Time evolution in quantum systems: a closer look at student understanding

Gina Passante, Benjamin P Schermerhorn, Steven J Pollock and Homeyra R Sadaghiani

Abstract
Time evolution of quantum systems has been shown to be one of the most difficult components of a typical undergraduate quantum mechanics course. In this work, we examine the current literature, and then take a closer look at the process that students use to determine how the quantum state of a spin-1/2 particle evolves with time. We divide the process of writing a time-dependent state into five elements and use these to both directly probe student understanding and guide our coding of student responses. We focus on three elements of this process, including knowledge of the Hamiltonian, the energy eigenstates and eigenvalues, and what basis should be used when writing the state as a function of time using the phase $e^{-iEt/\hbar}$. Analysis of four exam questions given at three institutions suggests that knowledge of the energy eigenbasis and its importance for time evolution may be a weak point in student understanding.

Supplementary material for this article is available online

Keywords: quantum mechanics, time evolution, physics education research, Hamiltonian, wave function
1. Introduction

The physics education research community has made strides in better understanding student thinking as they learn quantum mechanics, leading to curricula to improve student conceptual understanding [1–11]. Research has commonly shown that time evolution has proven to be a particularly difficult concept in undergraduate quantum mechanics [12–15], and yet it is necessary in order to understand the dynamics of quantum systems. For example, time evolution is of critical importance for explaining neutrino oscillations and interpreting the results of nuclear magnetic resonance experiments.

The time evolution of a quantum system can be determined from the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}|\psi(t)\rangle,$$

where $\hat{H}$ is the Hamiltonian operator. In situations with a time-independent Hamiltonian (which is all we consider in this study), it is possible to find a general solution for any starting state using the Schrödinger equation. The general solution is given as

$$|\psi(t)\rangle = \sum_n c_n |\phi_n\rangle e^{-iE_n t/\hbar},$$

(1)

where $c_n = \langle \phi_n | \psi(t = 0) \rangle$ are the probability amplitudes and $|\phi_n\rangle$ are the energy eigenstates with corresponding energy eigenvalues $E_n$. The energy eigenstates and eigenvalues can be found using the energy eigenvalue equation, also known as the time-independent Schrödinger equation.

Research-based quantum mechanics conceptual surveys have found that time dependence questions are exceptionally difficult for many students: the QM Visualization Instrument questions relating to time evolution had averages of approximately 25%, which is much lower than the test average [12]; on the QM Survey, 25% of students recognize that a general state is not a solution to the time independent Schrödinger equation [13]; and on the QM Concept Assessment (QMCA), questions relating to time evolution have some of the smallest success rates of approximately 35% [14]; the QM Assessment Tool (the open-ended precursor to the QMCA) had an average of approximately 40% on the time evolution questions, almost 20% lower than any other subset of questions, categorized as measurement, time-independent Schrödinger equation, wave functions and boundary conditions, and probability and probability densities [15].

In a study of incoming graduate students, Singh found that many students had difficulty with questions relating to time evolution of quantum systems. For example, when asked what was the most fundamental equation in quantum mechanics, Singh expected students to respond with the time-dependent Schrödinger equation, but found that instead, almost half of the students cited the time-independent Schrödinger equation as the most fundamental [16]. The same study found that 31% of students wrote a single phase for the time evolution (instead of a phase for each energy eigenstate as in equation (1)) and 9% believed a state provided at $t = 0$ should have no time dependence [16]. Emigh et al also reported that many students wrote a single phase for the entire wave function, and given any initial state and a time-independent Hamiltonian, they believed that there would be no time evolution [17]. On a multiple choice question asking what it means for a particle to be in a stationary state and/or energy eigenstate, no students (out of 10 surveyed) answered correctly [2]. The same work also found that after a measurement has been made, students have difficulty with the time-development of the system. For example, researchers have noted that some students believe
that after a measurement, the state returns to its pre-measurement state, or relaxes to the ground state [17, 18].

