Using Physics to Learn Mathematica® to Do Physics:
From Homework Problems to Research Examples

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Abstract

We describe the development of a junior-senior level course for Physics majors designed to teach Mathematica® skills in support of their undergraduate coursework, but also to introduce students to modern research level results. Standard introductory and intermediate level Physics homework-style problems are used to teach Mathematica® commands and programming methods, which are then applied, in turn, to more sophisticated problems in some of the core undergraduate subjects, along with making contact with recent research papers in a variety of fields.

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I. INTRODUCTION

Computational methods play an increasingly important role in the professional life of many working physicists, whether in experiment or theory, and very explicitly indeed for those doing simulational work, a ‘category’ that might not even have been listed separately when some senior Physics faculty were students themselves. That same reality is reflected in the curriculum requirements and course offerings at any number of undergraduate institutions, ranging from specific programming classes required in the major to entire computational physics programs [1] - [5].

At my institution, three of the five options in the Physics major require at least one programming course (from a list including C++, Visual Basic, Java, and even Fortran) offered by departments outside of Physics, so the majority of our majors typically have a reasonable amount of programming experience no later than the end of their sophomore year, in time to start serious undergraduate research here (or elsewhere, in REU programs) during their second summer, often earlier. Students in our major, however, have historically expressed an interest in a course devoted to one of the popular integrated multi-purpose (including symbolic manipulation) programming languages such as Mathematica®, Maple, or MatLab, taught in the context of its application to physics problems, both in the undergraduate curriculum, and beyond, especially including applications to research level problems.

In a more global context, studies from Physics Education Research have suggested that computer-based visualization methods can help address student misconceptions with challenging subjects, such as quantum mechanics [6], so the hope was that such a course would also provide students with increased experience with visualization tools, in a wide variety of areas, thereby giving them the ability to generate their own examples.

With these motivations in mind, we developed a one-credit computational physics course along somewhat novel lines, first offered in the Spring 2007 semester. In what follows, I review (in Sec. II) the structure of the course, then describe some of the homework-to-research related activities developed for the class (in Sec. III), and finally briefly outline some of the lessons learned and conclusions drawn from this experimental computational physics course. An Appendix contains a brief lecture-by-lecture description of the course as well as some data on student satisfaction with each lecture topic.
II. DESCRIPTION OF THE COURSE

Based on a variety of inputs (student responses to an early survey of interest, faculty expertise in particular programming languages and experience in their use in both pedagogical and research level applications, as well as practical considerations such as the ready accessibility of hardware and software in a convenient computer lab setting) the course was conceptualized as a one-credit “Introduction to Mathematica in Physics” course. The strategies outlined in the course syllabus to help achieve the goals suggested by the students are best described as follows:

(i) First use familiar problems from introductory physics and/or math courses to learn basic Mathematica® commands and programming methods.

(ii) Then use those techniques to probe harder Physics problems at the junior-senior level, motivating the need for new Mathematica® skills and more extensive program writing to address junior-senior level Physics problems not typically covered in standard courses.

(iii) Finally, extend and expand the programming experience in order to obtain results comparable to some appearing in the research literature.

This ‘vertical’ structure was intentionally woven with cross-cutting themes involving comparisons of similar computational methods across topics, including numerical solutions of differential equations, matrix methods, special functions, connections between classical and quantum mechanical results, etc.. In that context, the emphasis was almost always on breadth over depth, reviewing a large number of both physics topics and programming commands/methods, rather than focusing on more detailed and extensive code writing. The visualization of both analytic and numerical results in a variety of ways was also consistently emphasized.

Ideas for some lecture topics came from the wide array of ‘Physics and Mathematica®’ books available, [4] - [13], but others were generated from past experience with teaching junior-senior level courses on ‘core’ topics, pedagogical papers involving the use of computational methods and projects (from the pages of AJP and elsewhere), and especially from the research literature.
Given my own interests in quantum mechanics and semi-classical methods, there was an emphasis on topics related to those areas. On the other hand, despite many excellent simulations in the areas of thermodynamics and statistical mechanics, because of my lack of experience in teaching advanced undergraduate courses on such topics, we covered only random walk processes in this general area. Finally, the desire to make strong connections between research results and standardly seen topics in the undergraduate curriculum had a very strong affect on the choice of many components.

