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A double well on-line simulation and activities for active learning of introductory quantum mechanics

Sergej Faletič[1]

University of Ljubljana, Faculty of Mathematics and Physics, Jadranska 19, 1000 Ljubljana, Slovenia

E-mail: sergej.faletic@fmf.uni-lj.si

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Abstract

Teaching introductory quantum mechanics is challenging, especially to students who have limited knowledge of mathematics. The challenges and approaches are evidenced in a wide range of literature. Our goal is to develop an active engagement module for introductory quantum mechanics that would cover the most important concepts: indeterminism, incompatibility, the difference between superposition and statistical mixture and the role of measurement. To accomplish this, we developed a free on-line simulation of a double well—a (pseudo) two-state system—which is able to evidence all of the above concepts. Students perform simulated experiments and build their knowledge from their observations. We present the simulation and the proposed experiments to address the above concepts. We provide a description of the activities and their outcomes as tested with high-school students in different settings. Qualitative analysis of learning outcomes offers evidence that between 60% and 100% of students can reach the following conclusions on their own. (i) The particle is only ever detected in one of the possible states. (ii) The outcome of one experiment cannot be predicted, only its probability can be predicted. (iii) For some pairs of quantities, knowing the value of one quantity exactly precludes the possibility of knowing the value of the other quantity exactly. (iv) A statistical mixture (of eigenstates) is not the same as a superposition state. (v) The measurement affects the time evolution of the system. The most difficult conclusion for students to reach is how exactly the measurement affects the system. The success rates presented here lead us to conclude that the simulated experiments can be very useful when designing an active engagement course on the concepts of quantum mechanics. While the development is done in high-school, we believe the results are also relevant for introductory university level, especially for non-physics students.

[1]Author to whom any correspondence should be addressed.

Keywords: quantum mechanics, active learning, introductory level, high-school, simulation, ISLE

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

1. Introduction

Teaching introductory quantum mechanics is challenging. When students have limited mathematical skills or are discouraged by mathematics, the challenges are even greater. On the other hand, there is growing interest in introducing quantum mechanics at pre-university level and to non-physics students (especially engineers) at university level. This is becoming increasingly important [1–5]. One reason is that quantum technology has become a research goal and strategic agenda in many countries [6] and experts recognise that to increase the available expert workforce, quantum technology opportunities should be introduced to students before they make a career choice. In some cases, this could mean before enrolling in an undergraduate programme, while in others (for example, engineering degrees) it could mean at the beginning of the undergraduate programme. Due to the limited mathematical knowledge, approaches at these levels have to be tailored towards a more conceptual understanding. However, also in cases where the full mathematical description will be introduced later in the course or programme, building a conceptual understanding first can be beneficial. The approach with two-state systems is proposed due to its conceptual foundation and proved feasibility [2, 7–14]. It is also strongly related to quantum computing. It is well suited to introduce states, incompatibility (the uncertainty relation), the problem of trajectory, and in some cases, it can also be used to introduce entanglement. All the courses referenced above use simulations to provide active engagement and have shown that simulations are efficient in this goal.

The three most used two-state systems are the 'path' states in a Mach–Zehnder interferometer [8], the spin states in a Stern–Gerlach experiment [11] and polarization states in polarization experiments [14]. Spin (or angular momentum) and polarization are not necessarily part of high-school curricula. Therefore, they might introduce an additional cognitive burden on students even in the first year of university. Nonetheless, they are very efficient in introducing many of the key concepts of quantum mechanics. The polarization approach further allows for some simple real life experiments with the polarization system, which can be related to simulated experiments and a quantum description [15]. The Mach–Zehnder approach addresses position, but more precisely, it addresses 'path', and usually does not include a temporal component. None of the above approaches are suited to introduce the time evolution. Our goal was to build a simulation that would bring the 'mechanics' into the introduction of quantum mechanics, while still retaining the advantages of the two-state approach, thus addressing position and time, the quantities most associated with classical mechanics. Students could then compare and contrast quantum with classical mechanics, dealing with concepts that they should already be familiar with, such as position, trajectory and time. For the physical system we chose the double well. For almost degenerate energy states, and limiting ourselves to the lowest energies, this system can be approximated with two position states and two energy states, and includes the time evolution of states. More details are in the description of the simulation.

