

Conceptual Challenges of Discretizing Wave Functions: A Case Study

Christian D. Solorio, Elizabeth Gire

Department of Physics, Oregon State University, Corvallis, Oregon 97331, USA

To understand the conceptual challenges of discretization that students face, we present an instrumental case study of one student. This student took a junior-level quantum mechanics course and the accompanying computational lab course in the Winter 2021 term. The following year, she became an undergraduate teaching assistant for the computational lab course. Using a video elicitation interview, the participant reviewed a video clip of herself and a partner working on a kinetic energy operator computational activity. During the interview, she reflected on her understanding of discretization and identified two challenges associated with it: recognizing functions as column vectors and interpreting Δx . These challenges were productive for students in considering the nuances of discretization.

I. INTRODUCTION

The traditional position-first approach to teaching quantum mechanics uses the Schrödinger equation early on to introduce the position basis and the energy basis for the infinite square well (ISW), also known as the particle in a box. In the spins-first approach, the postulates of quantum mechanics are introduced in the context of sequential Stern-Gerlach experiments of spin-1/2 particles, which have a finite, discrete basis. The spins-first approach to teaching quantum mechanics has been shown to improve aspects of students' learning compared to the traditional position-first approach [1].

While there is good motivation for using the spins-first approach, instructors at Oregon State University have noticed students' difficulty in transitioning from discrete systems (like spin-1/2 particles) to continuous ones (like the ISW). Computation can be a powerful tool for facilitating this transition, as oftentimes continuous objects (like wave functions) and operations (like integration) must be discretized to be implemented into code. We developed a set of computational activities that introduced some of the ways continuous objects and operations can be approximated discretely. We believe that ideas of discretization can build a foundation for students and help them identify the connections between discrete and continuous systems. To explore this, we ask the following:

Research Question: *What are the conceptual challenges of discretization that students engage with?*

We answer this question by presenting an instrumental case study of a student, Mary (a pseudonym), who experienced a discretization-focused computational activity as both a student and an undergraduate teaching assistant (TA). Our qualitative analysis highlights some of the challenges of discretization students encounter and the productive elements of those challenges. This case study will inform the ways that instructors can support students' productive ideas of discretization, which may have implications for students' building connections between discrete and continuous quantum systems.

A. Instructional Context

Upper-division physics students at Oregon State University take an intensive five-week long, seven-contact-hour quantum mechanics course called Paradigms in Physics: Quantum Fundamentals. This course uses a spins-first approach to introducing quantum mechanics and the course ends with the ISW. In the Winter 2021 term, students concurrently took a computational physics lab course where they used numerical methods to solve quantum mechanics problems. Due to the ongoing COVID-19 pandemic during the Winter 2021 term, both of these courses were taught over Zoom.

B. Broader Research Context

In the Winter 2021 term, Mary was longitudinally observed by one of the authors in the computational lab course. One year later in the Winter 2022 term, Mary became a TA for the computational lab course. The rapport developed between Mary and the observing author perhaps helped her feel more comfortable sharing her thoughts during the interview. Additionally, the rapport was helpful during the analysis process because the authors had the additional context of Mary's experiences as a student.

II. METHODS

A. Video Elicitation Interview

In the Winter 2022 term, we conducted an in-person, one-hour-long, semi-structured interview with Mary. The interview employed video elicitation [2], also known as stimulated recall [3–5] where a participant views a video of themselves during an event. This method typically results in participants recalling their understandings and feelings and reflecting on their thoughts and actions during an event [2].

During the interview, Mary watched a 10-minute video clip of herself as a student working with a partner, Dave (a pseudonym), on a computational activity (described later in this section). Following the interview protocol, the video was paused at particular time stamps, and Mary was asked to reflect on the portion of the clip she saw, compare her understanding as a student and as a TA, and describe how she would assist students who had questions about the activity.

