OSP Quantum Mechanics:
Interactive Computer-Based Curricular Material

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Introduction

We have produced and class-tested interactive Open Source Physics-based curricular material in support of introductory, intermediate, and advanced courses in quantum mechanics. These exercises address both quantitative and conceptual difficulties encountered by many students in such topics as energy-eigenfunction shape, momentum space, time evolution, and classical/quantum-mechanical correlations. Because the materials are extremely flexible, these exercises are appropriate for use with a variety of levels and pedagogies. Examples of the curricular materials, the results of our preliminary assessment of their effectiveness, and future directions of this project are discussed.

OSP Quantum Mechanics

Although Physlets [1-4] are written in Java, they are not open source. Physlets are compiled Java applets that are embedded into HTML pages and are controlled using JavaScript. This paradigm works well for general-purpose programs, but fails for more sophisticated one-of-a-kind simulations that require advanced discipline-specific expertise.

The Open Source Physics (OSP) project [5-7] provides a consistent object-oriented library of Java components for anyone wishing to write their own simulation programs. The OSP Java library [6] contains numerical methods, user-interface components, and visualization tools. While this library was originally designed to teach computational physics [7], we have begun to modify the models in this book to enable them to be run as applets and are posting them on the Open Source Physics Web server [6] at Davidson College.

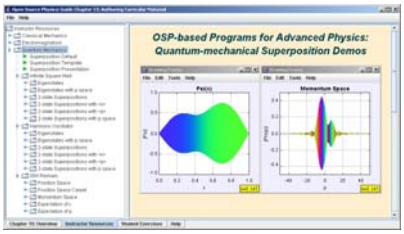


Figure 1: One of the features of this new material is its use of the OSP programs **`Launcher`** and **`LaunchBuilder`** to create Launcher packages, like that shown above, for organization and distribution of curricular material.

QMSuperpositionApp

One of the base computational packages for simulating quantum-mechanical phenomena within OSP is the **`QMSuperpositionApp`** Java program. This program calculates the position-space energy eigenstates and their energies either numerically, via the shooting method for any user-defined potential energy function, or calculated analytically for the special cases of the infinite square well, the periodic infinite well, and the simple harmonic oscillator.

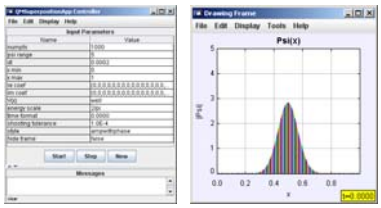


Figure 2: The controller and the result for the **`QMSuperpositionApp`** set up to show the dynamics of an initial Gaussian wave packet in the infinite square well.

Any arbitrary initial wave function can be programmed with the correct set of expansion coefficients. Figure 2 shows an initial Gaussian wave packet in the infinite square well using analytic eigenfunctions and eigenenergies.

Figure 3: Demonstration of the often uneasy coexistence between theoretical physicist and computational physicist. Using numerically determined eigenfunctions and eigenenergies, one is limited to the first 120 states in which to construct the superposition, while for an analytic basis, there is effectively no limit (>500).

One can also use numerically calculated energy eigenfunctions and eigenenergies. For any well, there is a coherence time, time to failure, for the numerically calculated states based on the fact that the time evolution is extremely sensitive to these energies. The table below shows the relationship between tolerance in the solver and the result for the well-studied infinite square well potential.

Tolerance	Time to Failure (T_{rev})
10^{-2}	0.25
10^{-3}	0.5
10^{-6}	3.0
10^{-9}	3.25
10^{-12}	4.25

Visualizations

Depending on the analysis one wishes to perform, one of the following programs based on **`QMSuperpositionApp`** can be chosen:

`ProbabilityApp`
`ExpectationXApp`
`ExpectationPApp`
`CarpetApp`
`MomentumCarpetApp`
`FFTApp`
`WignerApp`

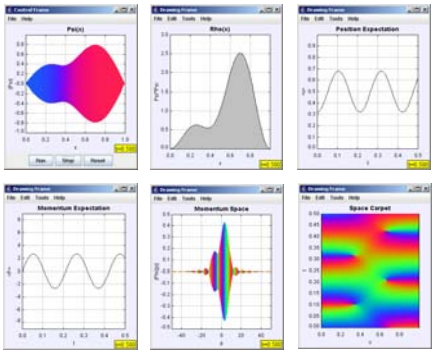


Figure 4: Several visualizations for the time development of a two-state superposition in the infinite square well.

