USING SPREADSHEETS IN CHEMICAL EDUCATION TO AVOID SYMBOLIC MATHEMATICS

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ABSTRACT

Traditionally, quantum theory has traditionally relied heavily on the use of mathematics. However, there is a significant cohort of students who are weak in mathematics, for example, students who are majoring in biochemistry, biological sciences, etc. This paper reports on the use of spreadsheets to generate approximate numerical solutions and visual (graphical) descriptions as a method of avoiding or minimizing symbolic manipulations, mathematical derivations and numerical computation. A specific example from quantum theory is provided. Some aspects of educational pedagogy of spreadsheet usage are discussed.

KEYWORDS

Physical chemistry
Quantum mechanics / Schrödinger equation
Mathematics in chemistry education
Computer-Aided Instruction
Spreadsheet
Teaching/Learning Aids

INTRODUCTION

Traditionally, quantum theory has been viewed as a “difficult” topic, mainly because of the symbolic-mathematical content. For example, Francl notes that two semesters of calculus is usually required for physical chemistry *(1)*, and this is certainly true for quantum theory. The traditional approach emphases the use of mathematical equations, derivations and calculations. How do we deal with non-chemistry majors who have a weak background in mathematics, but wish to study p-chem? Similarly, how do we deal with chemistry majors who have a weak background in mathematics?

Interestingly, the last 20-30 years has witnessed a paradigm shift in the *practice* of quantum chemistry. Leading up to the 1970s, quantum chemistry was monopolized by *theoretical* chemists, who were as much mathematicians as chemists. One had to be conversant with the mathematical methodology in order to perform a quantum calculation. More recently, the amazing increases in computing power have lead to graphical user interfaces, which has enabled a new group of *computational* chemists. These *computational* chemists are interested only in the significance of the *computed results*, not in the details of the mathematical methods used. However, the same paradigm shift in the *teaching* of quantum chemistry has *not* occurred yet: students are still required to be competent mathematicians.

The "new calculus" in mathematics education (eg, *2*) advocates the "rule of four" (numerical, graphical, symbolic and verbal descriptions) to deepen students' conceptual understanding (eg, *3*). This "new calculus" acknowledges that a predominantly symbolic approach to mathematics is suitable for some, but not all, students. The greater emphasis on graphical and verbal descriptions of a "problem" enables students to focus on the qualitative results. The numerical approach can refer either to approximate numerical solutions (cf modern computational chemistry software) or to specific numerical examples of more general symbolic equations.

This paper describes the use of spreadsheets to generate approximate numerical solutions and visual (graphical) descriptions as a method of avoiding or minimizing symbolic manipulations, mathematical derivations and numerical computation. The aim here is to teach the qualitative results that arise from quantum theory, but with less "math". The specific example of the one-dimensional Schrödinger equation and some aspects of the educational pedagogy of spreadsheet usage are discussed.

CASE STUDY: THE 1-DIMENSIONAL SCHRÖDINGER EQUATION

Quantum theory is a key part of chemistry. In freshman chemistry, students learn that:

- “Allowed” energy levels are quantized, but usually without a full appreciation of why;
- Electrons (and atoms?) exhibit both wave-like and particle-like behaviour.

Students are usually first introduced to quantum theory through the wavefunctions for the 1-dimensional Schrödinger equation. Exact solutions are derived for the particle-in-a-box (the Kuhn model (*4*)) and the simple harmonic oscillator model. The shapes of the potentials for these models are shown in Figure 1.

