Bound States
Design Outline
Draft 1

Sam McKagan

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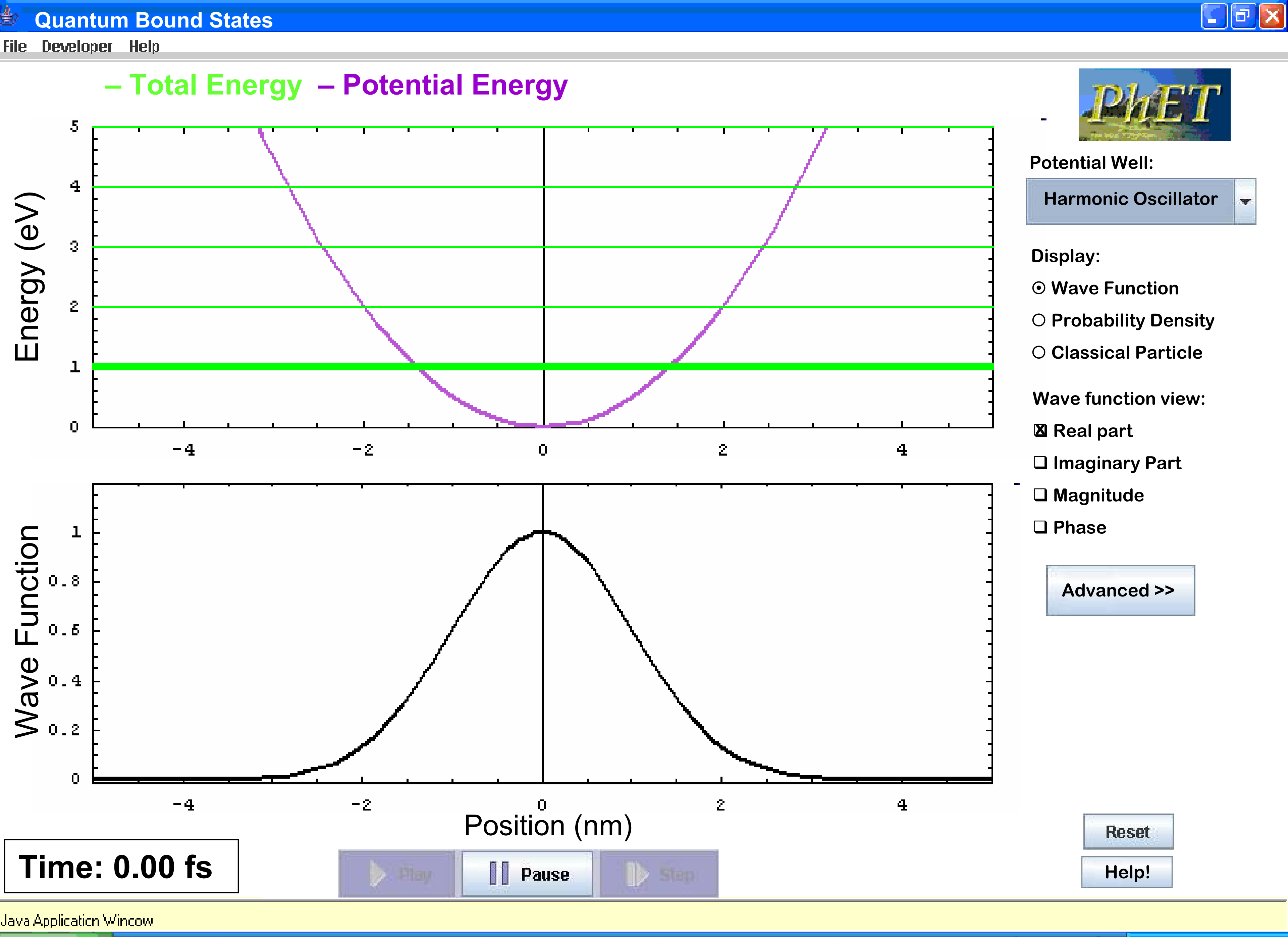
Learning Goals

- Visualize wave functions, probability densities, and energy levels for bound states in various potentials.
- Describe how multiple representations used for wave functions relate to one another.
- Relate quantum wave functions to corresponding classical systems.
- Explain what is and is not time-dependent for an energy eigenstate and a superposition state.
- Predict how the curvature and amplitude of the wave function and the spacing of the energy levels depends on the shape of the potential.

Similar Existing Simulations

- There are several simulations which together have all the desired features of this simulation, but these are extremely difficult to use. My goal is to take the best features from the following simulations and package them in a much more user-friendly interface.
  - falstad.com/qm1d/ OR falstad.com/qm1drad/
  - http://webphysics.davidson.edu/cise_qm/
    - click on "Time Evolution"
  - http://www.quantum-physics.polytechnique.fr/
    - click on panel 2.3
  - http://wps.aw.com/aw_young_physics_11/0,8076,898597-,00.html
    - click on “Particle in a Box” or “Potential Wells”



Quantum Bound States

Potential Well: Harmonic Oscillator

Display:

● Wave Function

○ Probability Density

○ Classical Particle

Wave function view:

☒ Real part

□ Imaginary Part

□ Magnitude

□ Phase

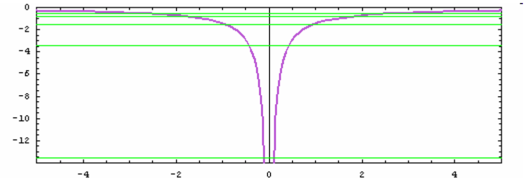
Time: 0.00 fs

Notes on Options

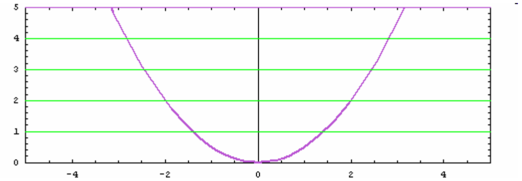
- If wave function/probability density selected for Display, bottom graph identical to the wave function/probability density graph in Quantum Tunneling.
- If classical particle selected, bottom graph displays a particle moving back and forth with kinetic energy equal to total minus potential.
- The wave function view options should be grayed out if classical particle selected.

Potential Wells

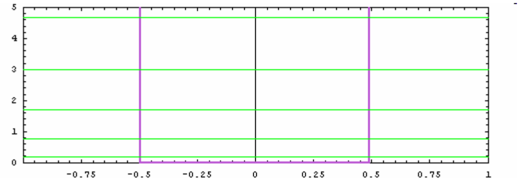
- Hydrogen Atom (Coulomb):
  - $U(x) = ke^2/|x|$



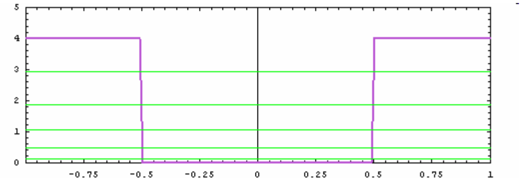
- Harmonic Oscillator
  - $U(x) = ½m\omega^2x^2$



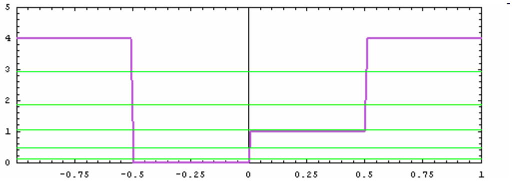
- Infinite square well
  - $U(x) = 0$ if $|x|<a/2$, ∞ if $|x|\geq a/2$

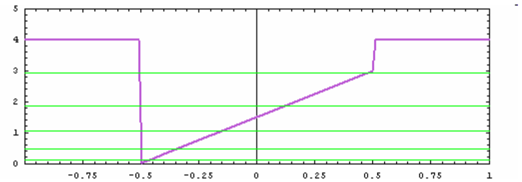


- Finite square well
  - $U(x) = 0$ if $|x|<a/2$, U_0 if $|x|\geq a/2$



- Asymmetric wells





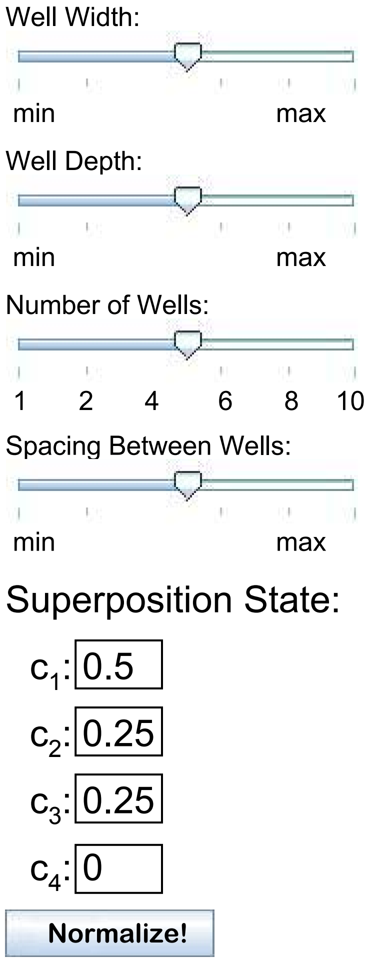
- Custom?

Stuff you can do:

- Choose energy eigenstate displayed in wave function graph by clicking on energy state in energy graph. The displayed energy eigenstate will be bold on energy graph as shown above.
- Create wave packets by clicking on point in wave function graph.
- Note that both these options are available in Falstad simulations, so you can see what they look like.

Advanced Options

- With these options the user can change the width or the depth of a well, or create an array of wells, or create a wave function which is a superposition of different energy states.
- We may also want to allow user to adjust slope/height difference of asymmetric wells.
- The user should be able to enter the coefficients for each possible state. Since the user may not enter values that fulfill normalization conditions, a normalize button is necessary.



Superposition State:

c_1: 0.5

c_2: 0.25

c_3: 0.25

c_4: 0

Implementation

- To find the energy eigenvalues of the Schrodinger equation and the solutions for a particular energy, we will need to solve the time-independent Schrodinger equation as an eigenvalue problem.
- Note that this is different from the method used in QT and QWI, in that in those simulations the initial state is always specified by the user, not determined dynamically.
- We may be able to get this feature for free by using a Schrodinger algorithm based on eigenvalues, such as that used by Falstad.
- We could avoid this by using only potential wells where the energies can be determined analytically ahead of time, but this would mean eliminating multiple wells and asymmetric wells.
- Will need to solve the time-dependent Schrodinger equation to implement wave packets.