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The Quantum Mechanical Particle-in-a-Box Experiment—A Revisit Using NMR Spectroscopy

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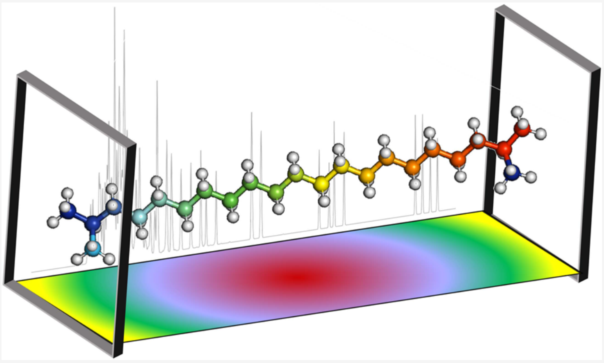

ABSTRACT: The particle-in-a-box experiment is a well-known method used to teach quantum mechanics concepts in physical chemistry laboratories for undergraduates. The investigation involves measuring the wavelength at maximum absorbance (λ_{max}) of electronic transitions in the UV−vis spectrum and linking it to the box length. As the electronic configurations directly influence the nuclear shielding, a computational approach to estimate the nuclear magnetic resonance (NMR) chemical shifts is shown to relate to the box length. This work revisits what Flewwelling and Laidlaw suggested over 50 years ago: NMR chemical shifts can indirectly be related to the box's length via electron density calculations. For a series of molecules (polyenylic ions) of increasing carbon chain length, the activity allows the students to develop a broader understanding of how Schrödinger's equation for a particle in a box model, electron density calculations, and NMR spectroscopy are all connected at the atomic level. Additionally, the open-ended computational procedure leverages easily accessible tools to estimate NMR chemical shifts, and this approach is suitable as a viable remote learning exercise that supplements traditional UV−vis experiments.

KEYWORDS: *Upper-Division Undergraduate, Physical Chemistry, Computer-Based Learning, Remote Learning, Particle-in-a-Box, Quantum Mechanics, NMR Spectroscopy*

INTRODUCTION

The particle-in-a-box model is a simple yet effective way to introduce undergraduate chemistry students to the Schrödinger equation and the principles of quantum mechanics. Moreover, this model can be applied to a physical chemistry experiment called the particle-in-a-box experiment, which uses the absorption spectra of polymethine dyes to determine the length of a one-dimensional box.[1,2] The apparent box length estimated in this exercise allows the students to relate the basics of the system's wavefunction, and the energy levels (eigenvalues) truly represent the boundary conditions of the Schrödinger equation. This topic has garnered much interest in this *Journal*, with over 25 manuscripts discussing the particle-in-a-box model, including the system's symmetry and degeneracy,[3−5] improved selection of molecules,[6−9] and expanded applications of the model.[10−15]

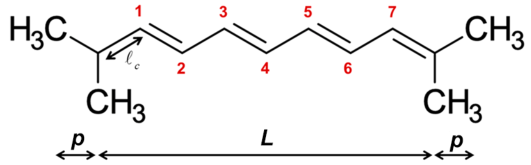

Figure 1. Theoretical estimation of the chain length. L is the calculated chain length from the average C−C bond length, and p is the penetration depth. The conjugated carbon atoms are numbered from left to right.

Delocalized electrons in a conjugated π-system can be approximated using the particle-in-a-box model by confining its location within the walls of a 1D horizontal box that spans the length of the conjugated chain, as shown in an example in Figure 1. To determine the experimental length of the conjugated π-system for linear carbon chain molecules like cyanine dyes,[2] polyenes,[6,16] or polyynes,[7,17] the wavelength of maximum absorbance in a UV−vis spectrum (λ_{max}) is related to the lowest energy transition. This experimental length is then compared to the calculated length of the molecule from its molecular structure, as shown in Figure 1, to validate the model system. However, the model's accuracy depends on the molecules chosen.[10]

