A Systematic Review of the Teaching and Learning of Quantum Mechanics: Implications for Mathematics Instruction and Research on Undergraduate Mathematics Education

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In this work, we review the literature on the teaching and learning of quantum mechanics situated in chemistry courses with the aim to provide a tool for education researchers and practitioners. We found that much of the research on quantum mechanics in the chemistry context involves students at the secondary level of instruction. Along with this, much of the research leans on mathematics and physics education research to support the claim that students have difficulties with mathematics; however, these claims require further investigation within chemistry education research.

Keywords: Quantum Mechanics, Chemistry, Interdisciplinary

Introduction

Physical chemistry is an upper-division course in the undergraduate chemistry curriculum that is notoriously challenging for students as it broadly focuses on three fundamental chemical concepts: kinetics, thermodynamics, and quantum mechanics (Holme, 2023). Briefly, kinetics is the study of rates of chemical reaction, thermodynamics is the study of energy and its movement in chemical systems, and quantum mechanics is the modeling of atomic and molecular structure. Many studies have been conducted investigating how students learn about thermodynamics (Bain et al., 2014) and kinetics (Bain & Towns, 2016) and have been reviewed to provide a tool for instructors and researchers teaching physical chemistry. In the review on thermodynamics, Bain et. al (2014) found that the literature investigating thermodynamics often posed alternative conceptions for the laws of thermodynamics, along with factors related to success in physical chemistry. Another finding in this study was that many papers focused on the mathematics used in physical chemistry, posing the need for interdisciplinary research collaborations. In Bain & Towns (2016), when reviewing chemistry education research on kinetics, they found that kinetics studies largely focus on secondary-level students' reasoning about chemical concepts. Along with this, they once more call for cross-disciplinary research, specifically between chemistry and mathematics, on students' reasoning of related rates and graphical representations (Bain & Towns, 2016).

The remaining topic in physical chemistry, quantum mechanics, has yet to be reviewed with a focus on the teaching and learning in chemistry contexts; however, outside the context of chemistry, quantum mechanics is a content area that has been widely studied in physics education. For example, a review of the physics education research regarding quantum mechanics found that students have difficulties understanding chemical concepts such as wave-particle duality, wave functions, and atomic structure. Along with this, students were found to have conflating ideas about classical and quantum mechanics (Krijtenburg-Lewerissa et al., 2017).

With this in mind, we aim to synthesize the chemistry education literature that investigates the teaching and learning of quantum mechanics in a chemistry context, with the goal of sharing our implications for practitioners and researchers. In this review, we identify the areas for further research and provide a detailed outline of the mathematical concepts and skills that are utilized in physical chemistry to provide insight to undergraduate-level mathematics instructors.

Data Collection and Analysis

Our approach for identifying articles to include in this review followed guidelines for reporting systematic reviews (Page et al., 2021). Articles were required to be peer-reviewed, empirical research studies (i.e., with research questions/aims, methods, and findings) that primarily focused on quantum mechanics topics, including both secondary and tertiary educational contexts. An overview of the data collection is provided in Figure 1. We searched the ERIC database, *Chemistry Education Research and Practice (CERP),* and the *Journal of Chemical Education (JCE)* using the search terms "chemistry" and "quantum mechanics", with our search last updated on January 13, 2025. After removing duplicates and articles that did not meet the inclusion criteria, we iteratively reviewed the citations and included additional articles that were within the scope of the review. In all, N = 50 articles were included in the review.

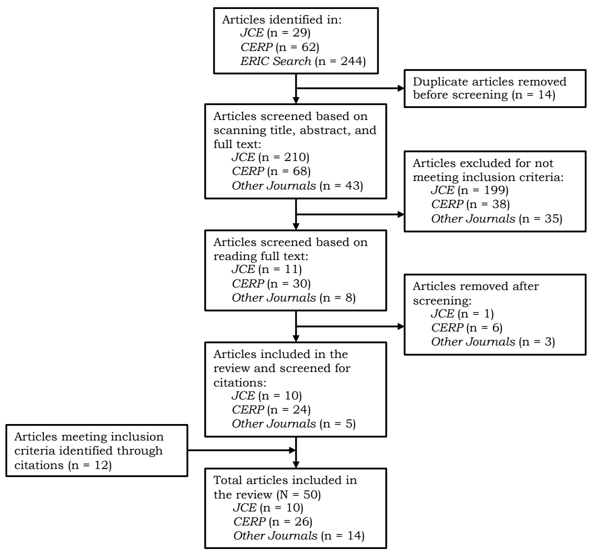

Figure 1. A PRISMA flow diagram detailing the article selection process. JCE is the Journal of Chemical Education, CERP is Chemistry Education Research and Practice, and ERIC is the Education Resources Information Center.