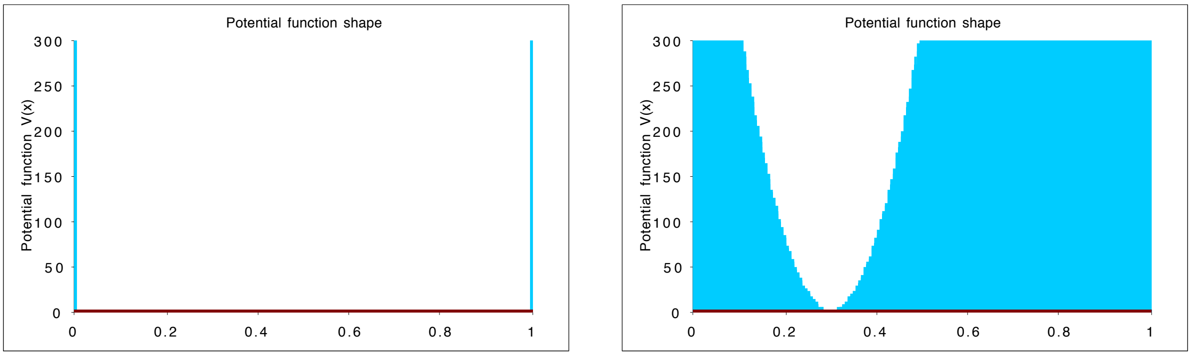


Figure 1. Potential functions for the particle-in-a-box model (left) and the simple harmonic oscillator model (right).

The exact wavefunction solutions for these models are of the form (eg *5*):

particle-in-a-box model: $$\psi = \left(\frac{2}{l}\right)^{1/2} \sin\left(\frac{n\pi x}{l}\right) \qquad \text{Equation 1}$$

simple harmonic oscillator model: $$\psi = \exp\left(\frac{-ax^2}{2}\right) H_n(x) \qquad \text{Equation 2}$$

where $H_n(x)$ is the Hermite polynomial of order n. The novice learner sees the *differences* between Equation 1 and Equation 2 and concludes that every potential is treated as a special case!

Potentials such has the triangular and stepped-valley models, shown in Figure 2, have no closed-form (ie analytic) wavefunction solutions. Similarly, the quantized energies cannot be given by any analytic equation. Here, the novice learner concludes incorrectly either that quantum mechanics does not apply, or that many systems are not quantized!

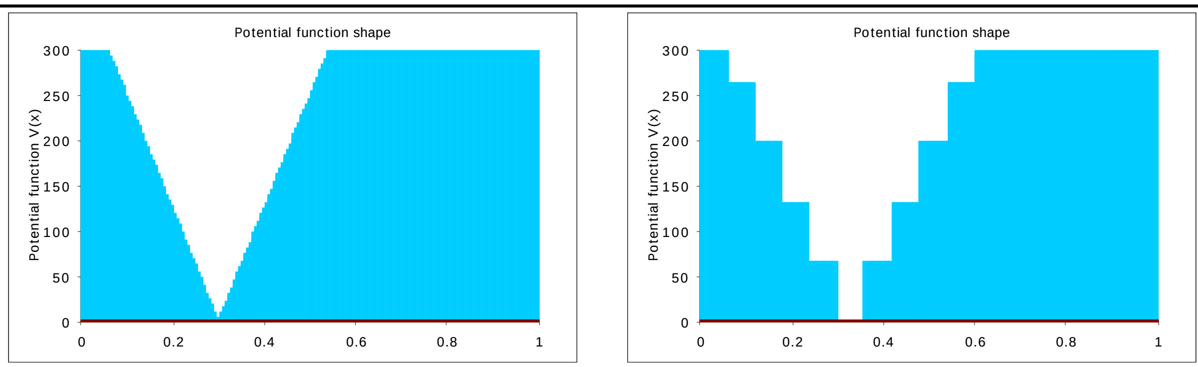


Figure 2. Simple piecewise-continuous potential functions for which the wavefunction does not have any closed form: a triangular potential (left) and a stepped-valley potential (right).

