

## Spreadsheets

# Using Spreadsheets to Teach Quantum Theory to Students with Weak Calculus Backgrounds

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### Abstract

*Quantum theory is a key part of the chemical and physical sciences. Traditionally, the teaching of quantum theory has relied heavily on the use of calculus to solve the Schrödinger equation for a limited number of special cases. This approach is not suitable for students who are weak in mathematics, for example, many students who are majoring in biochemistry, biological sciences, etc. This case study describes an approach based on approximate numerical solutions and graphical descriptions of the Schrödinger equation to develop a qualitative appreciation of quantum mechanics in an Australian University.*

### Level of Material: Second Year

## The Execution

The aim here is to teach the qualitative results that arise from applying mathematics to physical and chemical systems, but without the mathematical rigour: “teaching maths without the maths”. The “new calculus” advocates the “rule of four” (numerical, graphical, symbolic and verbal descriptions) to deepen students’ conceptual understanding. Students who have a weak background in mathematics do not have the knowledge of calculus required for the usual symbolic algebra approach to quantum theory. This case study illustrates how a combination of numerical, graphical and verbal descriptions can be used to overcome the lack of symbolic knowledge or ability.

Quantum theory is a key part of the chemical and physical sciences. In preceding semesters, students have collected spectra that show atoms and molecules only absorb (and emit) certain photon energies which are characteristic of that atom or molecule: other photon energies are not absorbed. Students have also learnt from classes and textbooks that:

- “Allowed” energy levels are quantised, but usually without appreciation of why.
- Electrons and atoms exhibit both wave-like and particle-like behaviour.

The Schrödinger equation for an electron-in-a-box (the Kuhn model) is introduced as two coupled first order differential equations. The derivative is explained as the “slope of a function”. The first order Euler method for generating numerical solutions is explained. No calculus is required as the Euler method can be derived from the definition of average slope. Students create their own spreadsheet (to find numerical solutions to the Schrödinger equation), or are supplied with a spreadsheet written by the lecturer.

The wavefunction solutions are classed as “valid” or “invalid” depending on whether the boundary conditions are satisfied as energy is varied (the shooting method). Students discover that energy determines the wavelength of the wavefunction, and that valid solutions require that only special (“allowed”) wavelengths will fit the dimension of the box. Further exploration shows that energies decrease as the box is enlarged (“delocalisation lowers energy”) and that energies increase as barriers are introduced (Kronig-Penney model).

The key results from the exploration activity are reinforced in class and generalised by considering other potential-energy functions, including functions (e.g. triangular-well potential) for which no analytical solution exists.

It is observed that the number of nodes (the zeroes or roots of the wavefunction) increases with energy and that the qualitative shape of the wavefunction can be generated from the nodal pattern. (One strategy in de Bono’s Lateral Thinking is to concentrate on what is not present — i.e. the nodes or zeroes — in order to obtain what should be present — the wavefunction). Wavefunctions can then be generated from nodal patterns in 2-dimensions and 3-dimensions. For example, the rotational wavefunctions are generated by considering nodal patterns (and hence wavefunctions) on the surface of a sphere (the original Hamiltonian model for waves on a spherical ocean. Note that these “spherical waves” correspond to combinations of the spherical harmonic functions, and are obtained from the symmetry — “topology” — of the nodal patterns).

## Pre-requisite Knowledge

The minimum mathematical knowledge required is to know about functions and to understand and manipulate the definition of average slope. All students entering university from secondary school (high school) will have this pre-requisite knowledge. Students also require some computer literacy and minimal knowledge of creating formulae in spreadsheets — see comments under “What Support Was Needed?”

# How Are Students With Different Mathematical Backgrounds Supported?

This topic has been designed for students with minimal mathematical background. Students who have a stronger mathematical background can be extended by emphasising the symbolic approach – solve the Schrödinger equation using calculus. Extensions such as numerical integration to test orthogonality of wavefunctions are also possible.