For the active engagement framework we chose ISLE (Investigative Science Learning Environment) [16, 17], because it is designed to let students build their own knowledge in an epistemologically authentic way [18]. The ISLE approach consists of letting students do the steps by which scientists do science for themselves. The main steps of this nonlinear process are (i) observation, (ii) generation of descriptions (models) or explanations (hypotheses), (iii) testing of the models or hypotheses by proposing testing experiments and making predictions for their outcomes based on the models or hypotheses, before performing the experiments, (iv) rejection or revision of hypotheses or models that make wrong predictions, and (v) application of accepted hypotheses or models to new problems. Experiments in the ISLE approach thus have clear roles: they can be *observational* experiments to address steps (i) and (ii), *testing* experiments to address steps (iii) and (iv), or *application* experiments to address step (v). We believe that such an approach, by letting students build their own models, might help them take ownership of the knowledge and overcome the usual difficulties in accepting the quantum description of reality [19, 20], and also build the fundamental concepts of the new way of thinking in quantum theory [21].

Research is done in the framework of design-based research [22, 23] by analysing student responses during the activities with the aim to identify students' difficulties and way of thinking in the building of specific concepts.

We contribute to the current literature by addressing a two-states system, the double well, that we have not encountered in literature, and by using the ISLE methodology to guide the development of activities and experiments. We perform most of the experiments in our own course and for those we can report the success rate of students in different activities. Our approach to the whole topic is beyond the scope of this article. Firstly, because the simulation has been successfully tested in very different settings with very different active engagement approaches and activities and is thus not limited to a particular course. Secondly, because the outcome of a course depends on many more factors than just the activities, which are the focus of this article. The research questions we want to answer in this article are thus as follows.

(a) How the features of the simulation offer opportunities for students to explore and to build basic concepts of quantum mechanics like indeterminism, probability, complementarity (uncertainty relation), collapse and the difference between a statistical mixture and a superposition?

(b) How successful are students in constructing the concepts of quantum mechanics using the simulation?

The research questions aim to give answer to the problem how can we help students take ownership of knowledge on quantum mechanics which has been identified as an important topic for research by a community of experts developing high-school courses in quantum mechanics [24]. So we contribute to the literature by addressing this question and offering an evidence based successful approach (tool).

2. The class settings and student engagement

The use of the simulated experiments with the double well has been experimented in various settings. (1) An active engagement course on quantum mechanics in high-school, where the experiments have been used for three consecutive years, each year in a class of approximately 30 students of grade 12 (17–18 years old) in Ljubljana, Slovenia. (2) A summer school for gifted grades 10–13 students ($N = 17$) from all over Slovenia. (3) A summer school for gifted grade 13 students ($N = 30$) from all over Italy. (4) A professional development course for in-service high-school physics teachers ($N = 20$). (5) A workshop for interested grade 12 students ($N = 34$) in Slovenia.

In this article we discuss how well students perform the experiments and whether they reach the intended conclusions. The way the experiments have been inserted in each course differs from implementation to implementation, and so does the way we collected data.

In setting (1), we prepared worksheets with specific questions or tasks[2] modelled after the ISLE worksheets found in the ISLE based textbook [25] and its accompanying active learning handbook [26]. For this setting, we report the percentage of students who arrived at the expected findings. The success rates are presented together with the proposed activities. We also add observations on alternative conclusions and difficulties that students encounter. Similar worksheets were used in settings (4) and (5), but were not analysed.

In settings (2) and (3) we just let the students explore the simulation for about 20 min and then report any findings that they arrived at. For these settings, we can only report whether a particular finding was reported in the discussion or not. A few of the experiments in these settings were performed by the instructor and also a few findings were arrived at following a whole class discussion. For these, we cannot report a success rate, but the experiments are still crucial to arrive at the whole class discussion and other steps in the epistemic process can be performed by the students.

3. The double well simulation

The simulation of the double well approximates a two-state system by using a barrier with such properties that the first two energy states are almost degenerate so that their superposition creates states that are almost entirely concentrated in either the left or the right well. The energy eigenvalues E_1 and E_2 are calculated from the settings ((H) in figure 1) with a numerical algorithm. The respective eigenstates are denoted $|\mathrm{E1}\rangle$ and $|\mathrm{E2}\rangle$. However, to obtain the position states as localized in one well as possible, the energy eigenvalues are very close together and the numerical calculation can fail to distinguish between the two roots of the equation. For this reason, some user adjustments of the well have been disabled for now. The default settings of the well are such that the period of transition of probability from one well to the other is almost exactly 60 fs.

In the simulated experiment we operate with two position states called $|\mathrm{L}\rangle = \sqrt{1/2}|\mathrm{E1}\rangle + \sqrt{1/2}|\mathrm{E2}\rangle$ for left and $|\mathrm{R}\rangle = \sqrt{1/2}|\mathrm{E1}\rangle - \sqrt{1/2}|\mathrm{E2}\rangle$ for right. These form a basis. Another basis is provided by the two energy states $|\mathrm{E1}\rangle$ and $|\mathrm{E2}\rangle$. These two bases are incompatible.

