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Student use of a quantum simulation and visualization tool

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Abstract

Knowledge of quantum mechanical systems is becoming more important for many science and engineering students who are looking to join the emerging quantum workforce. To better prepare a wide range of students for these careers, we must seek to develop new tools to enhance our education in quantum topics. We present initial studies on the use of one of these such tools, Quantum Composer, a 1D quantum simulation and visualization tool developed for education and research purposes. In particular, we conducted five think-aloud interviews with students who worked through an exercise using Quantum Composer that focused on the statics and dynamics of quantum states in a single harmonic well system. Our results show that Quantum Composer helps students to obtain the correct answers to the questions posed, but additional support is needed to facilitate the development of student reasoning behind these answers. We also show that students are able to focus only on the relevant features of Quantum Composer to achieve the task.

Keywords: quantum visualization, quantum education, quantum simulation tools

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 Supplementary material for this article is available [online](#)

(Some figures may appear in colour only in the online journal)

1. Introduction

Due to the recent attention on quantum technologies and their economic impact as a result of the so-called second quantum revolution [1], efforts are increasingly focused on educating the next generation of individuals who will make up the backbone of the quantum workforce. As such, current research is increasingly focusing on how higher education institutions can provide the preparation required for people to be successful in this emerging industry and to bring quantum technologies out of academic labs and into society [2, 3]. Additionally, the quantum workforce must draw from a wide range of backgrounds, requiring educators to build quantum literacy among individuals that have less mathematical background than the typical physics graduate.

To be able to meet this demand for a quantum literate workforce, the community needs to develop new quantum curricula at all levels [2, 4, 5], effective methods of teaching quantum mechanics to address common student difficulties in learning the relevant material [6, 7], and tools that allow students to visualize and explore quantum systems (e.g., those described in references [8–10]). If implemented effectively, these efforts will allow students to gain the skills necessary to contribute to the development and deployment of quantum technologies.

Here, we present a study of a new quantum software tool known as Quantum Composer (or simply Composer) [11]. Composer is an interactive and flexible flow-based programming tool designed to allow users to simulate and visualize the static and dynamic properties of one-dimensional quantum systems, including systems that are not readily analytically tractable. This study, which is an extension of preliminary work [12], was designed to identify how students used Composer to explore questions about 1D quantum mechanical systems. Previous work suggested that students used the visualizations contained within Composer to develop their conceptual understanding of a problem. The work presented here aims to probe the use of Composer more deeply.

In this study, we conducted think-aloud interviews with five students as they worked through an exercise designed to guide them through the statics and dynamics of quantum states in a quantum harmonic well system, and here we present the results from the single-well exploration. Our study sought to answer the following research questions:

- RQ1: did Composer help students determine correct answers and reasoning of problems in simple 1D quantum systems?
- RQ2: how did students interact with Composer to complete the tasks?

This study demonstrates the productive use of a new quantum visualization and simulation tool, while presenting the advantages and limitations of the tool with regards to students' abilities to provide correct answers and reasoning while exploring 1D quantum mechanical systems.

2. Background

2.1. Student learning of quantum mechanics concepts

Given the non-intuitive nature of quantum mechanics that arises due to concepts that are absent in classical physics (e.g., wave-particle duality, the quantization of energy levels, tunneling),

physics education researchers have studied extensively where common gaps in knowledge or misconceptions (i.e., interpretations inconsistent with common undergraduate-level instruction in quantum mechanics) arise. In order to develop an exercise that adequately tested the use of Composer for its capabilities, its limitations, and student learning, we drew from this literature and selected a subset of topics that our study could address. This is briefly summarized below, with an emphasis placed on the elements that featured components relevant to our work, that is, the statics and dynamics of stationary and superposition bound states (i.e., not scattering states).

