Incorporating Mathematica into an Introductory Quantum Mechanics Course

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Seeking a Visualisation Tool to Enhance Learning in PC2130

The introductory course PC2130 “Quantum Mechanics I” is a compulsory core module intended for second year physics majors. For those who are unfamiliar with the subject, quantum mechanics studies the mechanical evolution of atomic and subatomic particles. At such a scale, Nature behaves in a rather weird and counter-intuitive way. Take, for instance, the fact that electrons are behaving as particles and waves at the same time (a phenomenon known as wave-particle duality). To describe the state of such a “wave-particle” object mathematically, physicists came up with the notion of wave function, which essentially describes the probability of the electron being found at a particular position and/or momentum. These wave functions are solutions to a second-order partial differential equation (i.e. the Schrodinger equation), which itself is parameterised by various initial conditions and potential energy. If this sounds dry, tough and mathematically involved, it indeed does to the majority of the students taking PC2130. We identified that the learning-related issue may possibly lie with students having difficulty visualising the physical picture behind the mathematics. This prompted us to use the mathematical software Mathematica 9.0 (Wolfram, 2012) in the course as a visualisation and computation tool to help students gain a better grasp of the subject. In short, with the aid of Mathematica, we hope students are able to simulate the dynamics of this complex wave function.

Choosing Mathematica

When it came to selecting a visualisation tool to help us achieve the learning outcomes for PC2130, Mathematica was our software of choice. It was chosen over other mathematical software such as Matlab or Maple for three reasons:

1. It supports algebraic computation (which means that it can be used to solve equations in term of its variables);
2. It has a gentle learning curve as it comes with built-in Mathematica commands to perform sophisticated functions. For example, the “Manipulate[argument]” command in Mathematica enables the student to plot and interact with the “argument” (i.e. wave function, in our case) on a real-time basis; and
3. The software is freely available to NUS students through the academic site license. This is crucial as that means students are able to install the software on their laptops or home desktops, allowing them to use Mathematica to work on their project anytime and anywhere. We also hope that in the long run students would apply the skills they acquired beyond the course.

Recommended Citation

Incorporating Mathematica in the Syllabus as a Term Project

At the moment we have implemented this initiative over two semesters. In Semester 2 of AY 2011/12, Mathematica was introduced as a term project, which eventually contributed up to 20% of students’ final grades.

In this project, students had the opportunity to participate in peer learning, working in pairs and using Mathematica to visualise the evolution of wave function in a potential well. The instructions, together with the expected deliverables, were given early in the beginning of the semester. To further incentivise students to explore using the software beyond the minimum requirements in their projects, higher marks would be awarded to students who chose to work on more complicated initial conditions and potentials. In most cases, students picked up the computation skill required for the software by themselves. We did not hold a specific course on how to use Mathematica per se, but we integrated Mathematica into the lectures and tutorials. For instance, apart from providing a model solution to a particular problem in writing, we also provided the solution in Mathematica codes during tutorials. Students were then expected to pick up and modify the necessary Mathematica commands.

This self-exploratory way of teaching and learning Mathematica was sufficient for students to complete the basic requirements of the project. However, if the students decided to work on more challenging problems, they would face issues with regards to using the more advanced commands and optimising the programme (in order to shorten the computation time), which they would then have to resolve through self-exploration (e.g. browsing online discussion forums to find out how others solved similar problems). We also made ourselves readily available to students for consultation throughout the semester.

Students’ Response to Using Mathematica

At the end of the semester, a short survey was conducted to determine the impact the use of Mathematica has had on students’ learning for this project. Twenty-six students (out of 41 students in the class) responded. According to the survey results, 76% of the respondents agreed that they had a positive experience using Mathematica and had learnt a useful skill by going through the project despite the initial challenges and frustration in dealing with the software. When asked if they would consider resorting to Mathematica again to help them in their study or research work in future, 84% replied in the affirmative.

In the qualitative feedback collected from the survey, students reiterated that using Mathematica helped them gain a better understanding of quantum mechanics:

• “I think the project was pretty interesting, before the project, I had absolutely no idea what the potential well did, it was simply some mathematics to me, so I’m glad I managed to visualise something.”

• “I have learned quite a lot and we actually did more than we submit. We can plot all the wave function by Mathematica which is really awesome!”

• “Thanks for all the advice along the way. Overall I think even though the project was difficult and time-consuming, it was useful to help me understand [the concepts] better.”

They also appreciated the benefits of learning from their peers while doing the group project:

• “Although highly frustrating, the project did give me much valuable insight into quantum mechanics (e.g. energy eigen values etc) I like the freedom given to us to choose our wave functions. Of course, at the course of the project let my partner and I bond together, through the ups and
many downs and numerous meetings and rantings, and I appreciate the group work and camaraderie built up.”

However, students also expressed frustration at the difficulties they experienced using the software. For example, some had spent countless hours figuring out what they thought were fully functional programmes, and yet the system kept crashing or running into indefinite loops. In most cases, it turned out that the problem lay with the syntax and students being unfamiliar with programming semantics, which caused compilation or logical errors (Dewanto & Yeo, 2012).

In addition, although it was a semester-long project, most students only started work on the project near to the submission deadline, which caused much frustration towards the end of the semester when they were also preparing for their tests and facing other deadlines. In the survey, students also suggested improvements to the learning activities, including the provision of some training in Mathematica prior to the project to help them to better manage some of these difficulties:

• “This project is okay per se. Allows us to understand the concept more. But really need more training on how to use [M]athematica before we can afford to do more complex potential well or interesting initial wave functions. Independent studying is okay, I’m not asking to be spoon fed. But it’ll be good if we’re trained on [M]athematica before starting on the project. Think the focus should be on enabling us to visualise interesting physics situation rather than to figure out how to use a computer programme and how to resist the urge to throw my laptop out of the window (leave that to the computing students!).”

• “This project is supposed to make me understand more about the content of PC2130. I agree that this project helps a little bit. However, lecture quiz is much better than this project. if there is lecture quiz, I will study more the whole content of this module. This project only requires a small part of the concept taught in PC2130, not all. And also, the use of [M]athematica is quite difficult because I don’t have [the] skill in using [M]athematica and it tends to drive student only to look at the sample file the lecturer gave. So the students only learn about small part of [M]athematica. This project also tends to make student only look at the sample file and just copy it if they don’t understand it, not learn about the content. The lecture quiz tends to make student study hard because in the quiz they can’t cheat.”

Reflections on Using Mathematica for Future Cohorts

We had much to think about after our first attempt at incorporating Mathematica into PC2130. There is no doubt that learning Mathematica, as it would be the case when it comes to learning any other new software or programming language, would require a certain level of self-exploration and self-learning on the students’ part through trial and error. Conquering such a learning curve obviously takes time, which only the more motivated students would be willing to invest. As such, while students were generally positive about Mathematica’s usefulness in helping them understand key concepts in PC2130, the feedback indicated that we still had a way to go in terms of ensuring that this tool can comprehensively achieve the module’s learning outcomes. Nevertheless, we will continue to use Mathematica in PC2130, and will keep experimenting with various pedagogical strategies, such as incorporating Mathematica as part of continual assessment, to determine the best and most effective way to integrate the software into our teaching.

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Mr Andreas Dewanto, Dr Yeo Ye and Mr Kenneth Hong are teaching staff from the Dept of Physics. They do not subscribe to any particular pedagogy. However, throughout their years of teaching core as well as general education modules, they have been exploring various tools and medium to engage students, from interactive demonstrations that aid in the visualization of physical concepts to the utilization of mathematical software, such as the one presented here.

References