The simulation's graphical user interface (GUI) is shown in figure 1. The simulation allows the changing of the initial state of the particle (the preparation, (C) in figure 1), the choice of quantity to be measured (position, x, or energy, E), and the time of measurement ((D) in figure 1). It allows three measurement times with three separate displays of results ((F) in figure 1). The simulation also contains a switch ((E) in figure 1) to toggle whether the particle is reset between the measurements, effectively making them independent measurements, or not reset and leaving the particle in the state after the previous measurement. It is also possible to automatically repeat the experiment a selected number of times. The results are displayed in form of histograms for each measurement ((F) in figure 1), with the number of counts also displayed. A log of the results is also displayed to allow subsequent analysis ((G) in figure 1). It can be easily copy-pasted into a spreadsheet editor. The histograms for position measurements are in one colour and vertical, visually separating left from right, while the histograms for energy measurements are of another colour and horizontal, visually separating the lower and higher energy states.

[2] See https://fmf.uni-lj.si/storage/54807/Double_well_supplement.pdf.

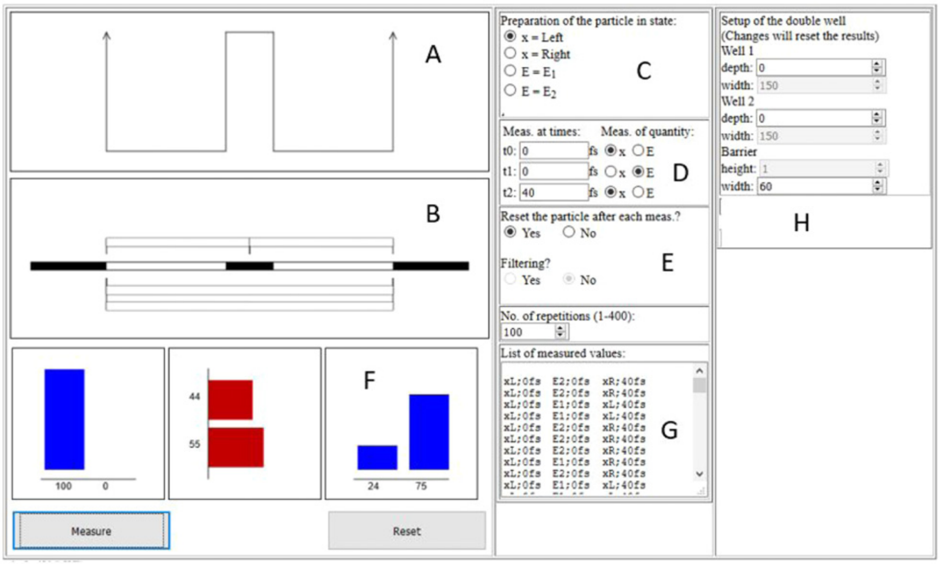


Figure 1. The graphic user interface of the double well simulation: (A) the representation of the potential, (B) the representation of a 1D double well, (C) the preparation settings, (D) the measurement settings, (E) resetting or not resetting the particle after measurement, (F) graphical representation of the results of the measurements, (G) log of the results and (H) parameters of the wells.

The simulation is written in HTML 5 to allow native portability to different platforms. It is available on-line [27] and can be run from portable devices, which is how students perform the simulated experiments.

3.1. Language, notation and introduction of energy states

In order to remain consistent and concise within the article and with students, we introduce the following terminology. A *quantity* is a physical quantity that we would like to measure, an observable. The *value* is the value of a quantity. In some literature this is called the property, but our students are unfamiliar with that use of the term, so to avoid unnecessary cognitive burden, we adopted a more familiar term. The value is usually an eigenvalue of the respective operator. However, in a double well we limit ourselves to two possible position values, which are not eigenvalues of the position operator, but we still treat them as such. Thus when we measure the quantity 'position' in a double well, we can get two values: either left well, denoted x:L or right well, denoted x:R. Likewise the energy values are denoted E:E1 and E:E2. We define the *state* as a collection of values of different quantities. By this definition, the difference between a classical and a quantum state is that the classical state can, in theory, be completely determined, while a quantum state cannot, because of the uncertainty relations.

We also use the term *pure state* (of a quantity), which we define as *the state for which the outcome of a measurement* (*of the quantity*) *is known with certainty*. In most cases this are eigenstates of the operator associated with the measured quantity. The states $|\mathrm{L}\rangle$ and $|\mathrm{R}\rangle$ still satisfy our definition of pure states in our settings of the well, even though they are not technically eigenstates.

To textually describe the resulting histograms, we use notation [A%], [B%], which means that the histogram shows A% of particles detected with the value x:L (or E:E1) and B% of particles detected with the value x:R (or E:E2).

