presents an opportunity to explore and compare how often students adopt and accurately apply the "quantum" framework they've learned versus primarily using "classical" reasoning. Explanations classified as quantum reasoning include statements about operators, their commutation relations, states and their time evolution via the time-dependent Schrödinger equation. Statements based on whether a system will exhibit precession were categorized as classical reasoning. Both were considered to be correct in this investigation, although our conversations with colleagues revealed that they value quantum reasoning more highly in these problems. For item 6, we did not make a distinction between quantum and classical reasoning since precession was explicitly mentioned. Below, we list some answers showing typical quantum, mixed and classical reasoning:

Quantum: Yes, as by [Ehrenfest's] theorem. Since $\hat{S_x}$ does not commute with $\hat{H}$ and since [it] is not a stationary state, the derivative of the expectation value of S_x with respect to time is not zero.

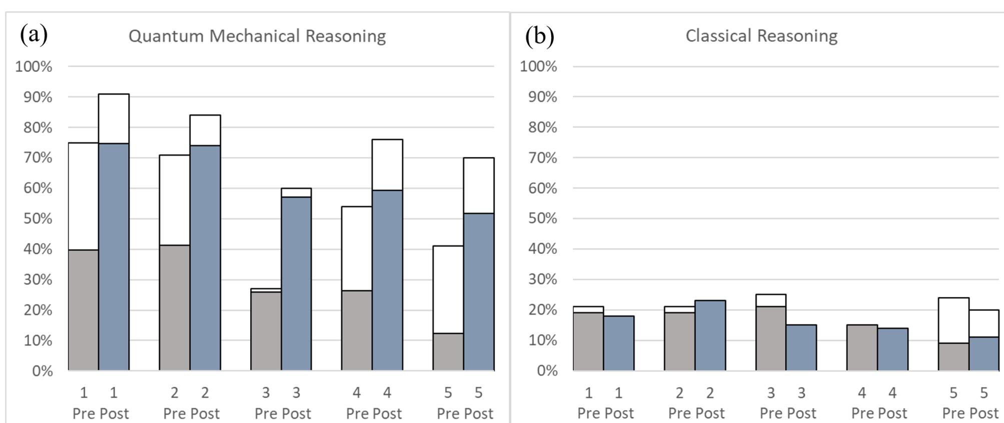
Mixed: No, since there is no longer precession about the z-axis. Eigenstates of $\hat{S_z}$ are stationary states.

Classical: (when asked if $\langle S_z \rangle$ depends on time) Yes, because the magnetic field causes an angular frequency ω and precession about z axis.

D. Grading Student Responses using Quantum and Classical Reasoning

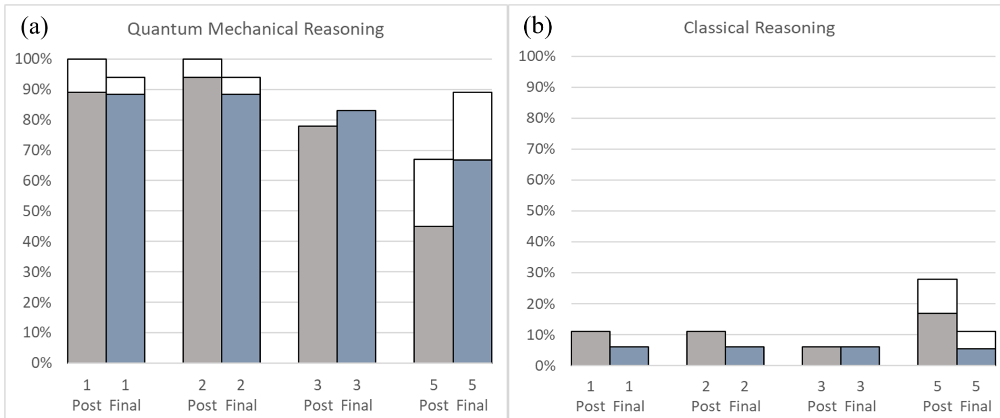
Figure 2 shows the percentage of total 95 students who used quantum mechanical reasoning and classical reasoning in the pre-test and post-test to answer items 1-5. As noted, for item 6, we did not make a distinction between quantum and classical reasoning. In Figure 2(a), the height of the bar represents the percentage of 95 students who used quantum reasoning to answer the item and the shaded region represents the subset who used quantum reasoning correctly. Figure 2(a) also shows that students used quantum mechanical reasoning much more frequently on the post-test relative to the pre-test. The correctness percentage also increased typically from pre-test to post-test. In contrast, Figure 2(b) shows that students used classical reasoning with comparable frequency in the pre-test and post-test. Typically less than one fourth of the total students used classical reasoning in either pre-test or post-test. Students who used classical reasoning had better performance than those who used quantum mechanical reasoning, especially in the pretest. Such a difference may be related to students' transfer of knowledge between classical mechanics and quantum mechanics. The percentage of quantum mechanical and classical reasoning for a particular question in a given test (e.g., pre-test) does not add up to 100% because some students used neither quantum mechanical nor classical reasoning and some students used both types of reasoning.