During the recent pandemic, remote learning has become essential for online laboratory experiments. Although UV−vis spectroscopy is still practical and vital, this article focuses on

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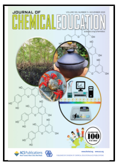

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Table 1. Molecules Used to Model the Quantum Mechanical Particle-in-the Box

PiB Model	Molecule (ion)	SMILE-Format	Number of conjugated carbons (n_c)	Number of electrons (n_e)	λ_{max} (nm) calculated
1	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 2$	CC(C)C=C(C)C	3	2	272.34
2	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 3$	CC(C)=CC=CC(C)C	5	4	316.10
3	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 4$	CC(C)=CC=CC=CC(C)C	7	6	406.56
4	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 5$	CC(C)=CC=CC=CC=CC(C)C	9	8	503.69
5	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 6$	CC(C)=CC=CC=CC=CC=CC(C)C	11	10	603.04
6	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 7$	CC(C)=CC=CC=CC=CC=CC=CC(C)C	13	12	703.40
7	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 8$	CC(C)=CC=CC=CC=CC=CC=CC=CC(C)C	15	14	804.30
8	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 9$	CC(C)=CC=CC=CC=CC=CC=CC=CC=CC(C)C	17	16	905.53
9	$(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}\ C(CH_3)_2$ $k = 10$	CC(C)=CC=CC=CC=CC=CC=CC=CC=CC=CC(C)C	19	18	1006.97

leveraging the manifestation of the electronic environment of a nucleus as an NMR chemical shift to predict the length of a particle-in-a-box approximation. We demonstrate that the wavelength at maximum absorption, defined by the electronic states of the molecule and the chemical shift changes based on the nuclear states, can be related to the length of the box (i.e., the number of carbons in a molecule's carbon chain).

NMR spectroscopy is a powerful and versatile technique used in various fields, from classroom applications in chemistry to advanced research in biotechnology and medicine. In particular, the chemical shift of a nucleus depends on its electronic environment, which is vital in protein structure determination.[18−20]

In measuring the electronic configuration of an atom, the electron density, determined by λ_{max}, affects the nuclear shielding, which is measured by NMR chemical shifts. We can associate a similar relation between chemical shifts and box length by establishing a linear relationship between electron density and box length. This approach supplements traditional methods when in-person experimental access is limited. A set of polyenylic molecules with varying carbon chain lengths was used to explore this relationship. For example, we have found that the chemical shifts of protons at the second and third (Figure 1) carbons are sensitive to box length. This exercise covers topics such as estimating electron density, introducing absorption and NMR spectroscopy, and numerical data analysis, which are relevant to undergraduate physical chemistry laboratory requirements.

■ EXPERIMENTAL DETAILS

Learning Objectives

Target Students. The target students had finished a one- or two-semester lecture course in physical chemistry. Students who completed prerequisite calculus and modern physics courses, taking physical chemistry lectures and laboratory courses concurrently, can also be considered. During the course, they learned about postulates of quantum mechanics, the time-independent Schrödinger equation, model systems such as particle-in-a-box, and broader spectroscopy principles. Additionally, they have completed lecture and laboratory organic chemistry courses, including an introduction and basic interpretation of NMR spectroscopy.

Learning Objectives.

1. Able to set up a boundary-value problem for the stationary Schrödinger equation of the particle-in-a-box model.
2. Able to derive an expression relating the eigenvalues of the Schrödinger equation and wavelength of maximum absorption (λ_{max}) to the length of the one-dimensional box.
3. Adopt a method to calculate the electron density using Worksheet-based (e.g., Excel) or other computer programs (e.g., Mathematica/Matlab/R).
4. Use the SMILE representation of molecules (polyenylic ions) to estimate the NMR chemical shifts of a selected set of molecular configurations.
5. Describe the physical meaning of the connection to electron density and chemical shifts and how it relates to the box length of the quantum mechanical model.