Interpreting the mathematics of time evolution requires working with a complex exponential, which, is known to be very difficult for upper-division physics students [19]. There is also evidence that some students confuse the time evolution of different quantities [17, 20]; believe that all superposition states have distinct phases (even if degenerate) [17]; misinterpret the mathematics (for example, interpreting the time-dependent phase as an exponential decay instead of a sinusoidal function) [17, 20, 21]. See Singh’s overview of student difficulties in quantum mechanics, including a section on time dependence [20].

There have been several research-based curricular activities designed to address student difficulties with the time evolution of quantum systems. For example, a Quantum Interactive Learning Tutorial (QuILT) on time development of wave functions was built on the research that shows students think there is one overall phase factor [1, 22]. Another example is a combined simulation-tutorial that was designed to improve student understanding of time evolution by focusing on a visual representation of the time evolution of the wave function. After the activity, performance on an exam question asking students if a probability density evolves with time revealed that students using visual reasoning were more likely get the question correct [21].

In almost all of the studies referenced above, the focus has been on whether or not students can correctly determine, identify, or draw conclusions regarding the time evolution of a quantum state. Very little work has been aimed at finding the root of this difficulty. Two studies that focus on the Hamiltonian shed some light on the situation. The first looked at time dependent perturbation theory and asked students if a particle that is initially in an energy eigenstate will have a probability density that depends on time as a perturbation is introduced to the system and then removed. They found that less than 25% of students were able to answer correctly, and identified a potential weak point in student understanding as the link between the Hamiltonian and the energy eigenvalues and eigenstates [23]. The second study investigated the resources students use when answering questions related to energy measurements. It was found that in response to spins-context questions asking for the probability of different energy measurements, the Hamiltonian was referenced by four times as many students as it was in response to a similar question asking about the probability of energy measurements in the wave function context [24].

The Hamiltonian is of central importance when discussing time evolution of quantum systems, and the link between the Hamiltonian, the energy eigenvalues, and energy eigenstates are crucial to being able to write a quantum state as a function of time. In this study, we aim to better understand why time evolution continues to be a difficult concept for students. For this purpose, we consider the process of writing a quantum state in a time-independent Hamiltonian as a function of time by isolating individual elements of this process. Before attempting to write the time-dependent state, you must have information about the physical system (which provides the Hamiltonian) and the state at an initial time (written in any basis). We note that these elements are not necessarily the process by which a novice or an expert might approach the problem of writing a state as a function of time, but they are one possible path to do so. These elements are as follows:

(i) Identify the Hamiltonian.
(ii) Determine (or solve for) the energy eigenvalues ($E_n$) and eigenstates.
(iii) Recognize that the state (at $t = 0$) should be written in the energy eigenbasis.
(iv) Write the state (at $t = 0$) in the energy eigenbasis (often requiring a change of basis).
(v) Multiply each energy eigenstate term in the superposition by $e^{-iE_n t/\hbar}$.
These elements guide our analysis and allow us to directly probe individual components of students’ work. In this study, we focus our attention on the first three elements to provide a finer grained examination of the initial stages of student problem solving.

This study looks at student responses to questions in the context of a spin-$1/2$ particle in the presence of a magnetic field. This decision was made in part because all data were collected in ‘spins-first’ QM courses where time evolution is taught first in the context of spin. Our research question is: in the context of spin-$1/2$ particles, what elements in the process of solving for the time-dependent quantum state cause the most difficulty for students?

The rest of the paper is organized as follows. The methods are described in detail in section 2. The data analysis is found organized by question in section 3 with a discussion of trends in section 4. Finally, we conclude with implications for instruction in section 5.