FIG. 2. The percentage of total students (N=95) who used quantum mechanical reasoning or classical reasoning in the pre-test and post-test to answer items 1-5. The height of the bar represents the percentage of 95 students who used quantum mechanical or classical reasoning to answer the item and the shaded region represents the subset who reasoned correctly.



For the items 1,2,3,and 5 administered in the final exam, Figure 3 presents the comparison of reasonings using either correct quantum mechanical reasoning and classical reasoning, respectively. The quantum mechanical reasoning is retained by a majority of students from post-test to the final exam. Students may consolidate their knowledge throughout the learning process, leading to improvements on certain items. Only one student changed from quantum reasoning to classical reasoning in the final exam. Also, very few students used classical reasoning to answer questions in both the post-test and final exam. These results suggest that students gain more expertise in quantum mechanical reasoning in this context by the end of the course.

FIG. 3. The percentage of students (N=18) who used quantum mechanical reasoning or classical reasoning in the post-test and final exam to answer items 1,2,3,and 5. The height of the bar represents the percentage of students who used quantum mechanical or classical reasoning to answer the item and the shaded region represents the subset who used reasoned correctly.



V. SUMMARY AND INSTRUCTIONAL IMPLICATIONS

Students have many difficulties with the time dependence of expectation values in quantum mechanics. The Larmor precession tutorial focuses on helping students learn about the time dependence of expectation values using a simple two state model. The pre-test and post-test data collected over several years show that student performance improved after working on the tutorial. Also, data on matched questions (same as pre-/posttest questions) administered to a subset of students on the final exam show that these gains are, on average, retained. These gains could likely be enhanced further, for instance, by having students submit the tutorials for grading, as the incentive of a grade may boost their engagement with the material.

The tutorial can be used by the instructors in many ways. Students can work on it in small groups and the instructor can move around to make sure that students engage productively. There can also be full class discussion after students have engaged with a set of questions addressing a certain difficulty. Instructors can also use some of these questions, both open-ended questions and hypothetical conversations, as think-pair-share questions in which students think individually about answers, then discuss in pairs, and finally share with the entire class. The multiple-choice questions can also be used as clicker questions. If class time is limited, the tutorial can be assigned as homework.

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Appendix A: The Pre- and Post test

Here we present version A of the pre-test and post-test. Version B is identical, except that all instances of $\hat{S}_x$ and $\hat{S}_y$ have been swapped. Students completed one version as a pre-test and the other as a post-test. We observed no statistically significant difference between performance on the two versions.

All questions below refer to the following physical system:
An electron is in an external magnetic field B which is pointing in the z direction. The Hamiltonian for the electron

spin is given by $\hat{H} = -\gamma B\hat{S}_z$ where γ is the gyromagnetic ratio and $\hat{S}_z$ is the z component of the spin angular momentum operator. *Notation:* $\hat{S}_z\left|\uparrow\right\rangle_z = \frac{\hbar}{2}\left|\uparrow\right\rangle_z$, and $\hat{S}_z\left|\downarrow\right\rangle_z = -\frac{\hbar}{2}\left|\downarrow\right\rangle_z$. *For reference, the eigenstates of $\hat{S}_x$ and $\hat{S}_y$ are given by:*
$\left|\uparrow\right\rangle_x = \frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle_z + \left|\downarrow\right\rangle_z)$, $\left|\downarrow\right\rangle_x = \frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle_z - \left|\downarrow\right\rangle_z)$
$\left|\uparrow\right\rangle_y = \frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle_z + i\left|\downarrow\right\rangle_z)$, $\left|\downarrow\right\rangle_y = \frac{1}{\sqrt{2}}(\left|\uparrow\right\rangle_z - i\left|\downarrow\right\rangle_z)$

1. If the electron is initially in an eigenstate of $\hat{S}_x$, does the expectation value of S_x depend on time? Justify your answer.