In p-chem classes at Deakin University, the derivative is explained as the "slope of a function". The 2nd order differential Schrödinger equation for an electron-in-a-box (the Kuhn model (*4*)) is explained as "finding the slope of a slope". The 1st 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. More-able students can construct an appropriate spreadsheet (to find numerical solutions to the Schrödinger equation), but mostly, spreadsheet quantum_well.xls <http://www.deakin.edu.au/~lim/KFLim/papers/2003_Spreadsheet_CCEN/quantum_well.xls>, implementing the Schrödinger equation, is provided as a "black box" to weaker students. (The pros and cons of black box methods are discussed below in the Discussion section.) Using the spreadsheet quantum_well.xls, students test how the shape of a trial "wavefunction" changes as the energy is varied (Figure 3). A copy of the instructions to students for this exercise can be found at <http://www.deakin.edu.au/~lim/KFLim/papers/2003_Spreadsheet_CCEN/Asgnt_1_6.pdf>. The wavefunction solutions are classed as "valid" or "invalid" depending on whether the boundary conditions are satisfied as energy is varied (the shooting method (*6*)).

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 potential (Figure 3). It is observed that, as wavelength decreases, the number of nodes (the zeroes or roots of the wavefunction) increases with energy. An extension of this exercise using a skipping rope easily verifies that it is more difficult (higher energy) to swing the rope with nodes present than without any nodes (lower energy). Since the sign of the wavefunction changes across a node, the qualitative shape of the wavefunction can be generated from the nodal pattern. (One strategy in de Bono's *Lateral Thinking* (*7*) is to concentrate on what is *not* present — ie 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 π molecular orbitals for cyclopentadienyl have, in increasing order of energy, no nodes, one node and two nodes respectively (Figure 4). Similarly, the rotational wavefunctions can be generated by considering nodal patterns on the surface of a sphere. Much of Schrödinger's original work was based on Hamilton's mathematical description of standing waves on a planet completely covered by ocean (ie water waves on a spherical surface). Note that these "spherical waves" correspond to combinations of the spherical harmonic functions, and can be obtained from the symmetry — "topology" — of the nodal patterns on the surface of a sphere.

On further exploration with the spreadsheet quantum_well.xls, students discover that the shapes of the allowed one-dimensional wavefunctions are similar (Figure 5), even for different potential models: ie, the lowest-energy wavefunctions all have one "bump", with no nodes.