2. Methods

We analyze several years worth of exam data at multiple institutions that asks students to perform various subsets of the elements aforementioned with different levels of scaffolding. For example, two exam questions (Q1 and Q2 in figure 1) were scaffolded in that they explicitly asked students to write the Hamiltonian, determine the energy eigenstates and energy eigenvalues, and then solve for the time-dependent state or the probability of measuring a particular spin value at a later time, which requires writing the full time-dependent state as part of their calculation. The other two questions (Q3 and Q4 in figure 1) only asked for students to write the quantum state at a later time. These elements guide our analysis and allow us to directly probe individual components of students’ work. In this study, we focus our attention on the first three elements to provide a finer grained examination of the initial stages of student problem solving.

Figure 1. Exam questions that were analyzed for the different elements of determining a time dependent quantum state. These questions were each given on different assessments. Questions 1 and 2 are scaffolded such that students are required to think about the relevant Hamiltonian and the energy eigenstates before being asked to write (or use) the quantum state as a function of time. We label these as ‘structured’ questions. Questions 3 and 4 do not provide the scaffolded structure, and instead ask directly for the state as a function of time. These are labeled ‘unstructured’ in the text. If a ket does not have a subscript indicating the basis, it is assumed to be in the $z$ basis.
Data were collected from three institutions in the USA, each using a Spins-first approach to quantum mechanics. Institution A is a selective, research-intensive, PhD granting institution, while institutions B and C are Hispanic-serving, primarily undergraduate institutions. The courses, taught by the authors follow the textbook Quantum Mechanics by David McIntyre\cite{25} and use a variety of interactive methods. A summary of which questions were administered at each institution is provided in table 1.

Each lettered part of the structured exam questions were coded independently. The first part of questions 1 and 2 were identical asnd coded for which spin operator the students wrote the Hamiltonian in terms of. Part b on Q2 asked students to specifically list the eigenstates and eigenvalues, whereas part b on Q1 asked if the given state was an eigenstate of the Hamiltonian and asked for an explanation. Both questions were coded for the basis they indicated was the energy eigenbasis. Part c on Q1 asked for the state at some later time, while Q2 specifically asked for the calculation of a probability at a later time. Part c was coded only for the basis in which they wrote the time evolved state, not for correctness of the exponential terms or the probability. We further analyzed for consistency across the three parts of these questions. Both unstructured questions (Q3 and Q4) only asked for students to write the time-evolved state. This question was coded specifically for whether or not students wrote the state in the correct basis. Coding was performed by the first two authors. Due to the objective nature of the codes, each response was coded by only one person.

Almost identical versions of Question 3 were given in two different years at the same institution with the same instructor. The only modification to the question was the initial state, in which the coefficient in front of the $|+\rangle_z$ was changed from 1 to 2 in one administration. There is no evidence that this change affected student responses, and therefore the results of the two administrations are aggregated here.

### 3. Results: analysis of student responses

In this section we summarize student responses to each of the questions individually, before discussing broader themes in section 4. When discussing different bases, we use the language of $x$-basis to refer to the eigenstates of the $S_x$ operator.

#### 3.1. Responses to Q1

Question 1 is a structured question that provides students with an initial state that is an eigenstate of $S_z$ (in the state $|+\rangle_z$), in a magnetic field oriented in the $+y$ direction. Table 2 summarizes the percentage of correct responses to each part of the question. On the first part

| Question label | School | Number of students | Given state at $t = 0$ | Direction of magnetic field |
|----------------|--------|--------------------|------------------------|-----------------------------|
| Q1             | A      | $N = 67$           | $|+\rangle_z$          | $+y$                        |
| Q2             | B      | $N = 14$           | $|+\rangle_z$          | $+x$                        |
| Q3             | C      | $N = 50$           | $N(1|+\rangle_z - 3|-\rangle_z)$ | $+y$                        |
| Q4             | A      | $N = 57$           | $|+\rangle_y$          | $-z$                        |

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of the question, 85% (57/67) of students correctly identified the Hamiltonian as being proportional to $S_y$. Ten percent (7/67) of the students wrote that the Hamiltonian was proportional to $S_z$ instead.