Weekly lectures (generated with LaTeX and printed into .pdf format) were uploaded to a course web site, along with a number of (uncompiled) Mathematica notebooks for each weeks presentation. Links were provided to a variety of accompanying materials, including on-line resources, such as very useful MathWorld (http://mathworld.wolfram.com) articles and carefully vetted Wikipedia (http://wikipedia.org/) entries, as well as .pdf copies of research papers, organized by lecture topic. The lecture notes were not designed to be exhaustive, as we often made use of original published papers as more detailed resources, motivating the common practice of working scientists to learn directly from the research literature. While there was no required text (or one we even consulted regularly) a variety of Mathematica books (including Refs. [8] - [13] and others) were put on reserve in the library.

While the lecture notes and Mathematica notebooks were (and still are) publicly available, because of copyright issues related to the published research papers, the links to those components were necessarily password protected. (However, complete publication information is given for each link so other users can find copies from their own local college or university subscriptions.) The web pages for the course have been revised slightly since the end of the Spring 2007 semester, but otherwise represent fairly well the state of the course at the end of the first offering. The site will be hereafter kept ‘as-is’ to reflect its state at this stage of development and the URL is www.phys.psu.edu/~rick/MATH/PHYS497.html. We have included at the site an extended version of this paper, providing more details about the course as well as personal observations about its development and outcomes.

A short list of topics covered (by lecture) is included in the Appendix, and we will periodically refer to lectures below with the notation L1, L2, etc. in Sec. III but we will assume that readers with experience or interest in Mathematica will download the notebooks and run them for more details.
III. SAMPLE ACTIVITIES

A. Learning Mathematica® commands

As an example of the philosophy behind the course structure, the first lecture at which serious Mathematica® commands were introduced and some simple code designed (L2), began with an extremely brief review (via the on-line lecture notes) of the standard E&M problem of the on-axis magnetic field of a Helmholtz coil arrangement. This problem is discussed (or at least assigned as a problem) in many textbooks [15] and requires only straightforward, if tedious, calculus (evaluating up through a 4th derivative) and algebra to find the optimal separation to ensure a highly uniform magnetic field at the center of two coils. A heavily commented sample program was used to ‘solve’ this problem, which introduced students to many of the simplest Mathematica® constructs, such as defining and plotting functions, and some of the most obvious calculus and algebra commands, such as Series[], Normal[], Coefficient[], Expand[], and Solve[]. (It helped to have a real pair of Helmholtz coils where one could measure the separation with a ruler and compare to the radius; lecture demonstrations, even for a computational physics course, are useful!)

This simple exercise was then compared (at a very cursory level) to a much longer, more detailed notebook written by a former PSU Physics major (now in graduate school) as part of his senior thesis project dealing with designing an atom trap. Links were provided to simple variations on this problem, namely the case of an anti-Helmholtz coil, consisting of two parallel coils, with currents in opposite directions, designed to produce an extremely uniform magnetic field gradient. We were thus able to note that the initial investment involved in mastering the original program, could, by a very simple ‘tweak’ of the notebook under discussion (requiring only changes in a few lines of code) solve a different, equally mathematically intensive problem almost for free.

B. Expanding and interfering Bose-Einstein condensates

One of the very few examples of an explicit time-dependent solution of a quantum mechanical problem in the junior-senior level curriculum (or standard textbooks at that level), in fact often the only such example, is the Gaussian wavepacket solution of the 1D free-particle Schrödinger equation. It is straightforward in Mathematica® to program readily available
textbook solutions for this system and to visualize the resulting spreading wavepackets, allowing students to change initial conditions (central position and momentum, initial spatial spread, etc.) in order to study the dependence on such parameters. Plotting the real and imaginary parts of the wavefunction, not just the modulus, also reminds students of the connection between the ‘wiggliness’ of the $\psi(x,t)$ solution and the position-momentum correlations that develop as the wave packet evolves in time \[16\]. This exercise was done early in the course (L4) when introducing visualizations and animations, but relied only on ‘modern physics’ level quantum mechanics, though most students were already familiar with this example from their junior-level quantum mechanics course.

