Discretizing wavefunctions for code is challenging and conceptually rich

Discrete and Continuous Challenges in Quantum Mechanics: A Reflective Interview

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Introduction

- Spin-first approach to teaching QM at OSU
- Connections that students make between discrete bases and continuous bases are unclear
- Wavefunctions are necessarily discretized in computer code when performing operations like integration
- Developed a computational lab course that is centered on wavefunctions
- **RQ:** What challenges about discrete and continuous quantum bases do students encounter in a computational lab course?

Reflective Interview

- Mary was a student in a computational physics course in 2021 and became a TA for that course in 2022
- Conducted a video elicitation interview with Mary using observational video data from when she was a student
- Video Context
  - Mary and her partner were doing a computational activity about the kinetic energy operator
  - The pair was told that the kinetic energy operator matrix should depend on Δx, but that was not reflected in their code
  - They began to discuss why in the context of the discrete psi column vector (see Figure 2) which would have the same number of rows as the kinetic energy operator
- Asked questions about her thought process during the observation and now after being a TA

> "…what I'm learning now is that delta x isn't actually like, not like on a bar graph where you have between two points, it's literally just a point on the graph. Like on this one that I drew [Fig. 2] it's not, it's not like a bar chart thing where you have a space it's just one point so even that might lead to misunderstanding about what our representation [Fig. 1] is"

> "[The instructor] just showed this in class where you have psi of delta x, psi of two delta x, psi of three delta x and so on. And that would map to like, um, like this one would map to a discrete point on like, the curve [underlines ψ(Δx) in purple and marks Δx on the plot in Fig. 2]. Like this is delta x and then this'd be some two delta x… 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."

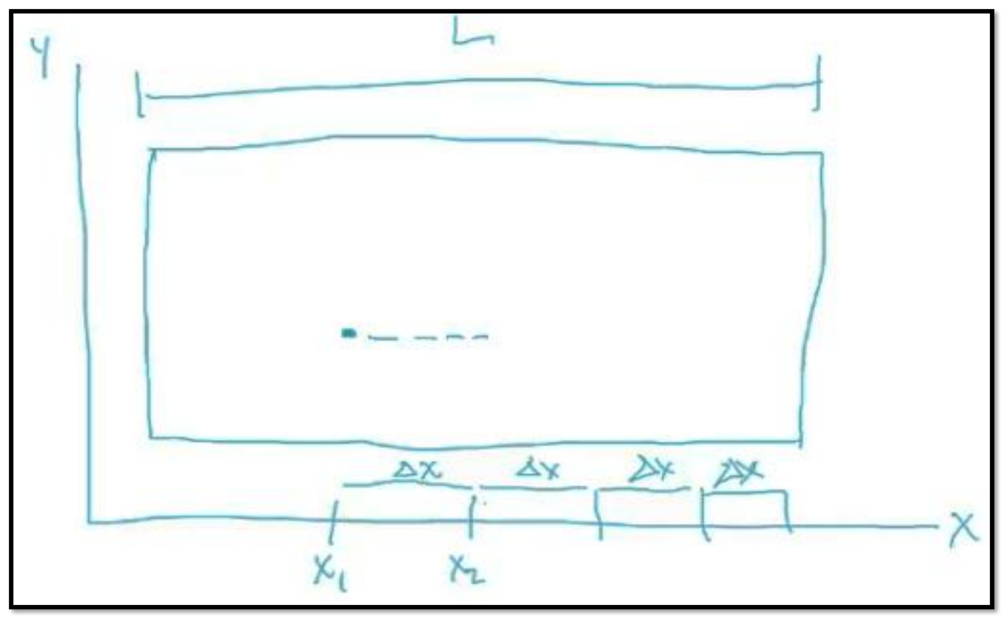

Fig. 1: A representation of a particle in a box drawn during the observational video.

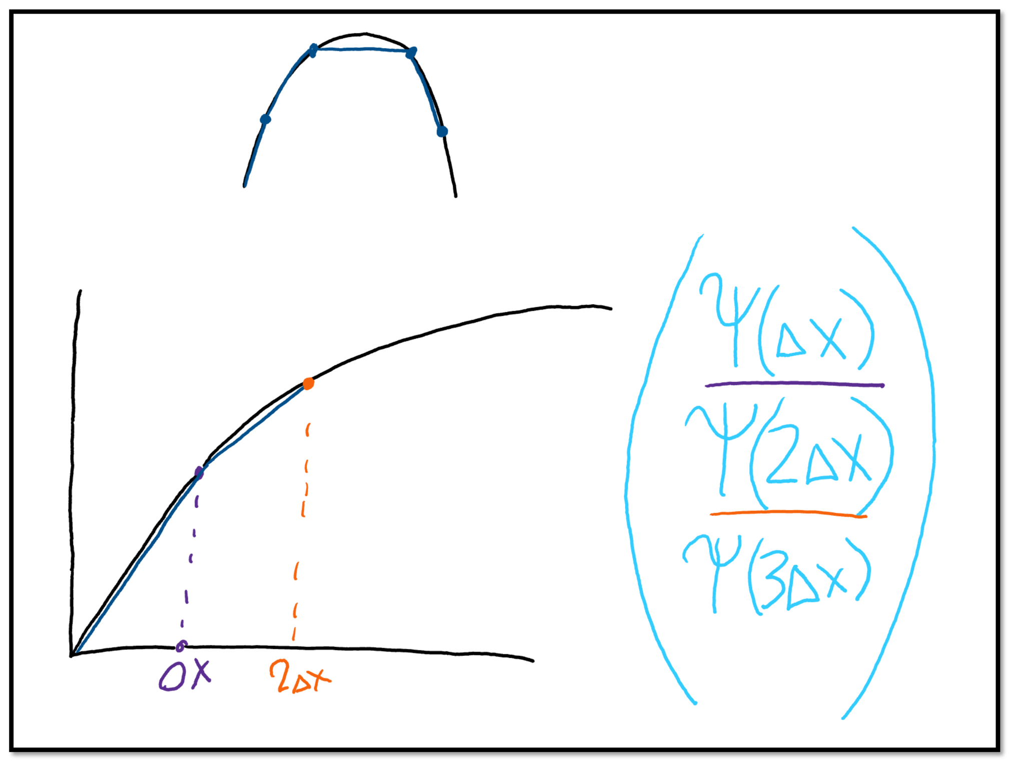

Fig. 2: A graphical representation of the discrete psi column vector drawn by the participant during the interview

Discrete to Continuous Challenges

Interpreting Δx

- Mary described two interpretations of Δx
  - The separation between points measurements (Figure 1)
  - A particular point on a graph (Figure 2)
- Δx is often used in the context of displacement rather than as a specific point

Recognizing $\psi(\Delta x)$ as value of a function

- Understanding $\psi(\Delta x)$ to be the wavefunction evaluated at Δx is challenging when Δx is understood to be the space between points

Writing a function as a column vector

- Discretized representations can't take any input, they must take integers of Δx
- Discretization means they are not "one-to-one", i.e., discretized wavefunctions are approximations

Representing the Particle in a Box

- "Box" has a 2-D connotation
- Drawing the "location" of the particle is not intuitive
- Labelling Δx on the box was productive reasoning that helped Mary understand the discrete psi matrix

Conclusions & Instructional Implications

- Discretizing a wavefunction encourages students to think about connections between discrete and continuous bases
- Students seek coherence between their code and physical understanding of a system

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