Example: Wigner Function

Wigner [8] was one of the first to address this issue and introduced a quasi-probability distribution defined by

$$P_W(x,p,t) \equiv \frac{1}{\pi\hbar}\int_{-\infty}^{+\infty} \psi^*(x+y,t)\,\psi(x-y,t)\,e^{2ipy/\hbar}\,dy\,.$$

This construct uses 'offset' position-space wave functions (it can also be written in terms of momentum-space wave functions).

The Wigner distribution is easily shown to be real: one of the desired properties of a probability distribution. Integration of $P_W(x, p; t)$ over one variable or the other is seen to give the correct marginal probability distributions for x and p separately. The calculation of P_W for energy eigenstates in the ISW is complicated by the limits of integration which are determined by the restriction that the wave functions are only non-vanishing only in the range $[0, L]$.

Figure 5: $P_W > 0$ at $t = 0$, $t = T_{rev}/4$, $t = T_{rev}/3$, and at $t = T_{rev}/2$ for a Gaussian in the ISW showing a fractional revival [10,11]. Calculation from Mathematica from Ref.[9].

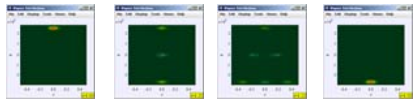


Figure 6: P_W at $t = 0$, $t = T_{rev}/4$, $t = T_{rev}/3$, and at $t = T_{rev}/2$ for a Gaussian in the ISW showing a fractional revival [10,11]. Calculation from **`QMSuperpositionWignerApp`**.

Example: Projection

If one does not know the expansion coefficients, one can use the **`QMSuperpositionProjectionApp`** to determine the coefficients and the dynamics.

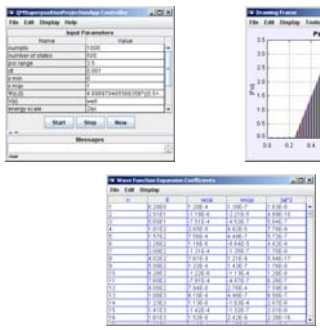


Figure 7: The **`QMSuperpositionProjectionApp`** showing the expansion for the initial "tent" wave packet. Like the Gaussian, or any other waveform in the infinite square well, the "tent" will revive. The table shows the energy and the real part, imaginary part, and amplitude squared of the expansion coefficients.

Example: Measurement

The OSP **`QMSuperpositionMeasurement`** program allows users to learn about measurement in quantum mechanics by simulating measurements on energy eigenstates, superposition of states, and wave packets. One can perform multiple measurements on a single system, or, by using the Reset button, perform a single measurement on a set of identically prepared systems (elements of an ensemble). The program allows one to measure the energy, the position, and the momentum. The measurement of the position and momentum are done with a finite precision, which can be set.

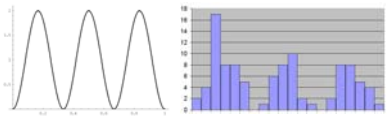
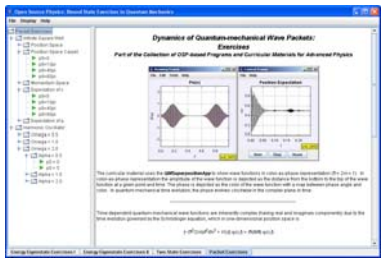


Figure 8: On the left of the Figure is the actual position-space probability density for the $n = 3$ energy eigenstate in the infinite square well. Shown on the right, the result of measuring position for different elements of an ensemble.

Figure 9: For the $n = 3$ energy eigenstate, the result of subsequently measuring x, then measuring p, and finally measuring x again, all on the same system.

Curriculum Packages

The OSP technologies that were developed to teach computational physics are now being used to create simulations for upper level physics. These simulations are distributed in Java archive (jar) files that can be executed by clicking (or double-clicking) on the file in a file-system browser if Java has been installed using default parameters. Although it would be possible to distribute every OSP simulation in its own jar file, this approach is not well suited for the distribution of curricular packages.



Launcher is a Java application that can launch (execute) other Java programs. We use *Launcher* to organize and distribute collections of ready-to-use programs, documentation, and curricular material in a single easily modifiable package. Delivering curricular material in *Launcher* packages has several advantages. First, the material can be made self-contained. Second, the material is only dependent on having a Java VM on a local machine and not on the type of operating system or browser used.

The OSP curriculum packages can be downloaded from the ComPADRE and the Open Source Physics websites.

References

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[11] D. L. Aronstein and C. R. Stroud, Jr., "Fractional Wave-Function Revivals in the Infinite Square Well," *Phys. Rev.* **A55,** 4526-4537 (1997).

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