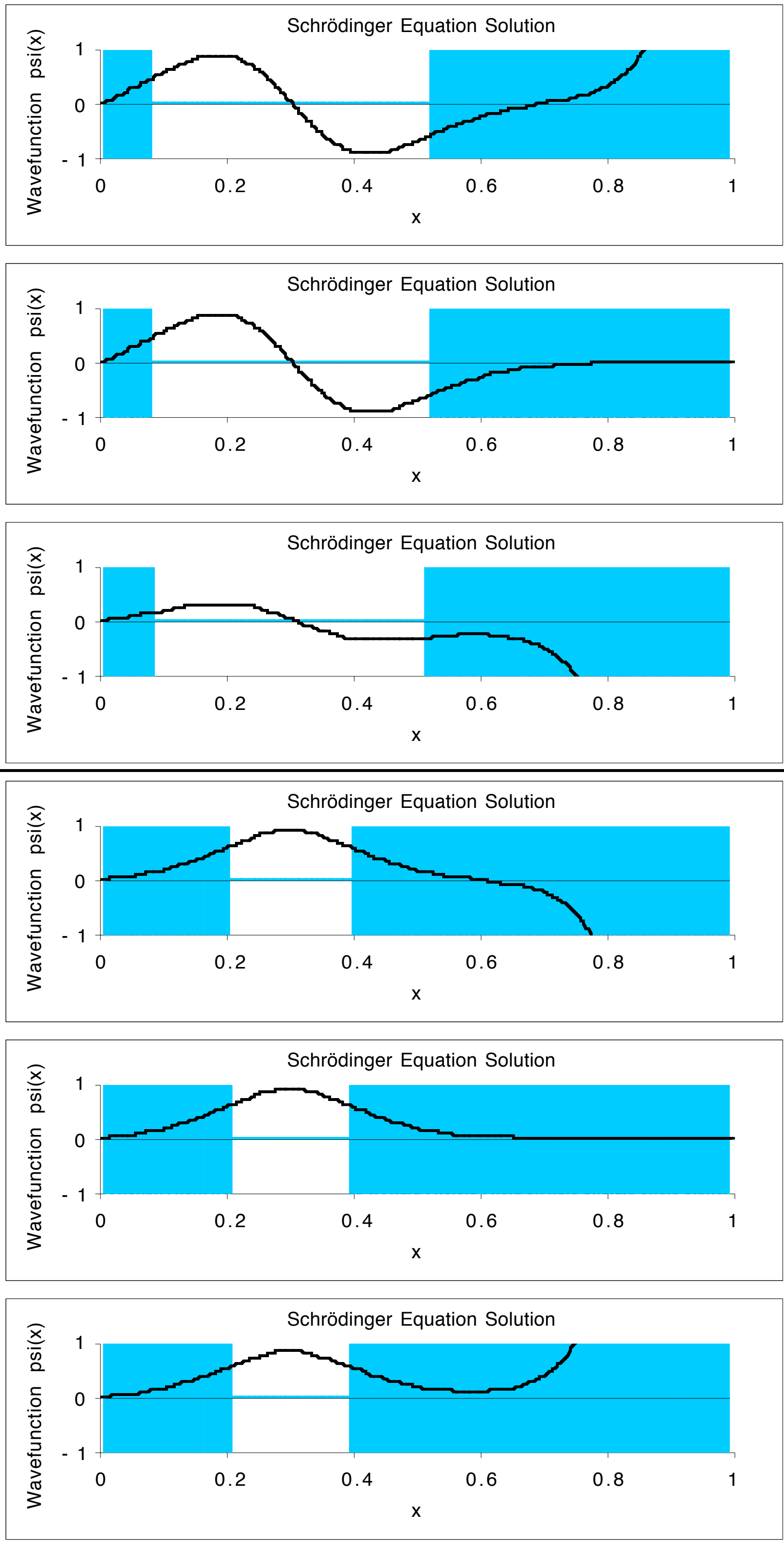


Figure 3. Approximate trial wavefunctions for the triangular potential (Figure 2), arranged from high energy (top) to low energy (bottom). Shaded domains are the forbidden region: $V(x) < E$.

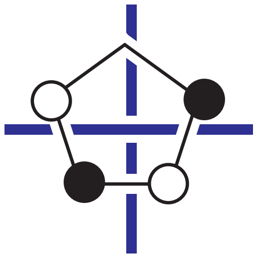
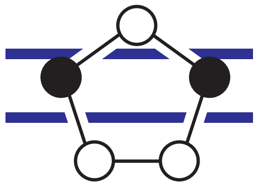
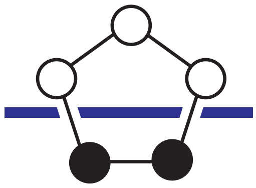
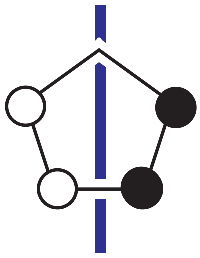
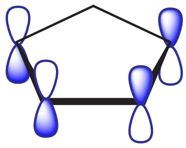
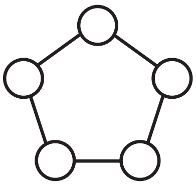
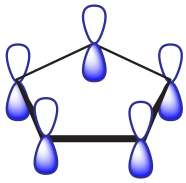
Highest energy π orbitals: Two nodes	 	
One node	 	eg 
Lowest energy π orbital: No node		eg 

Figure 4. π molecular orbitals for cyclopentadienyl. Shading of the circles in the centre panels represents the sign (direction) of the p_z orbitals. The p_z orbitals change sign across nodal planes, which are shown as blue lines.