3.2. The introduction of pure states

This is just a basic activity to introduce the simulation. We prepare one particle in a pure position state (for example $|\mathrm{L}\rangle$) and measure position at time 0. This is to show how the simulation works, how the results are displayed and how we set the initial state of the particle. In addition it shows that preparing in state $|\mathrm{L}\rangle$ and then measuring position will always return the value x:L, which is later used to introduce the pure states, but only after the students see in experiment E.1.1. that not all states are pure states.

3.3. Indeterminism and probability

There are various experiments that allow students to arrive at the indeterminism of single results and the predictability of the probability distribution. The experiments are presented in table 1. Each of the experiments leads to the same findings: undividability of a particle, mutual exclusivity of possible results, indeterminism of single results and predictability of the probability distribution. Students are very successful at arriving at all four findings. They seem to have some problems expressing the findings, but that can be improved with better phrasing of the questions.

3.4. Incompatibility

While many of the crucial concepts of quantum mechanics can be addressed with the simulation using only position states and measurements, incompatibility requires two incompatible quantities. This is the reason why we introduced energy into the simulation. The experiment is very simple and shown in table 2. The question for students is: ‘Is there a state that is both a pure state of position and a pure state of energy?’ In our last implementation most students concluded that no such state exists. In the summer school settings this finding was always reported.

3.5. Time evolution

The experiments in table 3 are observational and designed to let students arrive at a pattern for the time evolution of different quantities. Students are quite successful in all setting. In the last implementation, we noticed that some students might have been observing the single outcomes instead of the distribution pattern. We also noticed some observations by students that are the consequence of unfortunate statistical fluctuations, for example the number of particles in one well being smaller with each of the three repetitions, leading to a conclusion that the number in one well decreases with the number of repetitions. These can be smoothed out in two ways: (i) with more repetitions, and (ii) by comparing to results of other groups who did not find this pattern. An important concept to keep in mind for students is that the results must be reproducible. This is why we do not make predictions for single results. They are not reproducible.

3.6. Statistical mixture vs superposition

The difference between a statistical mixture and a superposition is one of the crucial concepts in quantum mechanics. A survey in the last implementation of our course showed that 64%

Table 1. Experiments to explore stochasticity of single results and predictability of probability distributions.

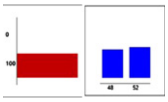
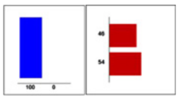
Experiment	Outcome	Observations and conclusions	Students' success
E.1.1. Prepare 1 particle in state $\|L\rangle$. Measure position at time 20 fs. Repeat measurements first manually, then automatically	(O.1.1) Both sensors never blink at the same time. (O.1.2) Some particles are found in the left and some in the right well. There is no pattern for single particles (this can also be analysed from the log). (O.1.3) The distribution is always [75%], [25%]	**(F1)** The particle is never in both wells—undividability of the particle, mutual exclusivity of values. **(F2)** One cannot predict the outcome of a single experiment—indeterminism. **(F3)** One can predict the distribution, probability of outcomes—predictability of probability	$N = 17$. (F1): 100%. (F2): 88%[a]. (F3): 76% identify a pattern in the distribution[b], 29% say that the distribution is predictable[c]
E.1.2. Prepare 1 particle in state $\|E1\rangle$. Measure position at time 0. Repeat measurements first manually then automatically	(O.1.1) and (O.1.2). (O.1.4) The distribution is always [50%], [50%]		In all settings students did report on all three findings

[a] Out of the 88%, 24% identified a probabilistic pattern without being asked. The other 12% (2 students) were unclear, but may have considered a probabilistic pattern.

[b] Another 12% (2 students) saw the pattern, but did not report it.

[c] The question stated only 'What can be predicted of the outcomes of future experiments with the same settings?' Some students may have only thought about single outcomes. A different phrasing could help.

Table 2. Experiments to explore incompatibility of some quantities.

Experiment	Outcome	Observations and conclusions	Students' success
E.2.1. Prepare 100 particles in state $\|E1\rangle$ or $\|E2\rangle$. Measure energy and position at time 0		**(F4)** There are no states which are pure states of energy and position at the same time	$N = 23$. 91%. This finding was reported in all settings.
E.2.2. Prepare 100 particles in state $\|L\rangle$ or $\|R\rangle$. Measure position and energy at time 0.			

($N = 26$) of the students hold the belief that 100 particles in a non-pure state is a statistical mixture of particles in pure states. The experiments in table 4 were developed specifically to address this idea. They show that a statistical mixture behaves differently than a superposition state.