Students can easily imagine that such Gaussian examples are only treated so extensively because they can be manipulated to obtain closed-form solutions, and often ignore the connection between that special form and its role as the ground-state solution of the harmonic oscillator. Recent advances in atom trapping have shown that Bose-Einstein condensates can be formed where the time-development of the wavefunction of the particles, initially localized in the ground-state of a harmonic trap, can be modeled by the free-expansion of such Gaussian solutions \[17\] after the trapping potential is suddenly removed. Students can then take ‘textbook-level’ Mathematica® programs showing the spreading of $p_0 = 0$ Gaussian solutions and profitably compare them with more rigorous theoretical calculations \[18\] (using the Gross-Pitaevskii model) showing the expected coherent behavior of the real and imaginary parts of the time-dependent phase of the wave function of the condensate after the trapping potential is turned off.

While this comparison is itself visually interesting, the experimental demonstration that the ‘wiggles’ in the wavefunction are truly there comes most dramatically from the Observation of Interference Between Two Bose Condensates \[19\] and one can easily extend simple existing programs to include two expanding Gaussians, and ‘observe’ the resulting interference phenomena in a simulation, including the fact that the resulting fringe contrast in the overlap region is described by a time-dependent spatial period given by $\lambda = \frac{ht}{md}$ where $d$ is the initial spatial separation of the two condensates; some resulting frames of the animation are shown in Fig 1. Since the (justly famous) observations in Ref. \[19\] are destructive in nature, a simulation showing the entire development in time of the interference pattern is especially useful.
C. Quantum wave packet revivals: 1D infinite well as a model system

The topic of wave phenomena in 1D and 2D systems, with and without boundary conditions, is one of general interest in the undergraduate curriculum, in both classical and quantum mechanical examples, and was the focus of *L5* and *L6* respectively. The numerical study of the convergence of Fourier series solutions of a ‘plucked string’, for example, can extend more formal discussions in students’ math and physics coursework. More importantly, the time-dependence of solutions obtained in a formal way via Fourier series can then also be easily visualized using the ability to *Animate*[] in *Mathematica*®.

Bridging the gap between classical and quantum mechanical wave propagation in 1D systems with boundaries (plucked classical strings versus the 1D quantum well), time-dependent Gaussian-like wave packet solutions for the 1D infinite square well can be generated by a simple generalization of the Fourier expansion, with numerically accurate approximations available for the expansion coefficients [20] to allow for rapid evaluation and plotting of the time-dependent waveform (in either position- or momentum-space.) Animations over the shorter-term classical periodicity [21] as well as the longer term quantum wave packet revival time scales [22], [23] allow students to use this simplest of all quantum models to nicely illustrate many of the revival (and fractional revival) structures possible in bound state systems, a subject which is not frequently discussed in undergraduate textbooks at this level. Examples of the early observations of these behaviors in Rydberg atoms (see, *e.g.* Ref. [24]) are then easily appreciated in the context of a more realistic system with which students are well-acquainted, and are provided as links.

D. Lotka-Volterra (predator-prey) and other non-linear equations

Students at the advanced undergraduate level will have studied the behavior of many differential equations in their math coursework (sometimes poorly motivated), along with some standard, more physically relevant, examples from their core Physics curriculum. Less familiar mathematical systems, such the Lotka-Volterra (predator-prey) equations [25], which can be used to model the time-dependent variations in population models, are easily solved in Mathematica using *NDSolve*[], and these were one topic covered in *L9*. The resulting solutions can be compared against linearized (small deviations from fixed population)
approximations for comparison with analytic methods, but are also nicely utilized to illustrate ‘time-development flow’ methods for coupled first-order equations. For example, the Lotka-Volterra equations can be written in the form

$$\frac{dr}{dt} = \frac{d}{dt} \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \alpha x(t) - \beta x(t)y(t) \\ -\gamma y(t) + \delta x(t)y(t) \end{pmatrix} = \begin{pmatrix} F(x, y) \\ G(x, y) \end{pmatrix} = V(r) \tag{1}$$

and one can use Mathematica functions such as `PlotVectorField[]` to plot $V(r)$ in the $r = (x, y)$ plane to illustrate the ‘flow’ of the time-dependent $x(t), y(t)$ solutions, themselves graphed using `ParametricPlot[]`. Note that the Lotka-Volterra equations can also be integrated exactly to obtain implicit solutions, for which `ImplicitPlot[]` can be used to visualize the results.

These methods of analysis, while seen here in the context of two coupled first-order differential equations, are just as useful for more familiar single second-order equations of the form $x''(t) = G(x(t), x'(t); t)$ by writing $y(t) = x'(t)$ to form a pair of coupled first-order equations, a common trick used when implementing tools such as the Runge-Kutta method. With this approach, familiar problems such as the damped and undamped harmonic oscillator can also be solved and visualized by the same methods, very naturally generating phase space plots.