Molecules (Polyenylic Ions) Investigated

This demonstration is developed using the list of polyenylic cations suggested by Flewwelling and Laidlaw:[21] The series of molecules (cations), $(CH_3)_2C{=}CH{=}(CH{=}CH{=})_{k-2}C(CH_3)_2$, $k = 2{-}10$. The molecules (polyenylic ions) are converted into the SMILES (Simplified Molecular Input Line Entry System) format to obtain the other calculations.[22] The first molecule in the series, with $k = 2$, will be $(CH_3)_2C{=}CH{=}C(CH_3)_2$, and the last in the series, with $k = 10$, will be $(CH_3)_2C{=}CH{=}(CH{=}CH{=})_8C(CH_3)_2$. Table 1 lists the molecules (polyenylic ions) and their respective SMILES format.

Estimation of Box Length and Electron Density

First, the length of the molecules (polyenylic ions) is calculated using a linear chain of conjugated carbons following the methodology of Flewwelling and Laidlaw.[21] Following the geometry defined in Figure 1, the length of the box is defined as

$$L = l_C \cos(30^\circ)(n_c - 1) + 2p \tag{1}$$

Table 2. Estimated Electron Densities and NMR Chemical Shifts

			Electron Density									Chemical Shifts of the Protons (ppm)								
PiB Model	λ_{max} Calculated (nm)	Estimated Box Length calculated (Å)	C1	C2	C3	C4	C5	C6	C7	C8	C9	C1	C2	C3	C4	C5	C6	C7	C8	C9
1	272.34	4.98	4.90×10^{-3}	3.11×10^{-2}																
2	316.10	9.96	7.22×10^{-3}	4.51×10^{-2}	1.09×10^{-1}							2.48								
3	406.56	14.93	8.50×10^{-3}	5.27×10^{-2}	1.25×10^{-1}	2.04×10^{-1}						2.48	5.79							
4	503.69	19.91	9.31×10^{-3}	5.75×10^{-2}	1.35×10^{-1}	2.18×10^{-1}	2.79×10^{-1}					2.48	5.74	6.02						
5	603.04	24.89	9.87×10^{-3}	6.08×10^{-2}	1.42×10^{-1}	2.27×10^{-1}	2.87×10^{-1}	3.10×10^{-1}				2.48	5.72	6.01	6.39					
6	703.40	29.87	1.03×10^{-2}	6.31×10^{-2}	1.47×10^{-1}	2.33×10^{-1}	2.93×10^{-1}	3.14×10^{-1}	2.99×10^{-1}			2.48	5.70	5.99	6.39	6.39				
7	804.30	34.85	1.06×10^{-2}	6.49×10^{-2}	1.51×10^{-1}	2.38×10^{-1}	2.98×10^{-1}	3.17×10^{-1}	3.00×10^{-1}	2.66×10^{-1}		2.48	5.68	5.97	6.39	6.39	6.39			
8	905.53	39.82	1.08×10^{-2}	6.63×10^{-2}	1.54×10^{-1}	2.42×10^{-1}	3.01×10^{-1}	3.19×10^{-1}	3.00×10^{-1}	2.66×10^{-1}	2.37×10^{-1}	2.48	5.66	5.95	6.39	6.39	6.39	6.39		
9	1006.97	44.80	1.10×10^{-2}	6.75×10^{-2}	1.56×10^{-1}	2.45×10^{-1}	3.04×10^{-1}	3.21×10^{-1}	3.01×10^{-1}	2.66×10^{-1}	2.38×10^{-1}	2.48	5.64	5.93	6.39	6.39	6.39	6.39	6.39	

where l_C is the length of the conjugated carbon−carbon bond (1.437 Å, average of C−C and C=C bond length), and n_c the number of conjugated carbon−carbon bonds. The cosine angle of 30° is incorporated to determine the horizontal length of each conjugated carbon−carbon bond. For this exercise, the penetration length is equal to l_C. The wavelength at maximum absorption using the particle-in-the-box model is then written as[21]

$$\lambda_{\max} = \frac{32 m_e c\,[l_C \cos(30^\circ)(n-1) + p]^2}{h\,(2n-1)} \tag{2}$$

where m_e the mass of the electron (9.11×10^{-31} kg), c velocity of light (2.99×10^{-8} m/s), h is Planck's constant (6.62×10^{-34} J·s), and p is the penetration depth (1.4 Å). Equation 2 is derived in the Supporting Material.