This interview differs from other video elicitation interviews in that the events of the video clip and the interview take place a year apart. Lyle suggests video elicitation interviews happen soon after the recorded event so that the study participant can better recall their thoughts and experiences [3]. At a few points during the interview, Mary mentioned not remembering what she thought in the moment as a student in the video clip. Because of this, the perspectives she gave during the interview were likely more informed by her experience as a teaching assistant rather than as a student.

Data captured during the interview included video and audio recordings of Mary, video of a nearby whiteboard that Mary wrote on during the interview, and a screen recording of the video clip. The interview was transcribed and reviewed to identify salient experiences, understandings, and perspectives that Mary shared related to our research question.

1. Activity Description

The computational lab course consisted of four activities in the quantum mechanics context developed by the instructor and one of the authors. Each activity of the computational lab course was related to the ISW. The third activity of the

computational lab course, taking place before students were introduced to wave functions in the Quantum Fundamentals course, focused on finding the eigenvalues and eigenvectors of the finite-difference approximation of the kinetic energy operator [6]. The goal of the activity was to demonstrate how a differential operator can be implemented computationally using a finite difference approximation and how wave functions can be discretized.

Students were tasked with first coding a matrix to represent the finite difference approximation of the kinetic energy operator $\hat{T}$. Students were given the equation below to show how the approximated operator acts on a wave function. The equation below shows the finite difference approximation of the kinetic energy operator $\hat{T}$ matrix acting on a wave function, represented by a collection of coefficients $\psi(n\Delta x)$ in a column vector.

$$\begin{pmatrix} \hat{T}\psi(\Delta x) \\ \hat{T}\psi(2\Delta x) \\ \hat{T}\psi(3\Delta x) \\ \hat{T}\psi(4\Delta x) \\ \vdots \end{pmatrix} = \frac{\hbar^2}{2m\Delta x} \begin{pmatrix} 2 & -1 & 0 & 0 & \dots \\ -1 & 2 & -1 & 0 & \dots \\ 0 & -1 & 2 & -1 & \dots \\ 0 & 0 & -1 & 2 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \psi(\Delta x) \\ \psi(2\Delta x) \\ \psi(3\Delta x) \\ \psi(4\Delta x) \\ \vdots \end{pmatrix}$$

Students were then asked to calculate the eigenvalues and eigenvectors of the $\hat{T}$ matrix and to observe what happens when the size of Δx is decreased. Because the ISW has a defined length, decreasing the step size Δx will increase the number of steps required to iterate over the entire box, resulting in a $\hat{T}$ matrix and a wave function column vector with more entries.

2. Video Clip Description

The video clip Mary watched during the interview opened with the observer asking Mary and Dave how the length of the ISW, the size of Δx , and the number of entries in the wave function column vector correspond to each other. The pair then looked at their wave function column vector composed of $\psi(\Delta x)$, $\psi(2\Delta x)$, $\psi(3\Delta x)$, and so on. They noticed that the number of entries in that vector did not change as they varied the step size Δx or the length of the square well. Mary was confused as to why that should be the case and Dave attempted to explain why through verbal descriptions and drawings.

B. Analysis

We used an instrumental case study to analyze Mary's interview responses. In instrumental case studies, a particular case is used to provide insight into a larger issue [7]. The case we present is that of a student, Mary, who has done a computational activity focused on discretization as both a student and a TA. We present two conceptual challenges that students

face when introduced to discretization identified by Mary during the video elicitation interview. This case will give further insight into the challenges students face in transitioning from working with discrete quantum systems like spin-1/2 particles to working with continuous quantum systems like the ISW.

Mary may be considered an extreme case [8] or an unusual case. She was part of a larger research project on the computational lab course and happened to later become a TA for that same course. She saw the course material multiple times with new coding and physics expertise being developed between taking the course as a student and being a TA for the course. This gave her more experience with the kinetic energy operator activity and a perspective that most students in the course would not have. Consequently, Mary was particularly valuable to interview because she gave the authors insights into the challenges of discretization that most students would not be able to articulate.