Early efforts to categorize student misconceptions in quantum mechanics were done by Styer [13] and Singh [14]. These studies focused on how quantum states are represented, evolve in time, and are measured. More comprehensive reviews of these student difficulties were recently compiled by Singh and Marshman [6] and Krijtenburg-Lewerissa *et al* [7]. In particular, both reviews discussed student difficulties with differentiating between a quantum state's energy, wavefunction, and probability density. Singh's review also found students had difficulties with answering questions about the time-dependence of systems; this result was confirmed by an earlier study by Cataloglu and Robinett [15] that focused on testing conceptual understanding and ability to work with visual representations in quantum mechanics; this work was later expanded on by Chhabra and Das [16, 17]. Singh found that this difficulty persists even beyond the introductory level and into graduate courses [18]. This study and others by Zhu and Singh [19, 20] also suggest that students face challenges with sketching the shape of the wavefunction. In later work, Emigh *et al* indicated that students fail to see the difference between the time evolution of wavefunctions versus probability densities, and they struggle to interpret a wavefunction's time-dependent phase factor(s) [21]. Student difficulties in interpreting complex exponentials were also identified by Wan *et al* [22]. Similarly, Emigh *et al* noted that students tended to misinterpret the physical meaning of the real and imaginary components of the wavefunction. This is supported by other work done by McKagan *et al* [23] and Passante and Kohnle [24], and both of these studies were framed in the context of visualization tools and their potential to assist student learning. In the supplementary material (SM), we provide a detailed overview of quantum visualization and simulation tools other than Composer, which we describe next.

2.2. Quantum Composer

In this study, we investigate the student use of a new quantum simulation tool: Quantum Composer. Composer was developed at Aarhus University (where this study was performed) and is available for free download for all major desktop computer platforms [25]. Rather than focusing on individual, curated simulations like the three projects mentioned in the SM, Composer is a flexible and interactive tool that enables educators and students to build and simulate one-dimensional quantum systems through a 'drag-and-drop' visual programming and execution interface. Composer is described in detail in reference [11] and relevant elements are discussed briefly here.

The interface consists of a simulation environment where elements are dragged-and-dropped and connected together sequentially, as shown in figure 1. These elements are referred to as *nodes* with interactive capabilities, e.g., entering scalars to create an arbitrary linear combination or defining a potential function. Composer also consists of a collection of visualization *nodes*, such as the *state comparison plot* that displays single eigenstates and superposition states, both in static and time-dependent configurations. The plots have checkboxes that enable the user to select which information they would like to see on the plot. For instance, one can visualize the real part, imaginary part, and the probability density of any wavefunction either

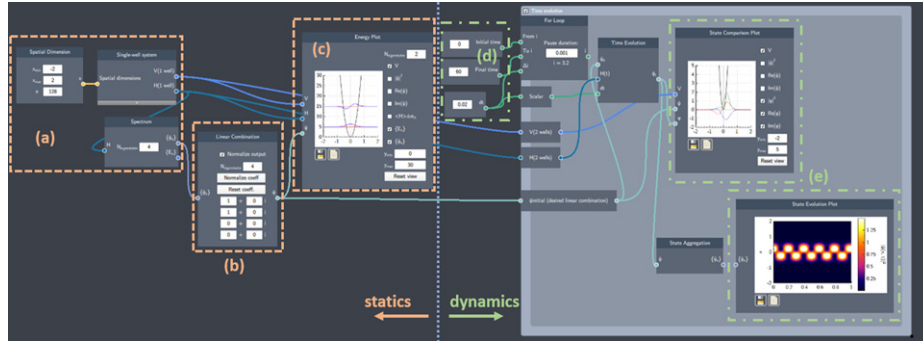


Figure 1. A screenshot of the *flowscene* for the single-well potential used by the interview participants. The blue dotted lines separate the time-independent parts of the simulation from the time-dependent dynamics that take place in the *time evolution* loop. All parameters shown in white boxes could be changed by the students. Students could observe the behavior of the system under study during (a) the time-independent parts of the scenario (orange, dashed box within ‘statics’) and (b) the time-dependent parts of the scenario (green, dashed box within ‘dynamics’). The plots in (b) updated continuously if the student initiated time evolution by pressing the play button (not shown).

simultaneously or one at a time by selecting the relevant checkbox. Composer is also capable of time-evolving a state given an initial state and potential. Once a simulation is built, it can be saved and loaded as a *flowscene*, which can be used by students for guided exploration.