Electron density on a carbon atom due to an electron on the m^{th} molecular orbital using the solution to the Schrödinger equation for a particle-in-the-box is given as

$$\rho = \int_{x=b}^{x=c} \psi_m^2(x)\,\mathrm{d}x \tag{3}$$

As there would be two electrons in each $(n-1)^{\text{th}}$ occupied orbital, the total electron density at a given carbon center 'r' is determined by summing the eq 3 over all the electrons as

$$\rho_r = 2\sum_{m=1}^{n-1}\left(\frac{2}{L}\right)\int_b^c \sin^2\left(\frac{m\pi x}{L}\right)\mathrm{d}x \tag{4}$$

The lower and upper limits of integration (b, c) are from the midpoints between carbon atom positions and the two carbon atoms on either side (see Figure 1). The electron density is calculated on each π-electron on the chain (σ-electrons are not included). The electron density given in equation 4 can be estimated straightforwardly, analytically, or numerically for each carbon center, with the integration limits spanning both sides of the carbon center over the length of the chain. Table 2 lists each carbon position's estimated $\lambda_{\max}$, box length, and electron density values.

Estimation of Chemical Shifts

The SMILE format of the molecules (polyenylic ions) was used to estimate the chemical shifts of the ^{1}H and ^{13}C nuclei in the open-source platform NMRDB.[23] Therefore, only the ^{1}H chemical shifts that show a variation in the molecular chain length were used for further analysis and are listed in Table 2. The combined calculations are easy to implement using MS Excel or programs R (Supporting Information).

Implementation in Physical Chemistry Laboratory Curriculum

Typically, students take a physical chemistry laboratory course during their senior year after completing a semester-long quantum mechanics and spectroscopy course. During the period of remote learning, educators were faced with new challenges and limitations in their teaching methods. To address this, a laboratory exercise was developed for 11 undergraduate chemistry students at Fresno State in the spring of 2021. The activity was designed to be open-ended, with the instructor providing background information and resources without step-by-step procedures to encourage student involvement (details are provided in the Supporting Information). First, the students were introduced to the quantum mechanical particle-in-a-box model and UV−vis-based experimental approach. Then, they were introduced to the concepts of NMR spectroscopy and posed the question: "Can NMR chemical shifts be used for spectroscopic investigation of the particle-in-a-box model?"

The students worked together to create a plan for the experiment, dividing into groups to focus on specific tasks such as researching relevant articles, selecting molecules (polyenylic ions), understanding their SMILE format, estimating electron density and wavelength, and estimating NMR chemical shifts. Using Zoom, they readily shared their computer screens and documents. Finally, a group was chosen to present an overview of the experimental methods and theoretical background for the rest of the class.

Before beginning the exercise, students were required to take a prelab quiz, which is included in the Supporting Information. Most students will need three to four laboratory sessions, each lasting 3 h, to complete the necessary tasks. Each student created an Excel worksheet summarizing the calculations, data fitting process, and overall results. Students shared their data, allowing them to combine results from replicated experiments. At the end of the exercise, all students took a postlab quiz, which is also included in the Supporting Information. The quizzes will serve as an indicator of overall improvement in their understanding of the exercise.

After the experiment, every student submitted a formal report that was evaluated with a grading guide based on the learning objectives. Based on the evaluation of a small sample size of 11 students, there was a slight improvement in the average score from 8.10 to 8.50. However, the p-value (t test) of 0.5 indicated this improvement was insignificant. Students submitted an Excel worksheet for assessment, and all reports were submitted online (the implementation process is described in the Supporting Information).