III. RESULTS: CHALLENGES OF DISCRETIZATION

The purpose of this case study is to highlight some specific struggles students face when engaging with discretization in a quantum mechanics computational activity. During the interview, Mary identified two challenges of discretization. The first was centered around the difficulty of recognizing that functions can be represented as a column vector with a finite number of elements. The second was centered around students' interpretation of Δx . She identified both these challenges to be productive for her understanding of wave functions and discretization.

In the following presentation of the challenges, all of the quotes are from Mary during the Winter 2022 (W22) interview rather than from the Winter 2021 (W21) observational video clip of her as a student.

A. Functions as Discrete Column Vectors

Of the four computational quantum mechanics activities, the kinetic energy operator activity was the first that required students to recognize wave functions can be represented as a column vector. Mary identified this as a challenge of discretization. During the interview, Mary stated that "...it's hard to think about what it even means to have the wave function in a matrix form and like have an operator in matrix form." Later in the interview, she described how the code she and Dave wrote approximates a wave function.

Mary: "Yeah, so we're approximating a continuous psi, which is an eigenfunction. We're approximating it with a discrete representation and rather than having some infinitely long set from like — er, yeah, infinite breaking up from 0 to L, because it is a particle in a box, it's not from negative infinity to infinity. But like we're breaking it

up into — we're only taking certain points along the line."

She described that typically the wave function has a defined value at each position along the length of the ISW, resulting in an uncountable infinite collection of coefficients. In the discretized case, however, she stated that the wave function is being approximated by sub-sampling the infinite set of coefficients. This allows the wave function to be represented by a finite set of coefficients. In the W21 observation video, she reached the same conclusion, but she more clearly articulated the approximation aspect of this during the W22 interview.

Part of the activity required plotting the eigenfunctions of the kinetic energy operator. Mary had identified this task as "unintuitive" in the following description.

Mary: *If you fed in $np.arange$ from 0 to L and just any number of x , you wouldn't have enough values for your eigenfunction to plot versus, so it would run an error on the code. That is very unintuitive for someone who's like 'Well, I should just be able to plot a function, and if you just give it any x value it should be able to spit something out.' There's just a lot of elements to it that are confusing I think.*

Because the wave function and kinetic energy operator had been discretized in the code, the calculated eigenfunctions had to be plotted against "certain points along the line". She described this as being unintuitive because typically wave functions have a value at every point along the length of the ISW, but the discretized wave function does not. In both the W21 observational video and the W22 interview, she found the challenge of understanding a wave function as a column vector productive to her understanding of discretizing a wave function. In particular, she noted her experience as a TA for the course helped her recognize that the size of Δx corresponded to how well the wave function was being approximated. She did not remember learning this in W21.

B. Interpreting Δx

In the W21 observational video, Mary was confused about why the number of elements in the discretized wave function changed with the value of Δx . Her partner, Dave, then drew a representation of the system on their shared virtual whiteboard, shown in Fig. 1. During the W22 interview, Mary was asked about her thoughts on Dave's drawing. She drew a plot on the whiteboard as shown in Fig. 2 and said:

Mary: *"I think just seeing Δx on a page is nice, because then you're like, 'Okay, what was Δx supposed to be?'. Um, except for that what I'm learning now is that Δx isn't actually like on a bar graph where you have between two points [sic]. It's literally just a point on the graph."*

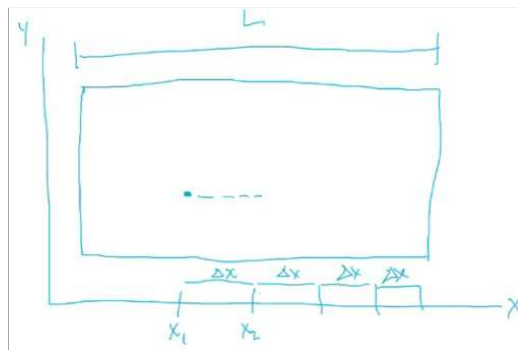


FIG. 1. Dave drew a graphical representation of the particle in a box and labeled Δx as the spacing between points x_1 and x_2 for the length of the box.