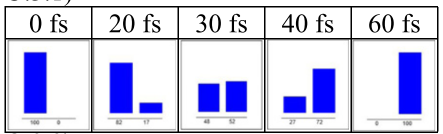
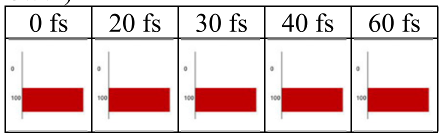
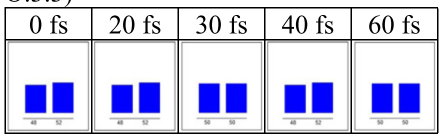
In our last implementation, the experiment was proposed as a testing experiment. We introduced the label $|LT30\rangle$ for the state 30 fs after the creation of a pure $|L\rangle$ state. This state has a probability for position results [50%], [50%]. The same is true for 100 particles of which 50 are prepared in state $|L\rangle$ and 50 in state $|R\rangle$. The hypothesis is that the state $|LT30\rangle$ is a statistical mixture. Students predict the result of the measurement 30 fs after state $|LT30\rangle$ is created based on this hypothesis (effectively they predict the outcome of experiment E.4.1.a). The prediction was made correctly by 40% ($N = 26$) of students. This is consistent with 48% ($N = 25$) of students being able to make predictions at all based on time evolution on their first attempt (we only had time for one exercise). Due to this, we first checked the prediction using a prepared statistical mixture (experiment E.4.1.a). After we very clearly summarised the result of E.4.1.a and presented it in a table, the comparison with the results of E.4.1.b led 65% of the students to the conclusion that a superposition state is not a statistical mixture. Responses from the rest of the students indicated that they do not see time evolution as being characteristic of a state. In other words, the fact that the two states evolve in different ways did not lead them to conclude that the states are different. We find the 65% success rate for such an important finding very good, but there is still room for improvement.

3.7. Trajectory

A one-dimensional trajectory is a sequence of positions at different times, or a sequence of pairs (x, t). In quantum mechanics using our notation this is a sequence of values, such as x:L;t:0fs, x:R;t:30fs, x:R;t:60fs. The possible values for position are x:L and x:R, while the t:... denotes the time of measurement. Table 5 presents experiments that show that just like any single measurement results, the trajectory (a sequence of single measurement results) is not unique or predictable. Therefore, the concept of trajectory as understood in the classical sense is not useful in quantum mechanics.

Despite finding that the trajectory is not predictable and that the final state is not the same, if trajectory is measured, some students still concluded that trajectory is a useful quantity. However, only half of these gave reasons that have something to do with physics, like: 'We can at least have some idea of how the particle travels'. The other half gave reasons such as: 'It is interesting' or 'Otherwise we would not discuss it', indicating that their conclusion was not based on their findings.

Table 3. Experiments to explore time evolution.

Experiment	Outcome	Observations and conclusions	Students' success
E.3.1. Prepare 100 particles in state $\|L\rangle$. Measure position at different times. Start with multiples of 10 fs	O.3.1) 	**(F5)** The probability distribution of position values changes with time. It has a period 2τ—time evolution	$N = 25$. >63%[a]
E.3.2. Prepare 100 particles in state $\|E1\rangle$. Measure energy at different times. Start with multiples of 10 fs	O.3.2) 	**(F6)** The probability distribution of energy values does not change with time	$N = 25$. >53%[b]
E.3.3. Prepare 100 particles in state $\|E1\rangle$. Measure position at different times. Start with multiples of 10 fs	O.3.3) 	**(F7)** The probability distribution of position values in an energy state does not change with time—stationary states	(F7) is very common in all settings

[a] Some of the remaining 37% of students observed single outcomes instead of distributions and correctly concluded that there is no pattern. Better instructions would probably help.
[b] Some students did not arrive to this experiment because they had trouble with E.3.1.

Table 4. Experiments to differentiate between a statistical mixture and a superposition state.