More generally, such examples can be used to emphasize the importance of the mathematical description of nature in such life-science related areas as biophysics, population biology, and ecology. In fact, ‘phase-space’ plots of the data from one of the early experimental tests of the Lotka-Volterra description of a simplified *in vitro* biological system are a nice example of the general utility of such methods of mathematical physics. Examples of coupled non-linear equations in a wide variety of physical systems can be studied in this way, *e.g.* Ref. [27], to emphasize the usefulness of mathematical models, and computer solutions thereof, across scientific disciplines.

Other non-linear problems were studied in L8 and L9 using the `NDSolve[]` utility, including a non-linear pendulum. The motion of a charged particle in spatially- or temporally-dependent magnetic fields was also solved numerically, to be compared with closed-form solutions (obtained using `DSolve[]`) for the more familiar case of a uniform magnetic field, treated earlier in L3.
E. Novel three-body problems in classical gravity

The study of the motion of a particle moving under the influence of an inverse square law is one of the staples of classical mechanics, and every undergraduate textbook on the subject treats some aspect of this problem, usually in the context of planetary motion and Kepler’s problem. In the context of popular textbooks [28], [29], the strategy is almost always to reduce the two-body problem to a single central-force problem, use the effective potential approach to solve for $\theta(r)$ using standard integrals, and to then identify the resulting orbits with the familiar conic sections.

Solving such problems directly, using the numerical differential equation solving ability in Mathematica®, especially NDSolve[], was the single topic of L10. For example, one can first easily check standard ‘pencil-and-paper’ problems, such as the time to collide for two equal masses released from rest [30], [31] as perhaps the simplest 1D example. Given a program solving this problem, one can easily extend it to two-dimensions to solve for the orbits of two unequal mass objects for arbitrary initial conditions. Given the resulting numerically obtained $r_1(t)$ and $r_2(t)$, one can then also plot the corresponding relative and center-of-mass coordinates to make contact with textbook discussions. Effective one-particle problems can also be solved numerically to compare most directly with familiar derivations, but with monitoring of energy and angular momentum conservation made to test the numerical accuracy of the NDSolve[] utility; one can then also confirm numerically that the components of the Lenz-Runge vector [32] are conserved.

It is also straightforward to include the power-law exponent of the force law ($F(r) \propto \hat{r} r^n$ with $n = -2$ for the Coulomb/Newton potential) as a tunable parameter, and note that closed orbits are no longer seen when $n$ is changed from its inverse-square-law value, but are then recovered as one moves (far away) to the limit of the harmonic oscillator potential, $V(r) \propto r^2$ and $F(r) \propto -r$ (or $n = +1$), as discussed in many pedagogical papers pointing out the interesting connections between these two soluble problems [33].

With such programs in hand, it is relatively easy to generalize 2-body problems to 3-body examples, allowing students to make contact with both simple analytic special cases and more modern research results on special classes of orbits, as in Ref. [34]. The two most famous special cases of three equal mass particles with periodic orbits are shown in Fig. 2 (a) and (b) (and were discovered by Euler and Lagrange respectively). They are
easily analyzed using standard freshman level mechanics methods, and just as easily visualized using Mathematica\textsuperscript{©} simulations. An explicit example of one of the more surprising ‘figure-eight’ type trajectories (as shown in Fig. 2(c)) posited in Ref. [34] was discovered and discussed in detail in Ref. [35]. It has been cited by Christian, Belloni, and Brown [36] as a nice example of an easily programmable result in classical mechanics, but arising from the very modern research literature of mathematical physics. In all three cases, it’s straightforward to arrange the appropriate initial conditions to reproduce these special orbits, but also just as easy to drive them away from those values to generate more general complex trajectories, including chaotic ones. For example, the necessary initial conditions for the ‘figure-eight’ orbit [35] are given by

\begin{align}
\mathbf{r}_3^{(0)} &= (0, 0) \quad \text{and} \quad \mathbf{r}_1^{(0)} = -\mathbf{r}_2^{(0)} = (0.97000436, -0.24308753) \\
\mathbf{v}_3^{(0)} &= -2\mathbf{v}_1^{(0)} = -2\mathbf{v}_2^{(0)} = (-0.93240737, -0.86473146).
\end{align}

The study of such so-called choreographed N-body periodic orbits has flourished in the literature of mathematical physics [37] and a number of web sites illustrate some very beautiful, if esoteric, results [38].