The purpose of this investigation is to explore the use of Composer as a tool for quantum visualization and simulation in an educational setting. Here, we extend previous developments on the use and impact of visualization and simulation tools in physics education research.

In this study, students answered questions related to the quantum harmonic oscillator based on an exercise (cf section 3.2) given to them with an accompanying *flowscene*. Their actions and thought processes during the exercise were captured through think-aloud interviews, and these data were analyzed to investigate the use and impact of Composer on student knowledge of quantum mechanics.

3. Methods

3.1. Research context

This study took place at Aarhus University, and the five students recruited for the study were enrolled in a second-year undergraduate quantum mechanics for nanoscientists course in Fall 2019. Students provided their informed consent prior to the study, and the consent form and study were approved by Aarhus University and is in compliance with the European Union General Data Protection Regulation. Course details and student exposure to Composer within the course can be found in the supplementary material, as can details on the interviews, which were done in the think-aloud style [26].

3.2. Interview protocol and exercise

The exercise that the students worked through in the think-aloud interview covered statics and dynamics in two separate scenarios using single- and double-harmonic well potentials

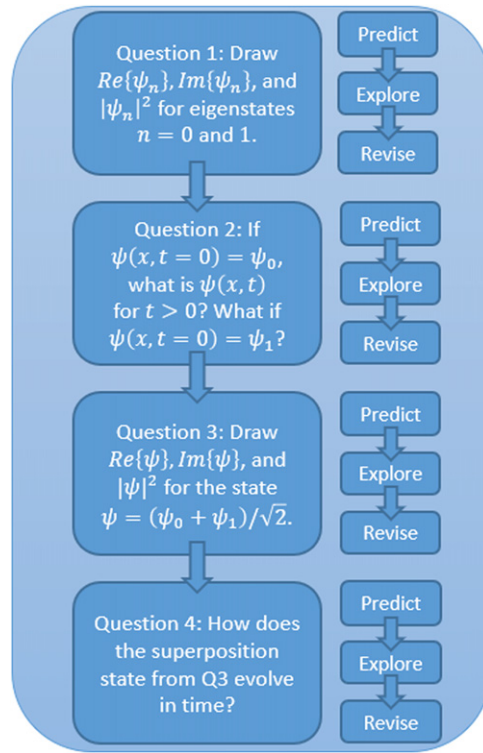


Figure 2. A simplified flowchart of the single-well exercise with the questions numbered as discussed in the results section and the *predict*, *explore*, *revise* phases associated with each question. The exercise asked students to consider statics, then dynamics, of single eigenstates before moving on to superposition states.

(see supplemental material for the full exercise prompt). In this study, we consider only the single-well part of the exercise, as shown in figure 2.

For the interviews, we provided a previously constructed *flowscape* for the participants to work with, as shown in figure 1. Additionally, we used the *scope* feature within Composer to hide unnecessary details of the simulation [11], in order to encourage students to focus on the important aspects of the simulation and avoid unnecessary cognitive overhead that would hinder their exploration [27].

The exercise was designed to use a *predict, explore, revise* framework. That is, before using Composer, students were asked to *predict* (using either words, equations, or sketches) specific aspects of the system under study. After making their predictions, the students were then prompted to *explore* the same system in Composer and finally, they were asked to *revise* their answer and reasoning if needed.

Students began the exercise by considering the eigenstates of the harmonic well. The exercise asked them to sketch the real part, imaginary part, and probability density of the ground state, $\psi_0(x)$, and first excited state, $\psi_1(x)$. Students were provided with a piece of paper with plots showing the harmonic oscillator potential on which they could sketch each state. After their sketches were completed, they then used Composer to produce plots of the same states and were prompted to compare the results they obtained in Composer with what they drew and revise any inconsistencies between their drawings and the Composer plots.

The exercise then prompted students to consider the time-dependence of the system. The exercise sheet reminded them that the n th eigenstate (with energy E_n) evolves in time as

$$\psi_n(x, t) = \psi_n(x) e^{-iE_n t/\hbar}. \quad (1)$$

The students were then asked to *predict* how the real part, imaginary part, and probability density of the ground and first excited states evolved in time, after which they went through the same *explore* and *revise* phases.

