# Chemistry Graduate Students' Problem Solving With Quantum Mechanical Models: "What Do I Plug in for Delta?"

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*In the chemistry curriculum, physical chemistry stands out as one of the most challenging given its reliance on calculus, particularly when using quantum mechanics to describe atomic and molecular structure. Though there is literature in chemistry education research that investigates students' conceptions of quantum chemistry, few of these studies focus on students' use of mathematics in this context. To this end, we interviewed graduate students (N = 23) about the "particle-in-a-box", one of the first quantum models discussed in physical chemistry. Preliminary analysis investigates phenomenographical categories of students' problem-solving strategies and their affective responses to the problem-solving task.*

*Keywords:* chemistry, quantum mechanics, calculus, interdisciplinary

There are few studies in the chemistry education literature that specifically focus on students' conceptualizations of quantum mechanical models (McAfee et al., 2025), and though these articles provide a great foundation for further research, they do not explicitly investigate students' use of mathematics. This gap does not insinuate that quantum mechanics is taught in chemistry without mathematics, but rather that chemistry education research often borrows findings from physics education research to contextualize students' conceptualizations of quantum mechanics. To this end, the aim of our study is understanding how students apply quantum mechanical models when problem-solving. For our study, we conducted semi-structured interviews with chemistry graduate students (N = 23) who received $50 gift cards for participating in a two-hour-long, in-person interview.

Preliminary data analysis, guided by phenomenography, focused on two major components of the graduate students' problem-solving: (1) their performance on the problem, and (2) their affective responses to solving the problem in front of a peer. To better understand their treatment of the molecule in the problem, we generated a rubric with a normative application of the particle-in-a-box model in which points were assigned to the graduate students' work based on correct decision-making during the task. The variation in model application shone through in the students' treatment of variable $a$, in which they needed to calculate the length of the molecule. Notably, none of the students applied the model completely normatively which speaks to the immense challenge quantum mechanics poses to students.

During the interviews, we noticed many affective responses from the graduate students such as nervous laughter, screams, qualifiers, etc. Given this, we inductively coded these responses which we frame as observed indicators of stress. Taken together with their problem-solving, three groups of students have emerged: (1) high performers with low observed indicators of stress, (2) low performers with low observed indicators of stress, and (3) low performers with high observed indicators of stress.

For next steps, we are interested in expanding our analysis to further understand the affective responses we observed form the graduate students and further describe the emergent phenomenographical groups.

## References

McAfee, S. C., Watts, F. M., & Rodriguez, J.-M. G. (2025). A review of research on the teaching and learning of quantum mechanics. *Chemistry Education Research and Practice*, *26*(3), 578–593. https://doi.org/10.1039/D5RP00030K