F. Statistical simulations and random walks

Students expressed a keen interest in having more material about probability and statistical methods, so there was one lecture on the subject (L11) which was commented upon very favorably in the end-of-semester reviews (but not obviously any more popular in the numerical rankings) dealing with simple 1D and 2D random walk simulations. This included such programming issues as being able to reproduce specific configurations using constructs such as the RandomSeed[ ] utility. Such topics are then very close indeed to more research related methods such as the diffusion Monte Carlo approach to solving for the ground state of quantum systems [39], but also for more diverse applications of Brownian motion problems in areas such as biophysics [40]. The only topic relating to probability was a very short discussion of the ‘birthday problem’, motivated in part by the fact that the number of students in the course was always very close to the ‘break even’ (50-50 probability) number for having two birthdays in common!
G. Gravitational bound states of neutrons

The problem of the quantum bouncer, a particle of mass $m$ confined to a potential of the form

$$V(z) = \begin{cases} 
\infty & \text{for } z < 0 \\
Fz & \text{for } 0 \leq z
\end{cases}$$

is a staple of pedagogical articles [41] where a variety of approximation techniques can be brought to bear to estimate the ground state energy (variational methods), the large $n$ energy eigenvalues (using WKB methods), and even quantum wave packet revivals [42]. The problem can also be solved exactly, in terms of Airy functions, for direct comparison to both approximation and numerical results. While this problem might well have been historically considered of only academic interest, experiments at the ILL (Institute Laue Langevin) [43], [44] have provided evidence for the Quantum states of neutrons in the Earth’s gravitational field where the bound state potential for the neutrons (in the vertical direction at least) is modeled by Eqn. (4), using $F = m_n g$.

In the context of our course, students studied this system first in L9 in the context of the shooting method of finding well-behaved solutions of the 1D Schrödinger equation, which then correspond to the corresponding quantized energy eigenvalues. The analogous ‘half-oscillator’ problem, namely the standard harmonic oscillator, but with an infinite wall at the origin, can be used as a simple starting example for this method, motivating the boundary conditions ($\psi(x = 0) = 0$ and $\psi'(0)$ arbitrary) imposed by the quantum bouncer problem. It can then be used as a testbed for the shooting method, seeing how well the exact energy eigenvalues, namely the values $E_n = (n + 1/2)\hbar \omega$ with $n$ odd, are reproduced.

The change to dimensionless variables for the neutron-bouncer problem already provides insight into the natural length and energy scales of the system, allowing for an early comparison to the experimental values obtained in Refs. [43], [44]. In fact, the necessary dimensionful combinations of fundamental parameters ($\hbar$, $m_n$, $g$) can be reduced (in a sledge-hammer sort of way) using the built-in numerical values of the physical constants available in Mathematica® (loading <<Miscellaneous‘PhysicalConstants‘) which the students found amusing, although Mathematica® did not automatically recognize that Joule = Kilogram Meter^2/Second^2. The numerically obtained energy eigenvalues (obtained by bracketing solutions which diverge to $\pm\infty$) can be readily obtained and compared
to the ‘exact’ values, but estimates of the accuracy and precision of the shooting method results are already available from earlier experience with the ‘half-oscillator’ example.

Then, in the lecture on special functions (L12) this problem is revisited using the exact Airy function solutions, where one can then easily obtain the properly normalized wavefunctions for comparison with the results shown in Fig. 1 of Ref. [43], along with quantities such as the expectation values and spreads in position, all obtained using the \texttt{NIntegrate[ ]} command. Once experience is gained with using the \texttt{FindRoot[ ]} option to acquire the Airy zeros (and corresponding energies), one can automate the entire process to evaluate all of the parameters for a large number of low-lying states using a \texttt{Do[ ]} structure. Obtaining physical values for such quantities as $\langle n|z|n \rangle$ for the low-lying states was useful as their macroscopic magnitudes (10’s of $\mu m$) play an important role in the experimental identification of the quantum bound states.

More generally, the study of the $Ai(z)$ and $Bi(z)$ solutions of the Airy differential equation provided an opportunity to review general properties of second-order differential equations in 1D of relevance to quantum mechanics. Topics discussed in this context included the behavior of the Airy solutions for $E > Fz$ (two linearly independent oscillatory functions, with amplitudes and ‘wiggliness’ related to the potential) and for $E < Fz$ (exponentially growing and decaying solutions) with comparisons to the far more familiar case arising from the study of a step potential.