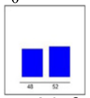
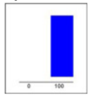
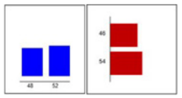
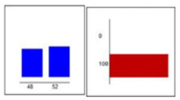
Experiment	Outcome	Observations and conclusions	Students' success
E.4.1.a: Prepare 50 particles in state $\|L\rangle$ ($t_0 = 0$), measure at 30 fs. Prepare additional 50 particles in state $\|R\rangle$, measure at 30 fs	t_0+30 fs 	A statistical mixture of 50:50 in 30 fs evolves into a state with distribution [50%], [50%]	$N = 26$. >65%
E.4.1.b: Prepare 100 particles in state $\|L\rangle$, let it evolve for 30 fs ($t_0 = 30$ fs) into state $\|LT30\rangle$ and then measure 30 fs later at 60 fs	t_0+30 fs 	The state $\|LT30\rangle$ in 30 fs evolves into the state with distribution [0%], [100%] (state $\|R\rangle$)	
E.4.1.a. and b. together: Compare the results of the two experiment and make a judgement whether the state $\|LT30\rangle$ is a statistical mixture		**(F8a)** The state $\|LT30\rangle$ is not a statistical mixture	
E.4.2.a: Prepare 50 particles in state $\|L\rangle$. Measure energy at time 0. Prepare additional 50 particles in state $\|R\rangle$. Measure energy at time 0	0 fs 	A statistical mixture with position distribution [50%], [50%] has energy distribution [50%], [50%]	This experiment was done frontally and explained
E.4.2.b: Prepare 100 particles in state $\|E1\rangle$ with a distribution of position values [50%], [50%]. Measure energy at time 0	0 fs 	The state $\|E1\rangle$ with position distribution [50%], [50%] has energy distribution [100%], [0%]	
E.4.2.a. and b. together: Compare the results of the two experiment and make a judgement whether the state $\|E1\rangle$ is a statistical mixture		**(F8b)** The state $\|E1\rangle$ is not a statistical mixture	

Table 5. Experiments to explore the concept of trajectory in quantum mechanics.

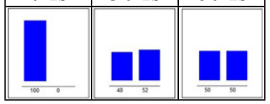
Experiment	Outcome	Observations and conclusions	Students' success
E.5.1. Prepare 100 particles in state $\|L\rangle$ and measure position at three different times (0, 30 fs and 60 fs) without resetting the state after each measurement	The log shows sequences like: x:L;t:0 x:L;t:30 x:R;t:60 x:L;t:0 x:R;t:30 x:R;t:60 x:L;t:0 x:R;t:30 x:R;t:60 x:L;t:0 x:L;t:30 x:L;t:60 The distributions are: 0 fs / 30 fs / 60 fs 	**(F9a)** The trajectory is not unique. **(F9b)** The distribution at 60 fs is no longer [0%], [100%] as in O.3.1. **(F9)** The trajectory is not a useful concept	$N = 24$. (F9a) 88%. (F9b) 73%. (F9) 50%

Table 6. Findings and reasoning to identify the role of measurement in quantum mechanics.

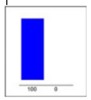
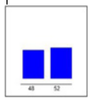
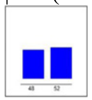
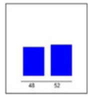
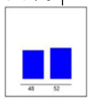
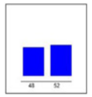
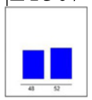
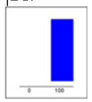
	Preparation	t_0 before measurement	t_0 after measurement or preparation	$t_0 + 30$ fs	Expected reasoning and students' success ($N = 15$)
(a)	|L⟩ 	|LT30⟩ 	|U⟩ (unknown) 		**(F10a)** From (a) and (b): the evolution of |U⟩ matches the evolution of a statistical mixture (73%).
(b)			50% |L⟩, 50% |R⟩ 		**(F10b)** From (a) and (c): state |U⟩ is not |LT30⟩ (60%). The state changes.
(c)			|LT30⟩ 	|R⟩ 	**(F10)** From the fact that a statistical mixture is a mixture of pure states: the measurement changes the state to make it a pure state (34%)

Table 7. Experiment to identify the role of measurement in quantum mechanics.

Experiment	Outcome	Observations and conclusions	Students' success
E.6.1: Prepare the particle in state $\|L\rangle$. Perform two position measurements in close succession (at times 23.0 fs and 23.1 fs) without resetting the state	The two distributions are exactly the same: [73%], [27%]. The log shows perfect correlation: x:L;t:23, x:L;t:23.1 x:L;t:23, x:L;t:23.1 x:R;t:23, x:R;t:23.1 x:L;t:23, x:L;t:23.1	All particles that have been measured with the value x:L at 23 fs have a distribution [100%], [0%] at 23.1 fs. Likewise for x:R. The state after the measurement is therefore $\|L\rangle$ if the measured value is x:L, and $\|R\rangle$ if the measured value is x:R	So far only done by the instructor

3.8. Collapse

From the experiments either about trajectory (table 5) or about measurement (table 6), students have concluded that the measurement affects the system. Students can arrive at how the measurement affects the system either by combining the findings from experiments E.4.1 (a and b) and E.5.1 (let us call this the *combo approach*) or from a specific experiment E.6.1 in table 7.