After considering single eigenstates, students then considered the superposition state

$$\psi_{\text{lin}}(x, t) = \sqrt{\frac{1}{2}} \left(\psi_0(x) e^{-iE_0 t/\hbar} + \psi_1(x) e^{-iE_1 t/\hbar} \right) \quad (2)$$

with the initial state at $t = 0$ given by

$$\psi_{\text{lin}}(x) = \sqrt{\frac{1}{2}} (\psi_0(x) + \psi_1(x)). \quad (3)$$

First, students considered the static case, and as before, they were asked to *predict* the real part, imaginary part, and probability density of $\psi_{\text{initial}}(x)$. However, they were also asked to *predict* whether or not the probability density of the state would evolve in time and why. Again, students were asked to *explore* and *revise* their predictions using Composer. This marked the end of the single-well part of the exercise.

3.3. Coding scheme

After all interviews were completed, the audio was transcribed by humans via an online transcription service [28]. The video, audio, and transcripts were all used during the coding process. In this context, coding refers to categorizing and labeling the students' vocalizations and on-screen actions. Extensive details on the coding scheme and the codebook used can be found in the supplemental material, and we include relevant aspects here.

In addition to coding the interviews, we documented the accuracy of students' responses to the questions in the *predict* phase to capture whether a prediction and the reasoning surrounding it were correct (including partially correct), completely incorrect, or not present. We included partially correct answers among the correct answers as there was a rather large spectrum of 'correctness' and it was difficult to place an answer on that spectrum, e.g., due to students' difficulties with the language of quantum mechanics.

4. Results

We address our research questions (outlined in section 1) in separate subsections. All exercise questions referred to in this section are labeled and briefly described in the flowchart in figure 2.

4.1. Impact of Composer on student answers and reasoning

Here, we address RQ1: does Composer help students determine correct answers and associated reasoning of problems in simple 1D quantum systems? To this end, we present in figure 3 categorization of students' responses to each question asked in the exercise. Additional details for each question are available in the SM.

As described in section 3.3, we categorized students' responses to the exercise questions as 'correct' if they were entirely or partially correct, 'incorrect' if the responses were completely

Question	Student 1	Student 2	Student 3	Student 4	Student 5
Q1, $\text{Re}(\psi_0)$	I	III	I	I	I
Q1, $\text{Im}(\psi_0)$	I	IV	IV	IV	I
Q1, $ \psi_0 ^2$	I	III	I	III	I
Q1, $\text{Re}(\psi_1)$	I	III	I	I	I
Q1, $\text{Im}(\psi_1)$	I	IV	IV	IV	III
Q1, $ \psi_1 ^2$	I	III	II	II	I
Q2, $\text{Re}(\psi_0)$	V	IV	III	II	IV
Q2, $\text{Im}(\psi_0)$	V	IV	II	II	II
Q2, $ \psi_0 ^2$	V	III	II	II	II
Q2, $\text{Re}(\psi_1)$	V	IV	III	II	IV
Q2, $\text{Im}(\psi_1)$	V	IV	II	II	IV
Q2, $ \psi_1 ^2$	V	III	II	II	III
Q3, $\text{Re}(\psi)$	III	II	III	II	II
Q3, $\text{Im}(\psi)$	II	II	II	II	IV
Q3, $ \psi ^2$	I	IV	IV	III	IV
Q4	I	III	II	II	V

Figure 3. Categorization of individual student responses for each question (cf figure 2), color- and Roman-numeral-coded by outcome: (I, yellow) corresponds to the case where the student gave the correct answer in the *predict* phase but provided no reasoning at any stage; (II, orange) corresponds to the case where students provided a correct answer with correct reasoning in the *predict* phase; (III, green) denotes where students provided correct reasoning after (but not before) using Composer in the *explore/revise* phase; (IV, red) marks cases where (a) the initial answer was incorrect or not provided and no reasoning was provided upon revision or (b) no answer was provided in the revision stage; and (V, blue) shows where students used Composer incorrectly at any stage of the process.

incorrect, or ‘not present’ if no response was provided. This categorization, when applied during the *predict* phase indicates the measure of students’ knowledge about the concept before using Composer, and when applied in the *explore/revise* phase indicates if Composer facilitated any improvement to their responses.