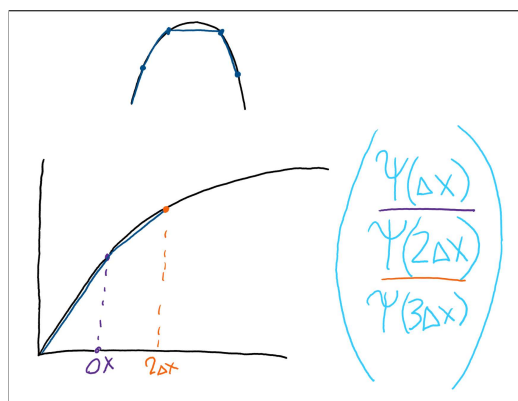


FIG. 2. During the interview, Mary drew a graphical representation of a wave function and discretized wave function. She used color to show how the element of the column vector corresponded to a point on the graph of the wave function.

In this quote, Mary reflected that Dave's drawing was helpful because it labeled what Δx was in relation to the length of the ISW. She then identified two interpretations of Δx that could impact one's understanding of the discrete wave function. The first was an understanding of Δx as the space "between two points", as reflected in Fig. 1. She compared this to a bar graph, where the bars occupy a space between two points. The second interpretation she offered, as drawn in Fig. 2, was that Δx , $2\Delta x$, etc. were single points with uniform spacing along the length of the ISW. In the W22 interview, Mary shared that as a TA she saw some students in the computational lab course use the "space between points" (SBP) interpretation and others use the "single point" interpretation. Mary noted that she had the SBP interpretation of Δx in the W21 observational video, but after an additional year of experience she developed the "single point" interpretation.

The SBP interpretation of Δx had implications on how Mary and Dave thought about other parts of the activity. Specifically, it affected how they understood $\psi(\Delta x)$ and how they graphically represented the ISW. Even with these implications, Mary reflected that the SBP interpretation was pro-

ductive for her in the W21 observational video because it helped her visualize the problem and connect the size of Δx to the number of elements in the discretized wave function.

The SBP interpretation of Δx introduced challenges to understanding $\psi(\Delta x)$ as a value of a function. During the interview, Mary said the following:

Mary: “[The instructor] just showed this in class where you have $\psi(\Delta x)$, $\psi(2\Delta x)$, $\psi(3\Delta x)$ and so on. And that would map to a discrete point on the curve [underlines $\psi(\Delta x)$ in purple and marks Δx on the plot in Fig. 2]. Like this is Δx and then this’d be some $2\Delta x$ [underlines $\psi(2\Delta x)$ in orange and then marks $2\Delta x$ on the plot in Fig. 2]. So then, I guess, I didn’t understand...why a discretized representation even worked. Like it isn’t a one-to-one, it’s just an approximation of the curve. I don’t think I had any understanding of that.”

She reflected that in W21 as a student with the SBP interpretation, she did not fully understand how to coordinate the discretized wave function with a plot of the wave function vs. position. With the understanding that Δx is a space between points, it was not clear to her in W21 how to evaluate $\psi(\Delta x)$. After experiencing the activity for a second time, in the W22 interview, Mary noted that the “single point” interpretation of Δx helped her understand that $\psi(\Delta x)$ is the wave function evaluated at a point.

Mary did, however, reflect that the SBP interpretation was productive for her and her partner. As shown in Fig. 1, Dave’s drawing of the ISW labeled Δx as the space between points. In the W21 observational video, the drawing helped Mary understand “breaking up L into Δx ” and how changing Δx would change the number of entries in the discrete wave function. Mary was asked to reflect on the drawing during the W22 interview. She explained that even though the drawing was not completely physically accurate, it did help her in W21 to understand the connection between Δx and the discrete wave function. Additionally, she noted the characteristics of the drawing that might be inaccurate or confusing for students, such as the x- and y-axes and the box not being aligned with the origin.