The reasoning for the combo approach is summarized in table 6. In our last implementation we were able to give students only 5 min to produce their idea about what is the effect of the measurement. In this time, 60% of students ($N = 15$) concluded that the measurement changes the state. More than half of these (34% of all students) further specified that the measurement transforms the state into a pure state. Only one student explicitly stated that the pure state is the state consistent with the result of the measurement, although we noticed that more students had the same idea. Some students spontaneously suggested testing experiments similar to E.6.1. to test their idea. A few students suggested that the state changes during measurement, but not due to the measurement itself, but rather due to the short time of undisturbed time evolution that it takes to make the measurement. These are not counted in the success rate.

The experiment E.6.1. was suggested by students also in one of the summer schools. The interpretation of the results so far has been left to the instructor. From the log, a perfect correlation is observed between the results of the first and the second measurement. This means that after the first measurement produces a value, for example x:L, the state is such that a subsequent measurement shortly after will produce the same result with certainty. This is the definition of a pure state, so the state after the measurement is a pure state.

3.9. Complex coefficients, Feynman phasors and probability

Some students quickly noticed that some states appear the same when described only with the probability distribution. For example, we can differentiate between three [50%], [50%] (position) states, as shown in figure 2. The states are $|E1\rangle$, $|E2\rangle$ and $|LT30\rangle$. Some students specifically asked whether the state $|LT30\rangle$ is $|E1\rangle$ or $|E2\rangle$ or neither. This introduces the discussion about the fact that the coefficients in the description of a superposition cannot be probabilities. Coefficients must be such that they can distinguish between the three states shown in figure 2. If during the introduction of the superposition we discuss that multiplying both

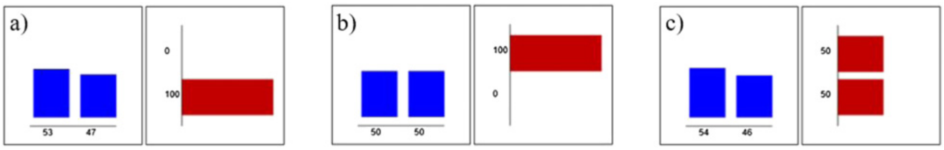


Figure 2. Three different states with equal probability for x:L and x:R (on the left of each diagram, blue). (a) $|\text{E1}\rangle$, (b) $|\text{E2}\rangle$ and (c) $|\text{LT30}\rangle$. On the right of each diagram there is a diagram of energy measurement distribution for each state (red). These are not equal for all states, which makes the states different.

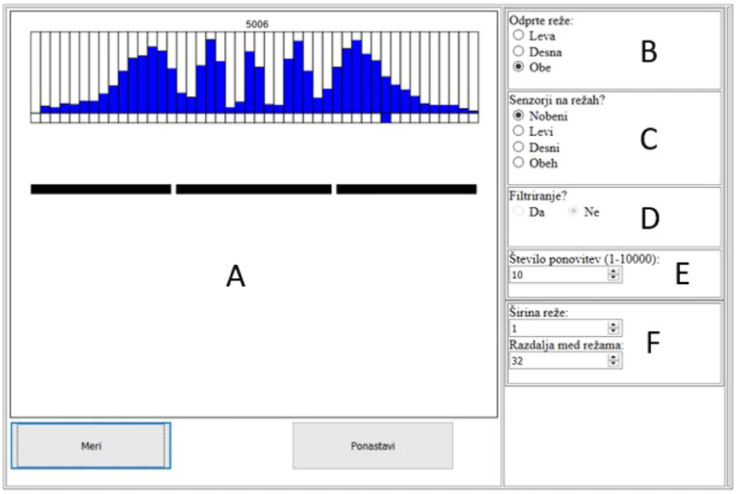


Figure 3. The graphic user interface of the double slit simulation: (A) the representation of the experiment with the histograms at the top, (B) the choice of open slits, (C) the choice of sensors on the slits, (D) the possibility of filtering out the particles coming through one slit or the other, (E) the number of particles, (F) the setup of the slits: width and distance between the slits. The distance from the screen cannot be changed at this time.

coefficients with the same number will not change the state, because the ratio of the coefficients remains the same, or if students are already familiar with linear independence, it becomes quickly clear that one cannot create three linearly independent states with two base states and real coefficients. When asked in a whole class discussion what else we could use, at least one suggestion arose in all settings to use complex numbers for the third state.

3.10. The double slit experiment, wave function and application of acquired knowledge

The experiments with the double well are useful to introduce descriptive rules of quantum physics. It could be argued that many high-school courses could stop here. However, since the wave function model can account for all the descriptive rules except collapse, we developed a simulation for the double slit experiment to complement the double well experiments and introduce the wave function. The simulation is basic, but it includes all the important features and intentionally resembles the double well simulation. The GUI is shown in figure 3. The building of the pattern is particle-by-particle to emphasize the statistical nature of the pattern.