The second part of the question asked students if the state was in an energy eigenstate at $t = 0$. Since the initial state is an eigenstate of $S_z$ and the Hamiltonian is proportional to $S_y$, the state is not an energy eigenstate. This question was answered correctly by 49% (33/67) of the students. An equal number of students (33/67) incorrectly stated that the state was an eigenstate of energy. Given that almost all students had correctly identified the Hamiltonian in the previous part, responses to this question suggest students are not necessarily connecting the Hamiltonian with the determination of energy eigenstates.

On the third part of the question, students were asked to write the state of the particle at a later time. On this question, 54% (36/67) of the students wrote the state in the $y$ basis (the correct basis for this question). When looking at all three parts of the question together, we find that 34% (23/67) of students identified the correct spin operator for the Hamiltonian, determined the energy eigenbasis, and wrote the state in the energy eigenbasis when writing it as a function of time.

In looking at responses to all questions, we find several types of inconsistent answers. There were 12% (8/67) students who correctly stated that the Hamiltonian was proportional to $S_z$, incorrectly identified $|+\rangle_z$ as an energy eigenstate, and then correctly wrote the time-dependent state in terms of the $y$ basis. A different type of inconsistent answers was provided by 15% (10/67) students: they correctly stated that the Hamiltonian was proportional to $S_y$, correctly indicated that $|+\rangle_z$ is not an energy eigenstate, but then used the $z$-basis to write the time-dependent state in part c.

### 3.2. Responses to Q2

Question 2 (shown in figure 1) was also structured and directly asked students to write the Hamiltonian. As in question 1, the initial state in Q2 was written in the $z$ basis, however the magnetic field was aligned along the $x$-direction. On this assessment, 64% (9/14) of students were able to identify that the Hamiltonian is proportional to the $S_x$ operator. One student wrote the Hamiltonian and the state abstractly in terms of $|E_+\rangle$ and $|E_-\rangle$. Then later in the question, they replaced $|E_+\rangle$ with $|+\rangle_z$ and $|E_-\rangle$ with $|-\rangle_z$, suggesting they did not connect the Hamiltonian to the magnetic field.

On the second part of this question, students were asked to write the energy eigenstates and energy eigenvalues. Half of all students (50% or 7/14) identified the energy eigenstates as $|\pm\rangle_z$, but only 21% (3/14) of the students identified both the correct eigenstates and eigenvalues. The other 29% (4/14) that did not write the correct eigenvalues did not include the necessary constants. A further 21% (4/14) of the students incorrectly wrote states in the $z$-basis, while 14% (2/14) wrote their answers in the energy basis without connecting them to the spin states.
On the final part of this question, students were asked to compute the probability of measuring spin down in the z-direction at a later time, which requires them to write the time-dependent state. On this question, 57% (8/14) of students correctly wrote the time-dependent state in the x-basis in order to perform this calculation. There were 36% (5/14) of students who incorrectly wrote the state in the z-basis instead. Of these five, only one had correctly identified the eigenstates in the previous part. The other four were consistent (but incorrect) in that they indicated the z-basis was the energy eigenbasis and then used that basis to write the time-dependent state.

3.3. Responses to Q3

Question 3 was an unstructured question that asked students to write the quantum state as a function of time without any 'helper' questions. On this question, 62% (31/50) of the students converted the state to the correct basis (the y basis). Of these students, 42% (13/31) structured their responses by listing the Hamiltonian and the eigenstates explicitly, even though the question did not ask for this information. A possible explanation for this behavior is that the course instructor labeled the elements of finding time dependence during lecture, and many students proceeded to write these elements on their personal equation sheet. Another 26% (8/31) of the students only wrote the Hamiltonian and not the eigenstates before writing the time-dependent state in the y basis.