H. 2D circular membranes and infinite wells using Bessel functions

Following up on L6 covering 2D wave physics, a section of L12 on special functions was devoted to Bessel function solutions of the 2D wave equation for classical circular drumheads and for quantum circular infinite wells. Many features of the short- and long-distance behavior of Bessel functions can be understood in terms of their quantum mechanical analogs as free-particle solutions of the 2D Schrödinger equation, and these aspects are emphasized in the first discussion of their derivation and properties in the lecture notes. Such solutions can then be compared to now-famous results analyzing the Confinement of electrons to quantum corrals on a metal surface [45] using just such a model of an infinite circular well.

The vibrational modes of circular drumheads can, of course, also be analyzed in this context, and a rather focused discussion of the different classical oscillation fre-
quencies obtained from the Bessel function zeros was motivated, in part, by an ob-
vious error in an otherwise very nice on-line simulation of such phenomena. The
site http://www.kettering.edu/~drussell/Demos/MembraneCircle/Circle.html dis-
plays the nodal patterns for several of the lowest-lying vibrational modes, but the oscillations
are ‘synched up’ upon loading the web page, so that they all appear to have the same oscilla-
tion frequency; hence an emphasis in this section on ‘bug-checking’ against various limiting
cases, the use of common sense in simulations, and the perils of visualization.

I. Normal mode statistics in 2D classical and quantum systems: Weyl area rule
and periodic orbit theory

The discussions of the energy eigenvalues (normal mode frequencies) for a variety of 2D
infinite well geometries (drumhead shapes) generated earlier in the semester, allowed us
to focus on using information encoded in the ‘spectra’ arising from various shapes and its
connection to classical and quantum results in L13. For example, the Weyl area rule [46]
for the number of allowed k-states in the range \((k, k + dk)\) for a 2D shape of area \(A\) and
perimeter \(P\) is given by

\[
dN(k) = \left[\frac{A}{2\pi} - \frac{P}{4\pi}\right] dk, \quad (5)
\]

which upon integration gives

\[
N(k) = \frac{A}{4\pi} k^2 - \frac{P}{4\pi} k. \quad (6)
\]

Identical results in quantum mechanics are obtained by using the free-particle energy con-
nection

\[
E = \frac{\hbar^2 k^2}{2m} \quad \text{or} \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (7)
\]

so that in the context of the Schrödinger equation for free-particles bound inside 2D infinite
well ‘footprints’, we have

\[
N(E) = \frac{A}{4\pi} \left(\frac{2m}{\hbar^2} E\right) - \frac{P}{4\pi} \sqrt{\frac{2mE}{\hbar^2}}. \quad (8)
\]

Given a long list of \(k\) (or \(E\)) values for a given geometry, it is straightforward to order them
and produce the experimental ‘staircase’ function

\[
N(k) = \sum_i \theta(k - k_i) \quad (9)
\]
and so the Weyl-like result of Eqn. (6) will be an approximation to a smoothed out version of the 'data'. A relatively large number of 'exact' solutions are possible for such 2D geometries, including the square, rectangle, $45^\circ - 45^\circ - 90^\circ$ triangle (isosceles triangle obtained from a square cut along the diagonal [46], [47]), equilateral ($60^\circ - 60^\circ - 60^\circ$) triangle [48] and variations thereof, as well as circular or half-circular wells, and many variations [49]. (We note that current versions of Mathematica give extensive lists of zeros of Bessel functions, by loading <<NumericalMath'BesselZeros', which allows for much more automated manipulations of solutions related to the circular cases.)

As an example, we show in Fig. 3a comparison between the ‘theoretical’ result in Eqn. (6) and the ‘experimental’ data in Eqn. (9) for the isosceles right triangle. In this case, the area and perimeter are $A = L^2/2$ and $P = (2 + \sqrt{2})L$ respectively, and the allowed $k$ values are $k_{n,m} = \pi \sqrt{n^2 + m^2}/L$ where $n > m \geq 1$, namely those for the square but with a restriction on the allowed ‘quantum numbers’.

