# Implementing PLTL in the quantum concepts semester of physical chemistry

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## Abstract

With an NSF dissemination seed grant, I have implemented the PLTL approach in the quantum concepts semester of the year-long physical chemistry course at Boston University, http://quantum.bu.edu/courses/ch352/workshops.html. Using PLTL has changed the nature of the course and the way I approach it. I have found that the allocation of time for course preparation, student discourse, the use of regular class time, and student performance have all changed from prior years. From the students' point of view, they have the opportunity and responsibility to work with methods and explore concepts more deeply. From my point of view, there have been four primary effects. First, the creation and then revision of the workshops based on input from the peer leaders takes significant time. Second, it is my impression that interaction in lecture is more sophisticated and students are more likely to steer lectures in interesting, unanticipated directions. Third, for the workshops to have a good balance of challenge and accessibility, I have had to structure preceding lectures very carefully, with about a two-week look ahead. Finally, the workshops have helped solidify for students foundation quantum concepts and so allowed me to present material at a richer level. My overall assessment is that there is no free lunch, but that the PLTL approach is a much better investment of student and faculty time than the traditional lecture and discussion approach.

## Logistics

The primary exposition of the course is based on my own notes, at http://quantum.bu.edu/notes/QuantumMechanics/index.html, and I structured the workshops elaboration of the material presented in the notes.

Workshops, summarized below, were held approximately weekly, on Thursdays for two hours, to six groups of five to six students each. The scheduling of the workshops, based on student and peer leader schedules took about a week to arrange.

Monday evening preceding each workshop the six workshop peer leaders worked through the initial draft of the workshop, with me acting as leader. This typically took a bit more than two hours. Based on the results of the peer leaders working through the draft, I revised the workshop over the next several days, and then distributed it to the leaders on Wednesday to hand out at their student workshop on Thursday. After their workshop, the leaders emailed me a detailed report on student experience in the workshop and their own observations. I also corrected any errors that were identified then posted the workshop to the class web, at http://quantum.bu.edu/courses/ch352/workshops.html. No answers were provided on the posted workshop. Finally, at the start of the next Monday training session, the leaders and I reviewed together their experience and suggestions based on the previous workshop.

## My experience

The creation and revision (based on feedback from leaders during the training session preceding each workshop) takes considerable time, perhaps as much as doubling the course preparation time.

To allow for a good balance of challenge and accessibility in the workshops, preceding class lectures need to be structured more carefully than I had anticipated, with about a bit less than a two-week lead time.

As the semester proceeded, interaction with students during class lectures became increasingly sophisticated, to the point where students were likely to steer lectures in interesting, unanticipated directions.

Workshops helped solidify for students foundation quantum concepts and this created a feedback loop that resulted in me presenting material at a richer level than I have in the past.

# Leader experience

The experience of the leaders in the training session preceding each workshop was crucial to the quality of the workshops. Typically the final version of the workshop was shortened considerably, questions were more finely focused, and clarifying questions were added.

As the course unfolded, leaders were challenged beyond their comfort level by the increased scope and sophistication of topics made possible by the workshop format. This was unexpected by the leaders, perhaps more so by those who had previously worked as leaders in general chemistry PLTL workshops.

# **Student experience**

Some students did not initially realize the workshops were an integral part of the development of the course, as opposed to, for example, problem practice sessions. Perhaps this reflects a perspective developed from their general chemistry PLTL workshops.

Accordingly, the opportunity to explore methods and concepts more deeply carried with it an unexpected responsibility to master the material presented in workshop.

Some leaders reported that students were less likely to work collaboratively than leaders had experienced in their general chemistry workshops. This may be a consequence of the differing comfort levels of the leaders.

## **Overall impression**

There was wide range in the response by the leaders to the challenge of the workshop material. At one extreme, some leaders attended preceding class lectures to refamiliarize themselves with material; at the other, they were not sufficiently prepared to effectively guide students.

Probably as a direct consequence of the variability in leader comfort with a workshop, there was a corresponding variation in the perceived quality and effectiveness of the workshops by the students. Students lead by confident, well prepared leaders generally reported a much more favorable experience.

This variability in turn has generated concern among faculty colleagues some students are not always getting the best possible "teaching." This is a valid concern.

The more challenging nature of the material and the variability of comfort with it among the leaders means that in future I will need to arrange things so that leaders are more uniformly prepared for each workshop.