■ RESULTS AND OBSERVATIONS

The Estimated ^{1}H Chemical Shifts Correlate Linearly with the Electron Density at the Carbon Position

The electron density calculated using Flewwelling and Laidlaw[21] and the estimated chemical shifts of the protons in the carbon chain show a linear correlation (Figure 2). Although the electron density of the first carbon showed a positive linear correlation with the box length, the estimated proton chemical shifts remain the same despite the increase in the electronic density. However, the electron densities of the second (Figure 2a) and the third carbons (Figure 2b) decrease

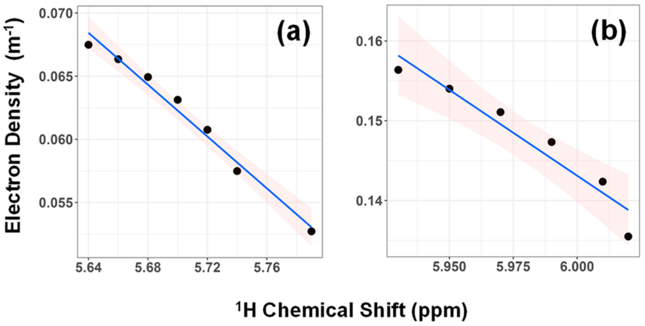

Figure 2. Correlation of chemical shifts and electron density. The plots of the proton chemical shifts at carbon positions (a) 2 and (b) 3 are a function of the estimated electron densities. The linear fits are shown as straight blue lines, and the pink bands represent the 95% confidence limit of the fits.

linearly with the increase of proton chemical shift, demonstrating the deshielding effect. For the ^{1}H on the second carbon, a linear fit yields a slope of $-1.02 \pm 0.06 \times 10^{-2}$ m^{-1}/ppm and an intercept of 0.65 ± 0.03 m^{-1} ($R^2 = 0.98$), while for the ^{1}H on the third carbon, it yields a slope of $-2.15 \pm 0.30 \times 10^{-2}$ m^{-1}/ppm and an intercept of 1.43 ± 0.18 m^{-1} ($R^2 = 0.91$). The chemical shifts of the protons on the fourth, fifth, and other carbons do not show a change with respect to electron density.

The Estimated ^{1}H Chemical Shifts Can Be Used to Determine the Length of the One-Dimensional Box

The basis of the particle-in-a-box model relies on a linear relationship between the wavelength at maximum absorption (λ_{max}) of the electrons in UV−vis and the box length of the one-dimensional well based on the eigenvalues of the Schrödinger equation of the system. As the electron densities of the carbons at the chain correlate with the nuclear chemical shifts (Figure 1), by corollary, the chemical shifts are indirectly related to λ_{max} and box length (Figure 3). The chemical shifts of the protons on the second carbon in the chain show a linear relation with the estimated (λ_{max}) (Figure 2a, slope: $-2.31 \pm 0.19 \times 10^{-4}$ ppm/nm; intercept: 5.86 ± 0.01 ppm; $R^2 = 0.96$) and the box length (Figure 2c, slope: $-4.66 \pm 0.37 \times 10^{-4}$ ppm/Å; intercept: 5.84 ± 0.01 ppm; $R^2 = 0.96$). The chemical shifts of the ^{1}H on the third carbon is much more sensitive than the second carbon with respect to λ_{max} (Figure 2b, slope: $-1.84 \pm 0.08 \times 10^{-4}$ ppm/nm; intercept: 5.11 ± 0.01 ppm; $R^2 = 0.99$) and box length (Figure 2d, slope: $-3.73 \pm 0.01 \times 10^{-3}$ ppm/Å; intercept: 6.01 ± 0.01 ppm; $R^2 = 0.99$).