3.4. Responses to Q4

Question 4 was another unstructured exam question, and the only question to align the magnetic field in the z direction (actually the −z direction in this case). In response to this question, 79% (45/57) of the students correctly wrote the state in the z basis (which is the energy eigenbasis for this problem) before multiplying by the time-dependent phases. We have previously seen (for example, on question 1, given at the same institution) that the basis the state in initially written in (at t = 0) is a common basis for students to use when writing the time-dependent state. In response to this question, only 5% (3/57) of the students incorrectly used the y-basis when writing the time-dependent state. It is possible that the fact that the magnetic field was in the z-direction contributed to the success on this question as the z-basis is the most familiar to students.

4. Discussion

In the previous section, we outlined student responses to each question individually. In this section, we will discuss trends across all questions. We will focus on the first three elements of writing a time dependent state as described in the introduction: (i) identify the Hamiltonian, (ii) determine the energy eigenstates, and (iii) write the state in the energy eigenbasis. The four different questions were administered to different students, in different courses, at different institutions, and therefore we will not be comparing performance across different questions, but rather be looking for overall trends in the responses.

We found that on the structured exam questions, the majority of students were able to correctly identify the Hamiltonian as proportional to the spin operator in the direction of the magnetic field (85% on Q1 and 64% on Q2). The most common incorrect answer was to write the Hamiltonian as proportional to the spin operator whose basis the initial state was written in (for both of the structured questions, that would be the z basis). With very few exceptions, only students who answered the Hamiltonian question correctly were able to go on to
successfully find the correct energy eigenstates and write the time-dependent state later in the problem. In this sense, it seems that correctly identifying the Hamiltonian was not the primary problem for the majority of our students, but a correct identification was by itself not a sufficient condition for then finding the time-dependent quantum state.

Both structured questions also ask students, in one way or another, to identify the energy eigenstates for the system. On both questions 1 and 2 approximately half of the students correctly identified the energy eigenbasis, most of whom correctly identified the Hamiltonian in the previous question part. In student written work we can see that those students who do not identify the correct eigenbasis are not referencing the Hamiltonian in their explanations.

All four questions required that the students write the state as a function of time (this is asked indirectly in Q2), and in our analysis we attended to the basis in which that students wrote the state. In order to multiply each term by a time-dependent phase as in the expression $|\Psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar} |\psi_n\rangle$, the state must be written in the energy eigenbasis, $\{|\psi_n\rangle\}$. In the structured questions, students had already been asked to identify the energy eigenbasis, and 57% (46/81) of all students on Q1 and Q2 wrote the final state in the correct energy eigenbasis. On the unstructured exam questions, 62% (31/50) of the students on Q3 and 79% (45/57) of the students on Q4 wrote the state in the correct energy eigenbasis. The most common incorrect answer is for students to write the state in the basis the state was initially written in. Performance on Q4 was better with respect to this element, possibly due to the energy eigenbasis being the $z$-basis, which is often used as a ‘special’ basis or direction.

Overall, we identified a common difficulty for our students with respect to the three elements is in the identification of the energy eigenstates, as half of our students made an error on this stage. We postulate that students do not necessarily connect the Hamiltonian of a system with the energy eigenstates and eigenvalues. That is, they do not necessarily consider the spin Hamiltonian when writing the energy eigenstates for a system, but instead may attend qualitatively to the direction of the magnetic field, which gives them a correct answer for the basis, but does not provide information about the eigenvalues and cannot be generalized to non-spin systems. Alternatively, and even more problematic, students may attend to the basis in which the state is initially written to determine the energy eigenstates. Furthermore, even students who correctly identify the energy eigenbasis do not always use this basis when writing the time-dependent state, and instead use the basis the state was initially written in. The converse is also observed, where some students do not correctly identify the energy eigenbasis, but nevertheless, correctly use the energy eigenbasis when writing the time-dependent state.