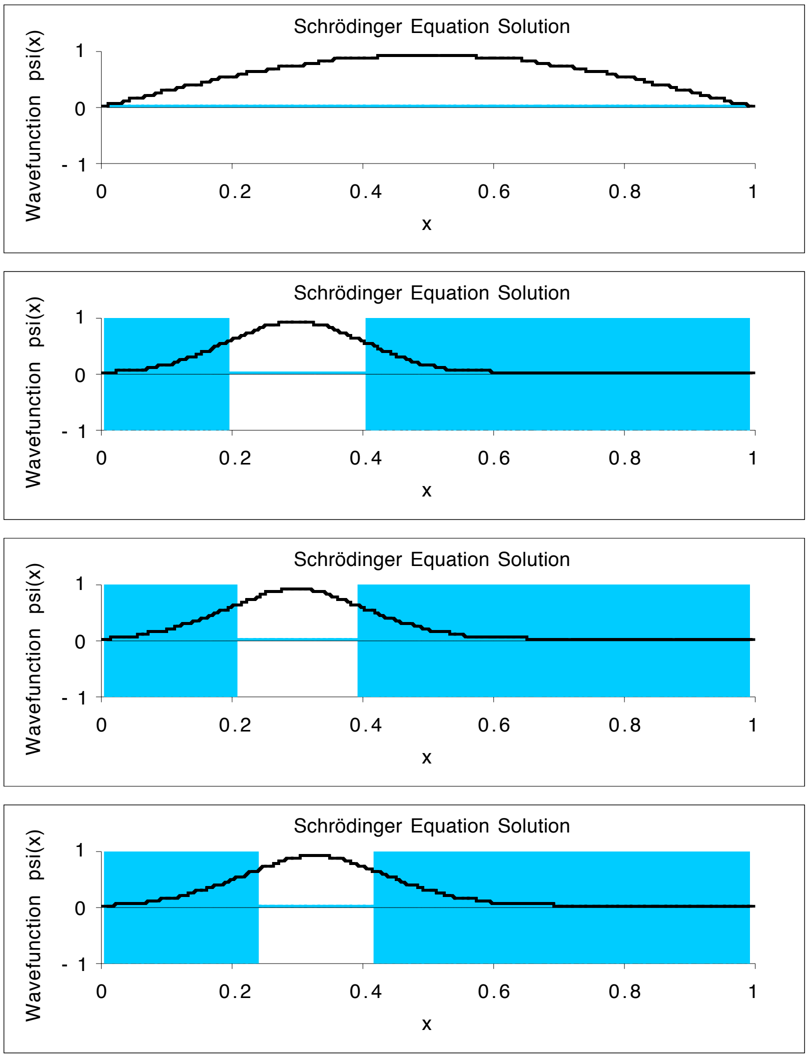


Figure 5. Lowest-energy approximate wavefunctions for the particle-in-a-box (top panel), simple harmonic oscillator (2nd panel), triangular (3rd panel) and stepped-valley (bottom panel) potentials of Figure 1 and Figure 2. Shaded domains are the forbidden region: $V(x) < E$.

It can be seen from the top three panels of Figure 3 that trial energies that are very close to exact energies result in wavefunctions that are very close in shape to the allowed wavefunction. This is also seen in the bottom three panels of Figure 3. The smaller the difference

$$\Delta E = E_{\text{trail}} - E_{\text{exact}} \qquad \text{Equation 3}$$

the longer it will be before students can distinguish visually differences between the "almost-right" wavefunctions and the "true" solution, resulting in the "lifetime-broadening" form of the Heisenberg uncertainty principle:

$$\Delta E\, \tau \approx \hbar \qquad \text{Equation 4}$$

Other concepts that can be illustrated by the spreadsheet quantum_well.xls are that:

- changing the shape of the potential well alters the spacing of the wavefunction energies;
- energies decrease as the potential well becomes wider. This is the "delocalization lowers energy" statement found in most organic chemistry texts (eg, *8*). Indeed, the electron-in-a-box model (the Kuhn model) was originally (*4*) developed to describe conjugated π systems;
- energies increase as barriers are introduced (eg Kronig-Penney model);
- wavefunctions can tunnel through barriers (eg Kronig-Penney model or Eckert potential); and
- the use of a series of square wells separated by barriers (extended Kronig-Penney model) illustrates that interactions between wells split energy levels. As the number of wells increases, the (single-well) energy splits into a quasi-continuous band of energies, giving rise to the band theory for conductors and semi-conductors.