While that type of analysis belongs to the canon of classical mathematical physics results, more modern work on periodic orbit theory has found a much deeper relationship between the quantum mechanical energy eigenvalue spectrum and the classical closed orbits of the same system [50], [51]. Given the spectra for the infinite well ‘footprints’ mentioned above, it is easy to generate a minimal Mathematica program [52] to evaluate the necessary Fourier transforms to visualize the contributions of the familiar (and some not so familiar [53]) orbits in such geometries; in fact, an efficient version of this type of analysis is used as an example of good Mathematica programming techniques in Ref. [54]. Links to experimental results using periodic orbit theory methods in novel contexts [55] are then possible.

These types of heavily numerical analyses, which either generate or make use of energy spectra, can lead to interesting projects based on pedagogical articles which reflect important research connections, such as in Refs. [56] and [57].

**J. Other topics**

In the original plan, the last two lectures were to be reserved for examples related to chaos. We did indeed retain L14 for a focused discussion of chaotic behavior in a simple deterministic system, namely the logistic equation, using this oft-discussed calculational example, which requires only repeated applications of a simple iterative map of the form
\[ x_{n+1} = cx_n(1 - x_n) \]
as one of the most familiar examples, citing its connections to many physical processes. The intent was to then continue in earlier studies of the ‘real’ pendulum (to now include driving forces) to explore the wide variety of possible states, including chaotic behavior.

Based on student comments early in the semester, however, there was a desire among many of the students (especially seniors) to see examples of Mathematica® programs being used for ‘real-time’ research amongst the large graduate student population in the department. One senior grad student, Cristiano Nisoli, who had just defended his thesis, kindly volunteered to give the last lecture, demonstrating in detail some of his Mathematica® notebooks and explaining how the results they generated found their way into many of his published papers. Examples included generating simple graphics (since we made only occasional use of Graphics[] elements and absolutely no use of palette symbols) to much more sophisticated dynamical simulations (some using genetic algorithm techniques) requiring days of running time. While some of the physics results were obviously far beyond the students experience, a large number of examples of Mathematica® command structures and code-writing methods were clearly recognizable from programs we’d covered earlier in the semester, including such ‘best-practice’ checks as monitoring (numerically) the total energy of a system, in this case, in various Verlet algorithms. Some of the Mathematica® notebooks and published papers he discussed are linked at the course web site.

IV. LESSONS AND CONCLUSIONS

Evaluation and assessment can be one of the most challenging aspects of any educational enterprise, and many scientists may not be well trained to generate truly meaningful appraisals of their own pedagogical experiments. In the case of this course, where the goals were less specific and fixed than in a standard junior-senior level course in a traditional subject area, that might be especially true. Since the course was not designed to cover one specific set of topics, the use of well-known instruments for assessment such as the FCI and others for concepts related to topics more often treated at the introductory level, or specialized ones covering more advanced topics, did not seem directly relevant.

Weekly graded homework assignments were used to evaluate the students, but during
the entire development and delivery of the course, there were also attempts at repeatedly obtaining student feedback, at regular intervals. Some of the results can be shared here, but we stress that they are only of the ‘student satisfaction’ type. We note that in the Spring 2007 semester, there were a total of 23 students enrolled in this trial offering, 12 juniors and 11 seniors, 4 female and 19 male, 21 Physics majors and 2 majors in Astronomy/Astrophysics.

Students in almost every course at Penn State are asked to provide anonymous ‘Student Ratings of Teaching Effectiveness’ each semester. Four questions are common to every form, including Rate the overall quality of the course and Rate the overall quality of the instructor, all on a scale from 1-7. For the initial offering of this Mathematica® course, the results for those two questions (obtained after the semester was over and grades were finalized and posted) were found to be 6.05/7.00 and 6.89/7.00 respectively. Additional ‘in-house’ departmental evaluation forms were used to solicit students comments, and were also only returned after the semester was completed. These forms are very open-ended and only include instructions such as In the spaces below, please comment separately about the COURSE and about the LECTURER. All of the resulting comments were positive, and consistent with similar feedback obtained from the ‘for-credit’ surveys. While such results are certainly encouraging, recall that the students registered for the course were highly self-selected and all rightly answered in the same surveys that this course was a true elective and not required in our major.