Importantly, students were not explicitly asked to revise initially correct answers that were provided without reasoning, and most students would provide correct answers without reasoning for some questions in the exercise. We note, however, that unless an answer was not provided in the *explore/revise* phase (which only occurred once), all students were able to provide a correct answer upon using Composer (provided they were using it correctly), indicating that students can, at the very least, use Composer to obtain the correct answer. Regarding the correct use of Composer: student 1 used Composer incorrectly during the first question that discussed time-evolution (Q2) due to the fact that they were not aware of the *play* button that would show wavefunction dynamics. Likewise, student 5 used the static (not dynamic) plot to answer Q4.

When examining at these data question-by-question, we see that difficulty with the imaginary part of Q1 was common. For example, student 4 stated

I can’t actually remember...about the imaginary part. I don’t remember if there is a imaginary part, so I’ll just skip that and maybe think about it later.

The student was, in the *explore/revise* phase, able to identify that the imaginary part of the wavefunction was zero, and this knowledge was correctly applied in later *predict* parts of the exercise. Interestingly, after looking at equation (2) while in the *predict* phase for Q2, the

student was able to apply correct mathematical reasoning to answer why the superposition state would have zero imaginary part in Q3. All but one of the other students were able to do the same, e.g., where student 1 states

So, as t increases, the exponential factor gets smaller. That's imaginary. Okay. I've only got the time and the exponential factor. We're introducing an imaginary part, so the imaginary part won't be zero anymore, I guess, at least.

The next question in the exercise involved time evolution. Unlike in the previous question, most students provided correct answers and reasoning for the imaginary part of the wavefunction in Q2, but we note that they were given the mathematical representation of the wavefunction in the exercise. An example of such a response is where student 1 states

So, as t increases, the exponential factor gets smaller. That's imaginary. Okay. I've only got the time and the exponential factor. We're introducing an imaginary part, so the imaginary part won't be zero anymore, I guess, at least.

On the other hand, students tended to make incorrect predictions for the time evolution of the real part of an eigenstate, even if they were all able to predict the $t = 0$ wavefunction (student 2 had a correct prediction without reasoning, but then provided correct reasoning upon revision). Many students predicted the real part to be static in time. Student 3 was one of these, but after using Composer, the student said

Of course it's changing in time as well, the real part... Because now we have a time dependency... for the real part, I actually didn't even think about the time dependency of the imaginary part working here on the real part. So it was actually nice seeing that. It had an influence because sometimes when I'm just looking at the equations it doesn't give you the interpretation of the wave functions.

Here, the student realized that the real part is time-dependent after looking at the dynamic *state comparison plot* in Composer. Additionally, the student mentioned that it was not obvious earlier that the real part would evolve in time, even though one may know the equations. The student was able to connect the visualizations of the wavefunctions shown in Composer with the underlying mathematics describing the physics of the system.

Similarly, student 2 initially did not predict that the probability density of the ground state would be stationary in time. Using Composer helped them to recall what they had learned in class, as shown below:

Oh, I need the probability density... and here we go. Let's see. There's something wrong... why isn't that moving more?... Oh, okay. So this part, I thought earlier would be moving. [It] doesn't move because it's the probability. But it makes sense, actually, from the theory that I have learned.

Later in the exercise, when asked to predict the dynamics of the first excited state, student 2 indicates a change in thinking, stating

Now I have learned that the probability density would also look the same [as time evolves].

Thus, the student has recalled additional knowledge in the earlier part of the exercise and applied this to make a correct prediction in another part of the exercise.