Notwithstanding the challenge to be met of having all leaders well prepared for each workshop, and the increased time needed on my part to incorporate PLTL, at this point I feel the workshop approach is a much better investment of student and faculty time than the traditional lecture-and-discussion format. The unsolicited request by several students in the course to be peer leaders for the next year of the course encourages me that we are making an important change. I anticipate that a second year would be a smoother experience for the leaders, since they will know first hand the kind of leader support that is needed, and so an even more positive experience for the students.

There is no free lunch-successfully implementing PLTL in physical chemistry is hard, careful work.

# Workshops summaries

1. *Probabilities, average values and uncertainties*: The work of Bohr and de Broglie led to the idea that matter must be represented in terms of wavefunctions, and Born introduced the idea that the squared magnitude of a wavefunction at a point determines the probability that the object described by the wavefunction will be found at that point. This workshop explores how to use these ideas to predict the spatial position, momentum and energy (and their uncertainties) of a particle from its wavefunction. See http://quantum.bu.edu/courses/ch352/workshops.html#1.

2. *Momentum of a quantum particle and the Heisenberg uncertainty principle*: In this workshop we will see how to compute particle properties that are represented as operators, and then explore the consequences of the position-momentum commutation relation on the simultaneous values of uncertainties of different particle properties. The most famous of these is the position-momentum (Heisenberg) uncertainty product. See http://quantum.bu.edu/courses/ch352/workshops.html#1.

3. Series expansion—A Swiss army knife for calculations and analysis: In this workshop we will explore series expansions and how they are helpful in analyzing quantum mechanical expressions and carrying out calculations with them. This workshop is based in part on McQuarrie and Simon, Physical Chemistry (University Science Books, 1997), MathChapter I. My hope is that once you have digested this workshop, you will have some confidence that you can actually use series expansions to do certain kinds of calculations and analyses much more easily. See http://quantum.bu.edu/courses/ch352/workshops.html#3.

4. *Particle on a ring*: A particle of mass m moving on a ring of radius r in the x y plane is an important model quantum system. It also provides nice examples of working with operators, the properties of their eigenfunctions and eigenvalues, and time dependence of wave functions. See http://quantum.bu.edu/courses/ch352/workshops.html#4.

5. *Approximate energies and wave functions* (two parts): We have learned how to find wave functions and energies by adjusting the total energy so the wave function is decays to zero in forbidden regions of infinite width or infinite potential energy. In numerical applications of quantum mechanics in chemistry, an alternative, flexible method of solving the Schrödinger equation is to approximate the wave function for a particular system in terms of those for a similar, so-called model system. A very nice feature of this approach is that the accuracy of the approximation can be systematically improved, by increasing the number of model wave functions used in the approximation. In this workshop we'll explore this method, for the example of a particle confined to an infinite well with a sloping bottom. The model system will be the corresponding infinity well with a flat bottom. See http://quantum.bu.edu/courses/ch352/workshops.html#5.

6. *One-electron-atom orbitals*: Three-dimensional wave functions of an electron in a one-electron atom are known as one-electron-atom orbitals. Electrons in many-electron atoms can be approximately represented in terms of these orbitals. The spatial properties of these orbitals are essential components in understanding the periodic properties of many-electron atoms, the bonding of diatomic molecules, and the shapes of polyatomic molecules. For these reasons it is important to be familiar with the three-dimensional structure of one-electron-atom orbitals. In this workshop you will explore the properties of these orbitals. See http://quantum.bu.edu/courses/ch352/workshops.html#6.

7. *Diatomic molecule vibrational and rotational spectra*: We have learned how the adiabatic and Born-Oppenheimer approximations allow us to separate the electronic, vibrational, rotational and center of mass contributions to the energy of a diatomic molecule. The key result is simple expressions for the electronic, vibrational and rotational contributions to the internal energy of the molecule. The purpose of this workshop is become familiar with these energy contributions and to see how to use them to understand vibrational and rotational spectra. See http://quantum.bu.edu/courses/ch352/workshops.html#7.

8. *Rovibrational and rovibronic spectra of gaseous HCl*: This workshop illustrates that rovibrational and rovibronic spectra of diatomic molecules are a rich source of information about their structure in their different electronic states. With experience, you will be able to tell with just a glance at a molecular spectrum quite a lot about the internal details of the molecule. See http://quantum.bu.edu/courses/ch352/workshops.html#8.

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