DISCUSSION

Although there has been a substantial history in the use of spreadsheet and graphical applications in education (eg *9,10*), the author believes that full utilization of the technology, especially in chemical education, has not been realized.

The aim of this paper is to teach the *qualitative results* that arise from applying mathematics to physical and chemical systems, but without the mathematical rigour: "teaching maths with minimal maths". The "new calculus" advocates the "rule of four" (numerical, graphical, symbolic and verbal descriptions) to deepen students' conceptual understanding (*2*). Students who have a weak background in mathematics do not have the knowledge of calculus required for the usual symbolic algebra approach to physical chemistry. 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.

The Logical-Mathematical intelligence is only one of multiple "intelligences" (*11*). By changing the emphasis away from mathematical calculus, the numerical-experimental activity, can also cater to those students who favour Spatial or Bodily-Kinaesthetic intelligences. A combination of this spreadsheet approach with the traditional calculus-based approach will enable more students (and students of more types of “intelligences”) to study quantum theory.

This paper has focused on the use of spreadsheets but, in principle, the simulations can be done using symbolic mathematical packages such as Mathematica, Maple or MathCAD. This would only be feasible for students who already have a strong mathematical background. This author prefers the use of spreadsheets for weaker students for the following reasons. The symbolic mathematical packages depend on the use of a symbolic, quasi-programming language, which can present an additional learning obstacle for many students (*12*). Furthermore, the access to symbolic mathematical packages is usually more limited than that of spreadsheets, which are widely available in home, business and community settings. The “worldware” (*13,14*) (also called “application-software” (*15*)) nature of spreadsheets means that students will have greater opportunities to use and become familiar with spreadsheets than with (eg) symbolic mathematical packages, leading to greater utility and expertise. Software that isn't designed for instruction can still be good for learning (*13*). (A “straw poll” of physical chemistry faculty suggests that significantly more faculty use spreadsheets in teaching and learning activities than symbolic mathematical packages (*16*).

While weaker students will use the spreadsheets, discussed in this paper, as “black boxes”, more-able students can construct similar, appropriate spreadsheets (eg *17,18,19*). Instructors will need to be careful in deciding to use the “black box” approach or to require students construct their own. *If successfully completed*, the latter approach will promote deeper learning (*19*), but the greater complexity of the task (*12*) may mean that some students cannot complete the task, resulting in frustration and lack of learning.

The key feature of using spreadsheets is that students do “numerical experiments”. (There is an interesting discussion of the use of numerical experiments in (*20-22*). Numerical experiments (eg *23*) were also a key part of the development of chaos theory (*20*).) By playing with “what-if” scenarios, students can test the validity of their concepts and ideas: the success of using spreadsheets in this way is supported by cognitive constructivist models of learning (*15,24,25*). The use of spreadsheets is intended to give students a qualitative appreciation of quantum theory, and does not serve as a pre-requisite to more advanced studies in quantum theory, for which a reasonable knowledge of mathematics is required.

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ABOUT THE AUTHOR

Kieran F. Lim (林百君) obtained his BSc (Hons) and PhD in theoretical chemistry from the University of Sydney. He was awarded an Archbishop Mannix Travelling Scholarship to Stanford University and been a faculty member at the University of New England, the University of Melbourne and Deakin University, where he is currently a Senior Lecturer in Chemical Sciences (equivalent to Associate Professor or Professor in North America). He is a Member (MRACI), Chartered Chemist(CChem) and Certified Practising Chemist (CPChem) of the Royal Australian Chemical Institute, and a Member (MACS) and Practising Computer Professional (PCP) of the Australian Computer Society.

Dr Lim is a recipient of the Royal Australian Chemical Institute's Division of Chemical Education Citation for significant contributions to chemical education (2002) and the Faculty of Science and Technology's Excellence in Teaching Award (1996 and 2000).

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