2. If the electron is initially in an eigenstate of $\hat{S}_x$, does the expectation value of S_y depend on time? Justify your answer.

3. If the electron is initially in an eigenstate of $\hat{S}_x$, does the expectation value of S_z depend on time? Justify your answer.

4. Consider the following statements from Student 1 and Student 2 when the electron is initially in an eigenstate of $\hat{S}_x$ (the x component of the spin angular momentum):
   Student 1: The electron will NOT be in an eigenstate of $\hat{S}_x$ forever because the state will evolve in time.
   Student 2: I disagree. If a system is in an eigenstate of an operator corresponding to a physical observable, it stays in that state forever unless a perturbation is applied.
   With whom do you agree? Explain.

   (a) Student 1

   (b) Student 2

5. If the electron is initially in an eigenstate of $\hat{S}_z$, does the expectation value of S_x depend on time? Justify your answer.

6. If the electron is initially in an eigenstate of $\hat{S}_x$, is there any precession of $\langle\vec{S}\rangle$ about the z axis? If your answer is yes, explain why and give an example of a situation where there will be no precession of $\langle\vec{S}\rangle$ about the z axis. If your answer is that there is no precession for the given case, explain why.

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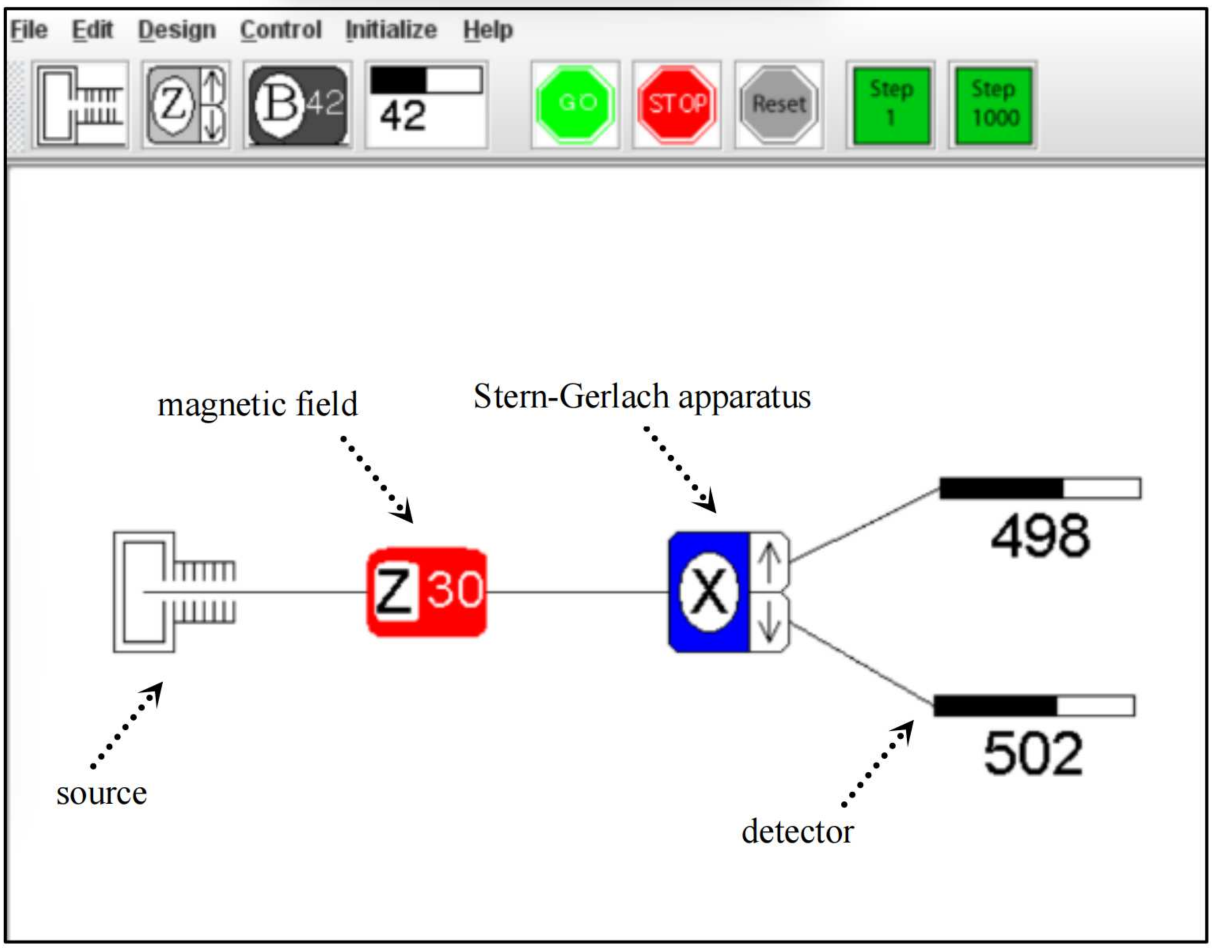
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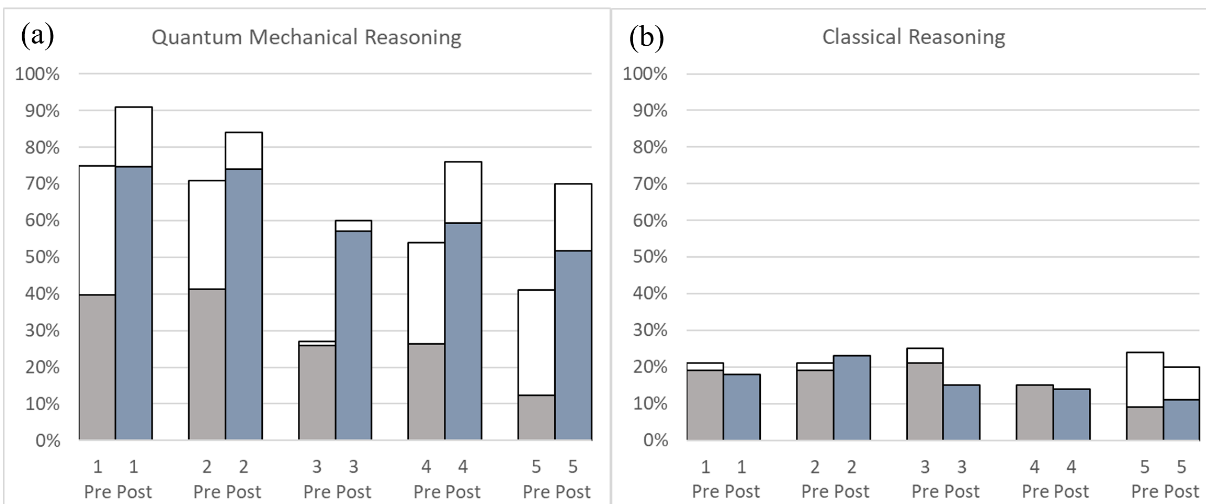
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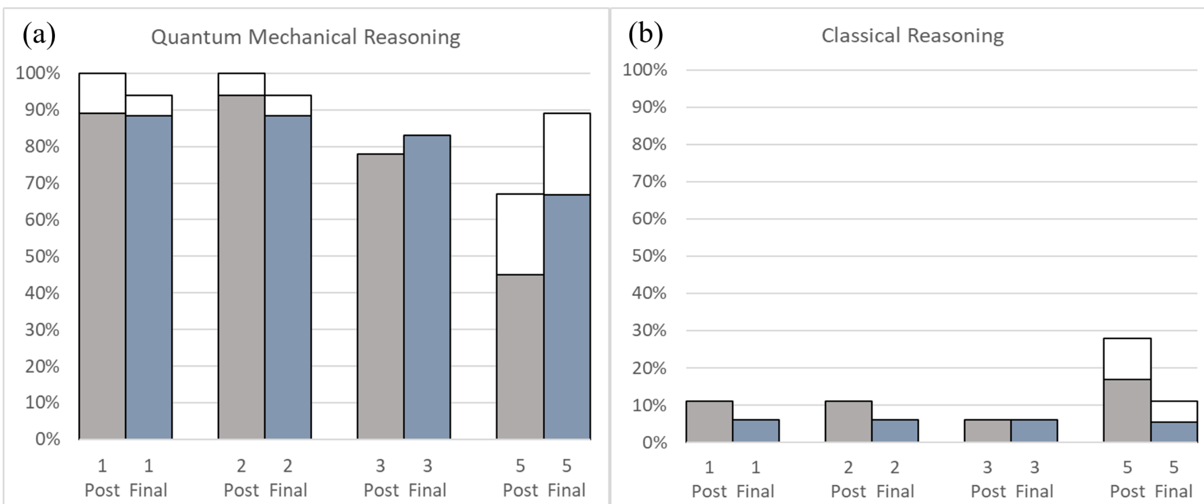
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