When considering a static superposition state, many students were able to determine the real and imaginary parts of the state, some with the help of Composer. However, the probability density proved more challenging to reason about. One notable exception is given by student 4, who states, upon using Composer:

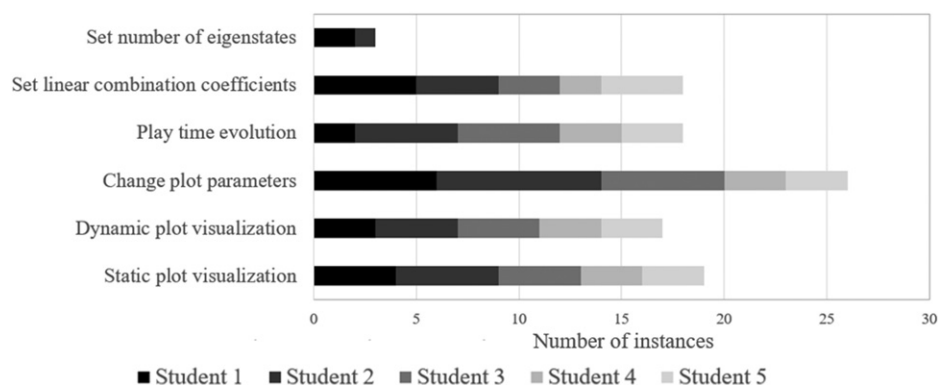


Figure 4. Bar chart showing the number of separate instances coded for each student's use of various Composer *interactions* and *visualizations* during the *explore/revise* phase of the single-well system exercise. The different colored bars in the charts show how often each student performed each *interaction* or made use of each *visualization*, and the stacked sum of all bars shows the total number summed across all students.

I can see that I was quite wrong, and it also makes sense because I can't just add the probability like before because that's not how it works. For the wavefunctions, I have to be able to draw it properly, and I can see it doesn't quite look like that. And then, I just I have to use this to make the norm square and to get the right answer, so I was quite wrong... I have learned that I just can't look at the probability density from the two eigenstates and then add it together.

The student has used the visualizations from Composer to correctly revise their reasoning about the correct answer in that they remember that they must take the modulus squared of the superposition state instead of adding the probability densities of the individual eigenstates. Thus, Composer facilitated their reasoning by making them confront the conflicting answers.

Holistically, we see that while Composer can facilitate the development of correct reasoning, this is not universal, as indicated by the roughly equal number of items in figure 3 corresponding to cases III (correct reasoning provided after using Composer) and IV (no reasoning provided upon revision or no answer provided upon revision).

4.2. Composer features

In this section, we address RQ2: how did students interact with Composer to complete the tasks? We do this to understand to what extent students are exploring all of the available Composer features or focusing only on the relevant aspects of the *flowscape*, and whether or not they focus only on one or two relevant features.

We quantified the use of Composer features by counting the number of separate instances coded for the different features. In this section, we consider six subcodes under the *exploration* code (denoted by * in the codebook, see the SM), as these are the features used during the exercise. We present the cumulative number of instances that were coded in all five interviews in figure 4.

The graph indicates that students engage regularly with all features with the exception of *set number of eigenstates*, which did not need to be changed to complete the exercise. We see that students work more extensively with the relevant features, including those related to visualization of the system, using each about the same number of times.

5. Discussion and implications for instruction

These results show that Composer allows students to visualize the correct behavior of a given system and facilitates their ability to make connections between what they learned in their coursework with the visualizations obtained from Composer. Additionally, by using Composer, students were able to better connect the underlying mathematics with the visualizations they were seeing. As they went through the exercise, almost all students were able to express the correct answers after using Composer, and a number of students indicated that the tool is a useful way to check their answers. Below, we discuss in more detail the results related to our research questions. Limitations of the study can be found in the SM.

First, we discuss our results relevant to RQ1: does Composer help students determine correct answers and associated reasoning of problems in simple 1D quantum systems? Perhaps most interestingly, our results show that students' use of Composer and the mathematical forms presented in the exercise (cf equation (2)) helps them to reason about the imaginary part of wavefunctions as they move through the exercise. This is particularly compelling, as it is common for students to struggle with visualizing the imaginary part of the wavefunction [21, 22], and this shows that, when used alongside the mathematical expressions, students can use Composer to reason about this concept and correctly apply their knowledge as they move through an exercise. This is supported by the following student quote:

And the imaginary part, yeah, so it also is constant at time equals zero. Okay. I'll just revise. So I think it's getting better, because I now have the knowledge from Composer, how they actually evolve, now I was able to answer more correctly than before. So I think it's working as it should.