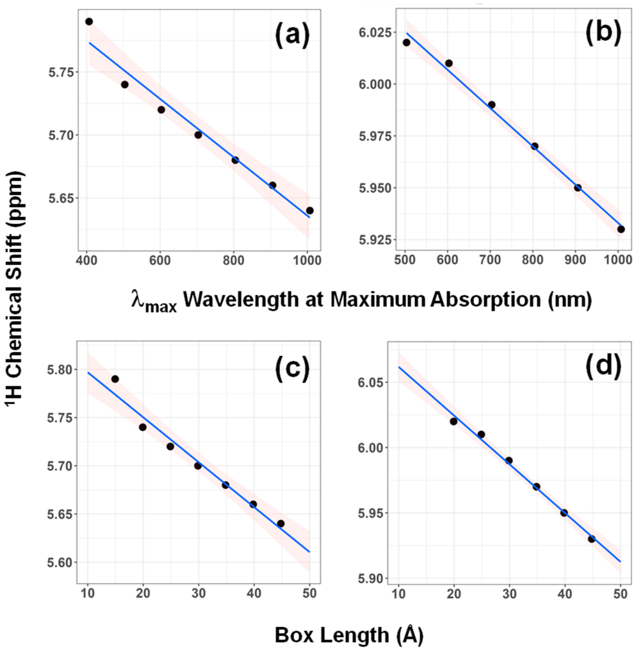

Figure 3. Correlation of chemical shifts with wavelength at maximum absorption and box length. The wavelength at maximum absorption shows a linear correlation with the estimated chemical shifts of protons at the carbon positions (a) 2 and (b) 3. Therefore, according to the particle-in-a-box model, the box length also shows a linear relation with the chemical shifts of the protons at the (c) second and (d) third carbons. The linear fit is shown as straight blue lines, and the pink bands represent the 95% confidence limit of the fits.

SUMMARY

In most universities, students majoring in chemistry usually take a physical chemistry laboratory course in their senior year. Typically, they would have already been introduced to NMR spectroscopy in their previous organic chemistry courses, and they are also required to complete the lecture courses in quantum mechanics and spectroscopy. This is to ensure that they have a good understanding of the concepts needed to achieve the goals of the investigation. Organic chemistry students struggle to learn and interpret NMR spectra.[24−26] However, several useful tools have been introduced and addressed pedagogical approaches for improved learning of NMR.[27−32] The exercises presented aim to help students appreciate that the chemical shift in the NMR spectra is not a single fixed parameter for a local configuration (such as the parts per million (ppm) values of a methylene group). Instead, it represents the molecule as a whole due to the interconnected nature of the electrons and nuclei and the overall representation of the molecular dimensions. For instance, students can learn how the chemical shift of a $-CH_2$ group changes systematically as a function of the molecular length.

While the proposed exercise is valuable for expanding traditional experimental approaches, the results demonstrate some notable limitations. The procedure yields dependable results for polyenyl molecules (polyenylic ions). Still, it does not provide reliable estimates for molecules (polyenylic ions) traditionally used in UV−vis spectroscopy, such as polymethine dyes,[6] when using database-derived chemical shift calculations. Though the ^{1}H and ^{13}C chemical shifts were estimated, only the ^{1}H ones tend to show a linear change with the box length. To improve the accuracy of the results, more advanced methods of calculating chemical shifts could be utilized.[33] Additionally, the estimated range of ^{1}H chemical shifts is small (~0.3 ppm), and experimental demonstrations may further be complicated due to the expected J-coupling effects between the protons in low to midfield NMR spectrometers (<400 MHz).

A classic experiment in the physical chemistry laboratory involves demonstrating the particle-in-a-box method using UV−vis spectroscopy on linear molecules (polyenylic ions) with a conjugated carbon chain. NMR-based demonstrations can be added to this exercise to enhance student learning and connect concepts infrequently linked in the traditional classroom. It is especially important for students to understand that molecules (polyenylic ions) comprise integrated systems of electrons and nuclei and that any changes in electronic configurations can influence other elements, such as protons. However, it is also worth noting the extraordinary intuition of Flewwelling and Laidlaw's findings[21] almost 50 years ago, before the age of modern NMR.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.3c00588.

Derivation of the wavelength at maximum absorption for the particle in the box model; overview of the open-ended laboratory; pre and postlab evaluation quizzes; answer keys; R-markdown for calculations (PDF)

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Notes

The authors declare no competing financial interest.

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