**TDSE: Propagation of Wave Functions Through Potentials**

**Intro:**

 In order to better understand the Time Dependent Schrodinger Equation (from here on out referred to as TDSE), our group has chosen to simulate the time-evolution of wave functions in the presence of some potential. We explore these bound states in two common potential wells: the Infinite Potential Well and the Quantum Harmonic Oscillator. By varying the coefficients of the stationary states and seeing how the wave function changes, we are able to obtain a more intuitive comprehension of Quantum Mechanics as a whole.

**Theory:**

 First, let’s take a look at the theory. The TDSE is used to solve for the physical states, or wave functions, permitted by a given potential, V. Upon deriving the position dependence and energy, we simply tack on the time dependence to obtain the complete wave function. To demonstrate this process, the infinite potential well solutions are derived below:
 Given the potential

$$V\left(x\right)=\left\{\begin{array}{c}0, 0<x<a\\\infty , elsewhere\end{array}\right.$$

We can solve the Schrodinger Equation separately in each of the three regions (within and on either side of the well). Clearly, though, where there is infinite potential there is zero probability of finding the particle and thus the wave function is simply zero. Slightly more interesting, though, is the region between 0 and a. The derivation of the wave function in this middle region (where V=0) is as follows:

$$-\frac{ℏ}{2m}\frac{∂^{2}}{∂x^{2}}ψ=Eψ$$

Substituting k:

$$\frac{∂^{2}}{∂x^{2}}ψ=-k^{2}ψ$$

Where:

$$k=\frac{\sqrt{2mE}}{ℏ}$$

As can be seen above, the differential equation admits a complex exponential eigenfunction of the form:

$$ψ\left(x\right)=Asin\left(kx\right)+Bcos(kx)$$

Due to continuity boundary conditions, however, we see right away that the wave function must be zero at the boundary and thus *the cosine term is unphysical*; therefore, *B=0*. In order for the sine term to “fit” correctly in the well, the wavelength must be an integer multiple of twice the width of the well. In other words, the sine term must be zero at the boundaries. In terms of the wave number, this condition is:

$$ka=nπ$$

or

$$k\_{n}=\frac{nπ}{a}$$

Where n is a positive integer.

From this quantization result, and the normalization of this solution (not shown), we obtain the position-dependent solution:

$$ψ\left(x\right)=\sqrt{\frac{2}{a}}\sin(\left(k\_{n}x\right))$$

 Using the quantized values of k, and the definition of k from the previous page, we obtain the quantization of energy condition:

$$E\_{n}=\frac{(nπℏ)^{2}}{2ma^{2}}$$

Now we can tack on the time dependence:

$$Ψ\left(x,t\right)=\sum\_{}^{}\sqrt{\frac{2}{a}}\sin(\left(k\_{n}x\right))e^{-iE\_{n}t/ℏ}$$

 Now that we’ve outlined the process for deriving complete wave functions in the presence of a potential, the Quantum Harmonic Oscillator solution is outlined below. For a potential:

$$V\left(x\right)=\frac{1}{2}mω^{2}x^{2}$$

We obtain a wave function of the form:

$$Ψ\left(x,t\right)=\sum\_{}^{}\left(\frac{mω}{πℏ}\right)^{1/4}\*\frac{1}{\sqrt{2^{n}\*n!}}\*H\_{n}\left(\sqrt{\frac{mω}{ℏ}}x\right)\*e^{-mwx^{2}/(2ℏ)}\*e^{-iE\_{n}t/ℏ}$$

Where the function H is a “Hermite Polynomial”.

**Simulation:**

 Our simulation is designed to illustrate the quantum mechanical superposition and time-evolution of up to three physically allowed states. The time-evolution, which occurs only in the imaginary plane, may be thought of as changing the probability amplitudes of each state, whilst preserving the normalization. Therefore, the inner product results in multiplication by unity as the conjugate imaginary exponentials simply cancel each other out.

 By illustrating the wave function with an interactive interface, the simulation allows for deeper insights into the evolution of the wave function and quantum mechanics as a whole. The display shows the wave function evolve with time in such a way that it is clear that higher energy states (corresponding to more nodes) rotate through complex space faster, much the same way a skipping-rope would with more nodes. One can view each individual state independently or view a superposition of states. Either way, the actual visualization is quite mesmerizing!

 Do note that, in our simulation, we ignore normalization, as it is not imperative for getting a feel for the behavior of the wave function. Indeed, the only things that really matter in this simulation are the eigenfunctions themselves, their relative weights (or probability amplitudes—again, non-normalized), and the energy of that particular state.

While on the topic of energy, it is also interesting to point out that the user can make a complicated wave function and, supposing he or she measured a specific energy, set the coefficients of all other states to zero to see the collapse of the wave function’s superposition of states down to a single state as dictated by the expectation of subsequent measurements of the system. The difference between the two wave functions is fairly interesting.

 Another interesting possibility is the coherent state of the quantum harmonic oscillator. These states most closely resemble the behavior of a classical oscillator. As a fun fact, this behavior satisfies the Correspondence Principle. These states can be explored via the simulation as well, and may be a good starting point for future programs.

**Users Guide:**

 Our simulation is relatively straightforward to use, offering an array of user-friendly sliders to adjust parameters. The simulation was designed in *Mathematica* because of its extensive library of helpful functions such as the simple “Plot” and “Animate”. With very few lines of code, many of which just outlined style preferences for the graphs of these wave functions, we were able to simulate the superposition and time-evolution of up to 3 states with variable energy levels and weights for both the infinite square well and the quantum harmonic oscillator.

 The wave function graphs for either potential may be adjusted without taking time-dependence into consideration, which allows the user to focus on studying the weights of each state and how this affects the amplitude of the superposition of these states. Without time-dependence, the user may also adjust the energy level (shape) of each state to focus on examining the affect this has on the shape of the superposition.

 Of course, each of these may also be observed if the user chooses to activate the time-evolution, either animatedly or controlled by the interactive bar. Taking the time-dependence into consideration, one may also observe the impact that adjusting the energy levels of each state has on the frequency of rotation in the complex plane, as well as how this affects the frequency and wobbliness (technical term) of the superposition of states.