IV. DISCUSSION AND CONCLUSION

We have presented two challenges of discretizing wave functions in a quantum mechanics computational activity as highlighted by a participant who has experienced the computational activity as a student and as a TA. The kinetic energy operator computational activity was productive and valuable in light of these challenges, as it encouraged students to engage with some of the nuanced ideas of discretization.

The first challenge we identified was in representing functions as discrete column vectors. A wave function, an un-

countably infinite collection of points, can be approximated with a finite set of points. Recognizing that wave functions are, by definition, a collection of points may be one of the reasons that the idea of discretization was challenging. According to an analysis of the structural features of quantum notations [9], wave function notation exhibits a low degree of individuation while matrix notation exhibits a high degree of individuation. Individuation refers to how well the important features of an object are represented as elemental pieces of a whole in a given notation. The uncountably infinite set of points comprising the wave function is obfuscated, which makes it more difficult to see how a function could possibly be represented by a column vector.

The second challenge was interpreting Δx . Some students interpret it to be the space or gap between points rather than a point. This led to some difficulty in understanding $\psi(\Delta x)$ as a value function and manifested in the graphical representation of the ISW. Mary mentioned that the course instructor drew a plot similar to the one in Fig. 2 that highlighted the connection between the Δx in the column vector and in the plot of a wave function. She said that this was helpful for orienting students to the activity, but it did not completely eliminate some students from understanding Δx as the space between two points. The “single point” interpretation of Δx was particularly productive for Mary as a TA because it allowed her to coordinate the discretized wave function with a graphical representation of the ISW.

We believe this study has further implications for highlighting the ways that continuous quantum systems like the ISW relate to discrete quantum systems such as spin-1/2 particles. Activities centered around turning a continuous object into a discrete object may illuminate the ways that common calculations like inner products, probabilities, and time evolution are isomorphic for discrete and continuous quantum systems. For example, writing Python code that calculates the inner product of two wave functions would require writing an integral as a sum, resembling an inner product for a spin-1/2 system.

We offer some implications for instructors, as informed by our study. Terms like Δx may carry connotations from previous courses which can affect students’ interpretations of them in a new context like a computational course. Additionally, providing multiple representations of wave functions (graphs, code, function representations, matrix representations, etc.) encourages students to consider the role of Δx in discretization. The study also provides evidence that students may benefit from additional instruction on the similarities of functions and vectors to facilitate students’ understanding of how a wave function can be represented as a column vector.

ACKNOWLEDGMENTS

This work is funded by the NSF DUE 1836604 and 1836603.

-
- [1] H. R. Sadaghiani, Spin First vs. Position First instructional approaches to teaching introductory quantum mechanics, in *The Proceedings of the Physics Education Research Conference* (Sacramento, 2016).
- [2] S. G. Henry and M. D. Feters, Video Elicitation Interviews: A Qualitative Research Method for Investigating Physician-Patient Interactions, *The Annals of Family Medicine* **10**, 118 (2012).
- [3] J. Lyle, Stimulated Recall: A report on its use in naturalistic research, *British Educational Research Journal* **29**, 861 (2003).
- [4] N. P. Dempsey, Stimulated Recall Interviews in Ethnography, *Qualitative Sociology* **33**, 349 (2010).
- [5] N. T. Nguyen, A. McFadden, D. Tangen, and D. Beutel, Video-Stimulated Recall Interviews in Qualitative Research, in *The Proceedings of the AARE Annual Conference* (Adelaide, 2013).
- [6] D. Roundy, [Kinetic energy](#).
- [7] R. E. Stake, *The art of case study research* (Sage Publications, Thousand Oaks, CA, 1995).
- [8] B. Flyvbjerg, Five Misunderstandings About Case-Study Research, *Qualitative Inquiry* **12**, 219 (2006).
- [9] E. Gire and E. Price, Structural features of algebraic quantum notations, *Physical Review Special Topics - Physics Education Research* **11**, 020109 (2015).