We could not use the excellent PhET simulation [28], because at this time it does not allow to hide the wave representation. Therefore, it cannot be used by students to build their own model.

Discussing all the experiment with the double slit simulation would exceed the scope of this article, but we want to mention the 'which way' experiment, because it relates to the learning outcomes of the double well experiments. In this experiment, sensors are placed on the slits to register which slit the electron passed through. The result is that the interference pattern is replaced by two independent one-slit patterns. When this experiment was shown to students who participated in the double well activities, some students spontaneously commented that a change of the pattern is to be expected due to the collapse of the wave function at the slit. This is encouraging and it indicates that the students have acquired some quantum intuition and that the concept of collapse might have become an important idea in their reasoning.

4. Discussion and conclusions

We have presented a double well simulation designed to address the basic concepts of quantum mechanics at an introductory level. It is written in HTML 5 and accessible online with full source code [27]. It runs on the client device, so very little data exchange with the server is needed. It can also be saved as an html page and run locally. It is designed for active engagement inspired by the ISLE framework, and can be used frontally or in a bring-your-own-device setting.

Our first research question was

(a) How the features of the simulation offer opportunities for students to explore and to build basic concepts of quantum mechanics?

We have presented a series of simulated experiments, which help students build these concepts on their own. The mutual exclusivity of the possible results emerges from the fact that in any experiment both sensors never blink simultaneously. The unpredictability of single results and the predictability of probability (or statistical) distribution of the results emerges from measuring a particle in a superposition position state multiple times and realizing that the sequence of the results is unpredictable, but the final distribution of the results remains the same, within statistical fluctuations. The time evolution and its patterns are discovered by performing measurements at different times, always starting from the same initial state. The time evolution is then used to differentiate states. By measuring the time evolution of states with same probability distributions, students discover that different states can have the same probability distribution. This can be used to introduce the probability amplitude as a value related to probability, but able to differentiate between states with the same probability distribution. Time evolution is also used to differentiate superposition states from statistical mixtures of states.

The effect of measurement, collapse, emerges from comparing the time evolutions of a superposition state, a statistical mixture of states, and a particle initially in a superposition state after a measurement has been performed. Students conclude that measurement transforms a superposition state into a statistical mixture of states. From this, the concept of collapse as the change of a state into the pure state consistent with the measurement result, can be easily introduced. Testing experiments for this hypothesis can be performed, for example measuring position two times in quick succession and revealing that the first and second result always match. This indicates that after the first measurement, the particle is in a pure position state so the second measurement can give the same result 100% of the time. The unpredictability of a trajectory emerges from simply measuring the trajectory multiple times. The fact that measuring the trajectory changes the final state of the system emerges from comparing the final states when trajectory measurements are performed and when they are not. It is also a natural consequence of collapse.

Introducing energy states gives a second possibility to differentiate states with the same probability distribution of position values, by comparing their probability distribution of energy values. It also allows the discovery of the uncertainty principle, as students discover that there are no states, which are pure states of position and energy at the same time. In our literature overview, we have found no other simulation capable of introducing all these concepts.

Our second research question was

(b) How successful are students in constructing the concepts of quantum mechanics using the simulation.

From the success rates presented in the tables it follows that most conclusions can be reached by more than 60% of the students without help from the instructor. The average success rate without the help of the instructor is about 70%, reaching above 90% for some activities. This indicates that the presented experiments can be used to let students construct their own ideas and concepts on quantum mechanics.

The simulation has been tested in different active engagement settings with different tasks and after the various pilots, we are confident that its usefulness is not limited to a specific course structure or didactic method. Given the success rates of high-school students, we are confident that the experiments can be implemented at university level. While the conceptual nature of the presented activities makes them particularly suited for courses where concepts are given priority, in our opinion even students in more rigorous courses could benefit from a conceptual introduction.

In setting (1)—high-school course—it took between 8 and 10 sessions of 45 min to complete the activities. However, in settings (2) and (3)—summer schools—and (4)—in-service teachers—it took four 45 min sessions. In setting (4) the same worksheets were used as in setting (1) indicating that participants with more physics background can progress through the activities faster. This leads us to believe that the experiments could be used in a regular course for physics students as an introductory active engagement module of four 45 min sessions to provide conceptual ideas on quantum mechanics and introduce terminology, before continuing to a more rigorous treatment of the topic.

A module, which uses the simulation and is based on the ISLE approach is being developed and we intend to report on it when the research is completed. With this paper, we wanted to offer the simulation to other teachers and researchers who might wish to use it to develop their own courses.

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ORCID iDs

Sergej Faletič https://orcid.org/0000-0002-5154-2868

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