In summary, there are a variety of issues that students experience in relation to the time evolution of quantum systems. Simply identifying the Hamiltonian is a small, but present difficulty. Determining the energy eigenstates and knowing that the energy eigenbasis should be used when writing the time dependent state are more common issues for our students. The fourth and fifth elements of writing the initial state in the energy eigenbasis and multiplying each term in the superposition by a time dependent phase are more nuanced than our data set allowed us to probe. However, these are important elements that warrant further study and encompass concepts such as change of basis, determining and associating eigenvalues with eigenstates, and how degeneracy can affect the time evolution of a state.

5. Implications for instruction

For our goal of looking carefully at where students falter when determining how quantum states evolve with time, we articulated five elements involved in this process. However, these
are not necessarily instructive for students. The first element is the identification of the Hamiltonian, a step that is commonly ignored when working with familiar potentials. For instance, it is common to solve for the energy eigenstates and eigenvalues for a given Hamiltonian (say for the harmonic oscillator) and then use the results each time that system is encountered. For some very common potentials, such as the infinite square well, instructors and students alike can recite the energy eigenstates from memory. At the same time, experts will be able to articulate how those energy eigenstates were determined. We believe that these results show that students do not necessarily connect these energy eigenstates with the Hamiltonian. It is for this reason that we articulate it as its own (important) element.

In the context of spin systems in an external magnetic field, the Hamiltonian has the form $H = \omega_0 S_n$, where $S_n$ is the spin operator in the direction of a magnetic field and $\omega_0$ is a constant that depends on the properties of the particle and the strength of the magnetic field. This relation allows students to take a shortcut that bypasses the Hamiltonian and allows them to arrive at a correct answer by relating the energy eigenstates to the direction of the magnetic field. While there is nothing inherently incorrect with this shortcut, it can further weaken the important connection between the Hamiltonian and the energy eigenstates. Regardless of the context in which students are initially taught time evolution, the fact that the solution to the time-dependent Schrödinger equation is a superposition of energy eigenstates, which are in turn found by solving the time-independent Schrödinger equation, is an important connection for students to make. This becomes especially important as students move to more advanced study involving perturbation theory, where changes to the Hamiltonian result in changes to the energy eigenstates and eigenvalues.

Although we did not investigate wave function contexts in this work, there is a similar disconnect between the Hamiltonian and energy eigenfunctions. When dealing with wave functions, there are a limited number of situations that can be solved exactly, and in an undergraduate quantum mechanics course, the number of solutions that students encounter can be counted on one hand. In each case, the student, instructor, or textbook will solve the time-independent Schrödinger equation and arrive at the energy eigenstates. It is rare that this procedure is repeated, but rather, students simply use the results in future questions. For example, when asked for the probability of measuring the ground state energy in an infinite square well problem, students are expected to simply write down the ground state eigenfunction and use it to solve for the probability, rather than first re-derive it. It should then not be surprising that students might forget that they initially used the Hamiltonian to solve for the energy eigenstates.

Our instruction should continually reflect that the energy eigenstates and eigenvalues are determined from the Hamiltonian using the time-independent Schrödinger equation. We suggest following the lead of D. McIntyre’s Quantum Mechanics textbook [25] and using the term ‘energy eigenequation’ instead, which helps to reinforce this connection. It may also be useful to discuss how small changes to the Hamiltonian might affect the energy eigenstates and/or eigenvalues. For example, in the context of spin, this could take the form of a magnetic field in a slightly different direction, or with a different field strength. In the context of wave functions, the harmonic oscillator potential could change width. These types of questions have the added benefit of preparing students for future instruction in perturbation theory.
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ORCID IDs

Gina Passante https://orcid.org/0000-0002-3718-3387
Benjamin P Schermerhorn https://orcid.org/0000-0002-6936-4932
Steven J Pollock https://orcid.org/0000-0002-2462-8164
Homeyra R Sadaghiani https://orcid.org/0000-0002-3800-7465

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