One of the very few explicit goals was to try to encourage students to make use of Mathematica® in their other coursework, and a question related to just such outcomes was posed in a final survey. The vast majority of students replied that they had used it somewhat or even extensively in their other courses that semester. For juniors, the examples were quantum mechanics (doing integrals, plotting functions), the complex analysis math course (doing integrals to compare to results obtained by contour integration) and to some extent in the statistical mechanics course. For seniors, the typical uses were in their Physics elective courses (especially the math intensive Special and General Relativity elective), a senior electronics course (where the professor has long made use of ‘canned’ Mathematica® programs) and senior level Mathematics electives being taken to fulfill the requirements of a minor or second major. At least one student used Mathematica® techniques to complete an Honors option in a course he was taking, but the majority seemed to use Mathematica® in either ‘graphing calculator’ or ‘math handbook’ modes, and not for further extensive programming.
Finally, while I used Mathematica® as the programming tool, set in a LINUX classroom, for the development and delivery of this course, these choices were only because of my personal experience with the software and the readily available access to the hardware, as I have no very strong sectarian feelings about either component. I think that many Physics faculty with facility in languages such as Maple or MatLab, access to a computer lab/classroom facility, and personal interests in modern research in a wide variety of areas can rather straightforwardly generate a similar course. I only suggest that the approach, namely using introductory Physics and Math problems to motivate the use of an integrated programming language, which can then be used to bridge the gap between more advanced coursework and research results, can be a fruitful one.

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APPENDIX A: COURSE OUTLINE

We include a rough outline of the course material, organized by lecture, but remind readers that the entire set of materials is available on-line at the web site mentioned in Sec. [II]. The numbers (with error bars) after each lecture are the results of student evaluations of each lecture, asking for ratings of “...interest, understandability, and general usefulness...” on a scale from 1 (low) to 3 (medium) to 5 (high), combining all aspects of each presentation. Differences in the ratings between the junior and senior groups were typically not significant so the results for all students have been combined, except for L12. The last two lectures which covered material which students hadn’t ever seen in their undergraduate coursework, were somewhat less popular, although some seniors cited L14 as the most interesting of all.
L1 - Introduction to the course (4.0 ± 0.8)
L2 - Getting started with Mathematica® (4.4 ± 0.7)
L3 - Exactly soluble differential equations in classical physics (4.2 ± 0.7)
L4 - Visualization and animations (4.6 ± 0.6)
L5 - 1D wave physics (4.3 ± 0.7)
L6 - 2D wave physics (4.3 ± 0.8)
L7 - Vectors/matrices and Fourier transform (4.0 ± 0.8)
L8 - Numerical solutions of differential equations I (4.4 ± 0.8)
L9 - Numerical solutions of differential equations II (4.2 ± 0.7)
L10 - Classical gravitation (4.2 ± 0.7)
L11 - Probability and statistics (4.0 ± 0.8)
L12 - Special functions and orthogonal polynomials in classical and quantum mechanics (4.7 ± 0.5 for juniors, but 3.9 ± 0.7 for seniors)
L13 - Normal mode (energy eigenvalue) statistics in 2D classical and quantum systems (3.9 ± 0.7)
L14 - Chaos in deterministic systems (3.9 ± 0.8)
L15 - Guest speaker: Graduate student use of Mathematica® in research (No data available)
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FIG. 1: Position-space probability density for a two-Gaussian solution of the free-particle Schrödinger equation, modeling the interference of two expanding Bose-Einstein condensates as observed experimentally in Ref. [19]. The solid curve corresponds to $|\psi(x,t) = \psi_1(x,t;x_0 = -d/2) + \psi_2(x,t;x_0 = +d/2)|^2$ with contributions from each harmonic potential, while the dashed curve is that for a single isolated expanding Gaussian, similar to the presentation of the experimental results in Fig. 4 of Ref. [19].
FIG. 2: Special classes of equal mass three-body periodic orbits studied in Ref. [34] including trivial and non-trivial quantum braiding. The numerical values for the initial conditions giving the special case in (c) were discovered in Ref. [35] and are given in Eqns. (2) and (3).
FIG. 3: Comparison of the Weyl prediction in Eqn. (6) (solid curve) for the number of states, $N(k)$ versus $k$, with the numerically obtained ‘staircase’ function in Eqn. (9) for the isosceles right ($45^\circ$-$45^\circ$-$90^\circ$) triangle. For this geometry one has $A = L^2/2$ and $P = (2 + \sqrt{2})L$ and we have used $L = 1$ for definiteness. The dashed curve corresponds to the Weyl prediction, but ignoring the perimeter correction term.