## What Support Was Needed?

The Information Technology Services Division runs computer-training sessions during Orientation Week at the start of the academic year. The university is investigating the implementation of on-line self-paced modules associated with the International Computer Driving Licence (ICDL), which includes training in the use of spreadsheets. The use of spreadsheets is demonstrated to students who are still not confident in their use at the start of this topic.

## The Barriers

In some Australian states, it is possible to complete high-school mathematics without any calculus. At many Australian universities, students choose statistics as their first-year mathematics. Hence, traditional approaches to quantum theory are not practical.

Physical chemistry, and especially quantum theory, are viewed as difficult topics within the chemistry course because of the level of mathematics (second order PDEs, basis sets, etc.) required. This has been overcome by de-emphasising the traditional symbolic approach and instead focusing on the numerical, graphical and verbal descriptions of the topic.

## The Enablers

The major enabler is the use of spreadsheet software to generate numerical solutions of differential equations. For mathematically weak students, spreadsheets are preferred over MathCAD, Mathematica and similar programs, because spreadsheets are perceived as being more “ordinary” and easier-to-use.

Most students have access to spreadsheet software at home, without incurring additional licensing cost for the student or the university. In other topics, spreadsheets are also used for data analysis and plotting, again in preference to more specialised programs like SPSS or Minitab, etc.

## Evidence of Success

The evidence of success is that students who have no knowledge of calculus are able to complete this introductory topic.

## How Can Other Academics Reproduce This?

Examples of spreadsheets and other documents are located at the unlinked URLs in the references below.

Similar approaches using numerical solutions can be used to teach the differential equations associated with chemical reaction kinetics.

## Quality Assurance

Second and third-year subjects (units) at Deakin University undergo formal student feedback/evaluation at least biennially, with informal feedback/comment to teaching staff. Students who have no knowledge of calculus are able to complete this introductory topic.

## Other Recommendations

The use of specialised software (such as Origin, SigmaPlot, MathCAD, Mathematica, SPSS, Minitab, etc.) should be deferred until students undertake research programs. Until then, generalist software (“worldware”) should be used across all disciplines to foster expertise in software that is in common usage in the general workforce outside universities. However, surveys of students at Deakin University indicate that they are less confident with the use of spreadsheets than other common generic software types, e.g. word processors, web browsers, electronic mail. Further, the skill level with each type of software is highly variable.

### References

The approach described in this case study has been influenced by the American M.U.P.P.E.T. program and the “new calculus”:

“Student programming in the introductory physics course: M.U.P.P.E.T.” *American Journal of Physics*, 1993, 61, 222-232, Redish, E. F. and Wilson, J. M. (1993) <http://www2.physics.umd.edu/~redish/Papers/mupajp.html>

University of Maryland, Published papers describing *M.U.P.P.E.T.* <http://www.physics.umd.edu/ripe/muppet/papers.html>, Redish, E.F. (1995) (accessed 20 December 2001).

Preparing for a New Calculus, *Mathematical Association of America*, Washington (DC), vol. 36, Solow, A.E. (ed.) (1994).

“Introduction” to: Stewart, J., *Calculus*, 4th Edition, Brooks/Cole, Pacific Grove (CA), Stewart, J. (1999).

### URLs

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Asgnt\\_1.pdf](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Asgnt_1.pdf)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Asgnt\\_1\\_soln.pdf](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Asgnt_1_soln.pdf)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Jillian.xls](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Jillian.xls)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Jillian\\_demo.xls](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Jillian_demo.xls)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/quantum\\_well.xls](http://www.deakin.edu.au/~lim/teaching/quantum_mech/quantum_well.xls)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Morse.pdf](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Morse.pdf)

[http://www.deakin.edu.au/~lim/teaching/quantum\\_mech/Morse\\_exercise.XLS](http://www.deakin.edu.au/~lim/teaching/quantum_mech/Morse_exercise.XLS)