Once the dataset was finalized, we read the articles and grouped them based on the main topics of the articles. Throughout the process of reading the included articles, we took detailed notes and memos on the key findings to identify preliminary categories that arose. The first three categories that emerged were related to the quantum chemical concepts that the articles investigated: (1) Students' reasoning related to atomic and molecular structure; (2) Students' reasoning related to spectroscopy; and (3) Students' reasoning related to commonly discussed quantum mechanical models (e.g., particle-in-a-box, quantum mechanical harmonic oscillator, etc.). Any article that mentioned multiple categories (i.e., students' interpretations of the particle-in-a-box quantum mechanical model and atomic structure) was included in both relevant categories. In consideration of space, we will only discuss findings related to students' interpretations of quantum mechanical models, contextualizing it for the mathematics education research community.

Preliminary Findings

Overview of the Data

The findings presented in this section discuss the preliminary categories stemming from analysis of the data. To begin, we briefly provide an overview of the sample. We found that 48% (n = 24) of the articles used qualitative methods, 6% (n = 3) of the articles used quantitative methods, and 46% (n = 23) were mixed-method. Along with this, we identified the country that where the research was conducted, along with the associated participants' level of instruction. Most of the studies in our review were conducted in the United States (40%, n = 20) with many conducted in Greece (28%, n = 14). As for level of instruction, we found that articles typically involved students in introductory chemistry courses (Figure 2); however, a notable number of the articles investigated students' reasoning at the secondary level.

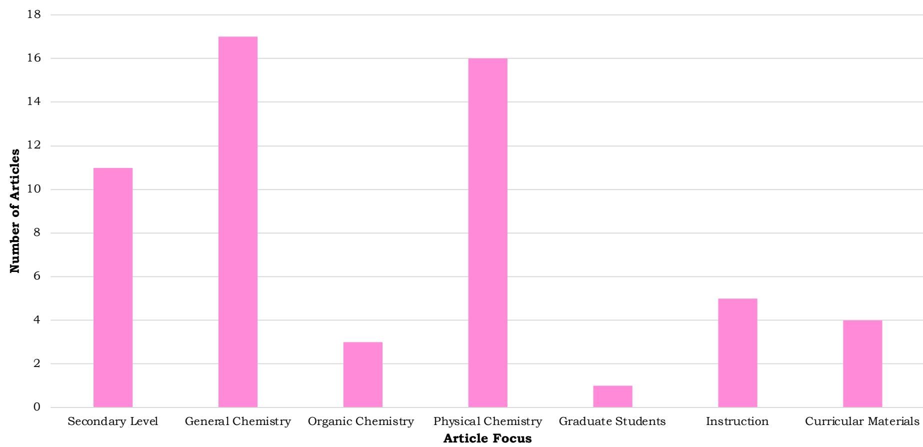

Figure 2. A bar graph showing the focus for each article. The total number of articles in this graph is greater than number of articles in the review, since each article may have multiple datasets.

Students' Reasoning About Commonly Discussed Quantum Mechanical Models

We discuss the key findings related to how students reason about common quantum mechanical models that are presented in a physical chemistry course. Though there are few, for clarity, we structure our discussion around the quantum mechanical model that is under focus.

Particle in a Box. Three articles in the sample focused on students' interpretations of the particle-in-a-box quantum mechanical model (Beck et al., 2020; Muniz et al., 2018; Muniz & Oliver-Hoyo, 2014). This model is often used in physical chemistry courses when introducing quantum theory to students as it describes the translational movement of a particle in a theoretical, one-dimensional box. To describe the particle's movement, students are taught their first application of the Schrödinger Equation, which is an eigenfunction that involves the use of partial derivatives. This eigenfunction takes the sum of the particle's kinetic and potential energy, called the Hamiltonian, and multiplies it by a wavefunction to produce the energy eigenvalue of the model. However, for the particle in a box model, the particle is assumed to have no potential energy, only kinetic energy. During classroom discussions, it is common in physical chemistry courses to discuss the mathematical treatment necessary to normalize and square the wavefunction to find the probability of locating the particle in its one-dimensional box which can be difficult for students. This typically includes walking through partial derivatives and integrations of the wavefunction with students. When students are learning about the particle-in-a-box model, there are many difficulties that have been identified in the literature. The primarily reported challenge is students' conceptualizing that more complex models are more suited, or more accurate, than simpler models (Muniz et al., 2018). Students were also found to struggle with the representations that are used in this model (e.g., eigenfunctions, etc.)