Therefore, we believe that Composer could be particularly beneficial in addressing questions concerning the time evolution of states, as it allows students to visualize the time evolution for the real part, imaginary part, and the probability density; this can assist with the difficulties identified in references [6, 7]. Moreover, features like the *state comparison plot* (coded as *dynamic plot*) help students compare the behavior of a quantum state in the static and dynamic cases. This assists students in determining the differences between the two cases, although Composer alone is not necessarily well-suited to helping students to express their reasoning behind their answers, a finding echoed in other work on engaging students in electronic learning tutorials [29]. Part of this is due to how our exercise was worded in that students who expressed the correct answer initially were not asked to reason about the problem upon revision, and we found that many students would simply provide correct answers without reasoning, particularly in the initial phases of the exercise.

Thus, Composer is likely, as with most other quantum visualization and simulation tools, best used in conjunction with a textbook, exercise, lecture, or other tool that focuses on elucidating the reasoning behind the physical behavior of the system under study, as is done in references [10, 30–32]. For example, student reasoning may be better developed in an exercise where students work out a problem using mathematical representations and check their answers in Composer before being asked to reason about the problem. This can help them to build insight into problems where they connect what they see in Composer with what they have worked out mathematically. Additionally, these exercises should help students develop better reasoning through guiding questions that connect the math to the visualizations [33].

We note, however, that when students use Composer, they can get the wrong answer, which, in the worst case, can facilitate the development of incorrect reasoning. This indicates the need for comprehensive onboarding during Composer use in the classroom, and instructors should look out for students who are using the tool incorrectly.

Now, we briefly discuss the results related to RQ2: how did students engage with Composer to complete the tasks? Our finding show that students generally focus only on relevant aspects of the Composer *flowscene*, suggesting that Composer is laid out in such a way to support student use of the tool. In addition, students focus largely on the visualization aspects provided in Composer (i.e., the last four lines in figure 4), which suggests that they are using the tool as intended, that is, to visualize the system at-hand. Thus, Composer as-is is sufficient to aid students in their exploration of 1D quantum physics, although this does not rule out the possibility of future improvements that can be made to the interface.

6. Conclusion and outlook

The aim of this study was to probe whether Quantum Composer can be used as a tool to increase students' knowledge of quantum mechanics in a single harmonic well system. The exercise covered questions related to the static and dynamic case of the real part, imaginary part, and probability density of single eigenstates and superposition states. The study used a think-aloud protocol with five students, where we found that all students could determine or revise answers to problems in quantum mechanics by changing parameters and visualizing the system in Composer. Overall, we were able to demonstrate the constructive use of a new quantum visualization and simulation tool and show how student responses to questions about quantum systems was aided by exploration in Composer, in particular, with regards to their ability to provide the correct answers to questions posed.

This work bolsters previous studies on the impact of quantum mechanics visualization tools. First and foremost, the use of tools like Composer can facilitate students' ability to articulate the correct answer, but more effort is required to ensure that students are properly reasoning about the behavior of a given quantum system. Thus, we recommend that the use of such tools be coupled directly to other course materials and environments (e.g., guided tutorials, homework exercises) that help students connect their answers to the underlying reasoning.

As this was just our first exploratory study of the benefits and limitations of using Composer to aid in student learning of 1D quantum mechanical systems, there are many opportunities for more in-depth research studies. Future work will include a larger number of student participants with different demographics and educational backgrounds. Additionally, we could examine clickstream-type data to better understand how exactly students interact with all of Composer's features. We could also create new types of exercises that help develop and elicit student reasoning around these topics. Given Composer's unique flexibility, we could also study how students and educators create and/or modify *flowscenes*, as they illustrate or explore different concepts. Ultimately, we hope to be able to not just refine Quantum Composer so that it is more useful for students, but we also hope to understand the best way to incorporate Composer in quantum mechanics courses for all science and engineering majors, including those focused on a career in quantum information science and technology.

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