along with conceptualizing the meaning of quantum number *n* (Muniz & Oliver-Hoyo, 2014). It was also observed that students tended to conflate the particle-in-a-box model with other models, which leads to misapplications of the model to real-world phenomena (Beck et al., 2020; Muniz et al., 2018).

Quantum Mechanical Harmonic Oscillator. There were a few studies that investigated students' interpretations of another model, the quantum mechanical harmonic oscillator (Beck et al., 2020; Muniz et al., 2018). This model is another fundamental quantum mechanical model that describes the vibrational movement of particles, which is often taught after students learn about the particle-in-a-box model and requires a similar mathematical treatment. The main difference with this model from the previously described particle-in-a-box model is that vibrational movement requires students to consider how to model kinetic and potential energy with the Schrödinger equation. As discussed previously, students have shown difficulties with model application and model conflation (Beck et al., 2020; Muniz et al., 2018). Along with this, students tended to avoid mathematizing models when possible (Muniz et al., 2018), and when they do use math, they focus primarily on surface features of quantum mechanical models, both lexical (e.g., the language used when describing the model) and complex (e.g., the intensity of the mathematics that is shown in the model) (Muniz et al., 2018). When describing the kinetic and potential energies of the harmonic oscillator, students used classical mechanics to build explanations (Beck et al., 2020).

Two-Dimensional Rigid Rotor. There were a few studies that investigated students' interpretations of the two-dimensional rigid rotor model (Beck et al., 2020; Muniz et al., 2018). The two-dimensional rigid rotor is taught sequentially after the quantum mechanical harmonic oscillator. This model describes the rotational movement that a particle can experience. This model requires a similar mathematical treatment of the Schrödinger equation, including the use of the potential energy component of the Hamiltonian. The main difference in the mathematical treatment of this model is that it includes polar coordinates in the wavefunction. In these studies, students were found to conflate vibrational and rotational motion when applying the model (Beck et al., 2020; Muniz et al., 2018). When using the two-dimensional rigid rotor system to predict and explain molecular rotation, students were found to focus on incorrect aspects of the model causing misapplication of the model (Beck et al., 2020).

Discussion and Next Steps

The three quantum mechanical models described above are not the only models that physical chemistry students learn. After instruction on these introductory models, students move on to find the analytical solution to the hydrogen atom using the Schrödinger equation, discuss the challenges with quantum mechanics that arise with the three-body problem, and learn approximation methods that allow for exact solutions to the Schrödinger equation when modeling multi-electron atoms. As can be seen in our findings, there is a need in the literature for more studies that investigate students' interpretations of the models in physical chemistry.

The models that are taught in physical chemistry require a robust amount of mathematics skills. However, the included studies rarely investigated students' conceptualizations or reasonings regarding the mathematics that they are applying in physical chemistry. When comparing our quantum mechanics review to the quantum mechanics reviews that exist in physics education literature (Krijtenburg-Lewerissa et al., 2017), there is a jarring difference in the way mathematics is discussed. In the physics education reviews on quantum mechanics, findings from investigations conducted on students' use of specific mathematical operations are discussed in detail whereas these findings are largely absent from our review. Instead, the articles in our sample rely on this prior work as support for understanding and explaining physical chemistry students' difficulties with quantum mechanics.

Although physics and mathematics education research has provided a clear pathway and foundation for this research, there is a need for more research investigating chemistry students' interpretation and use of the mathematics present in physical chemistry courses. Considering the interdisciplinary nature of the topics in physical chemistry, it is necessary for more interdisciplinary education research to be conducted on these topics. With more interdisciplinary research collaboration, a better understanding of students' difficulties with the content in physical chemistry may provide new pathways for instruction. For instructors, we have presented on the mathematics concepts and skills that are relied upon in physical chemistry to clarify how they are used in chemistry courses. The next step for our project includes analyzing the remaining categories that emerged in our study to further review the chemistry education literature related to the teaching and learning of quantum mechanics.

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