Bound States Design Outline Draft 4

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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.
- 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 and the mass of the particle.
- Gain an intuition for how band structure results in a lattice of many wells.
- Gain an intuition for how to go from the microscopic potential of a single atom to the macroscopic potential of a solid.

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”

One Well Panel:

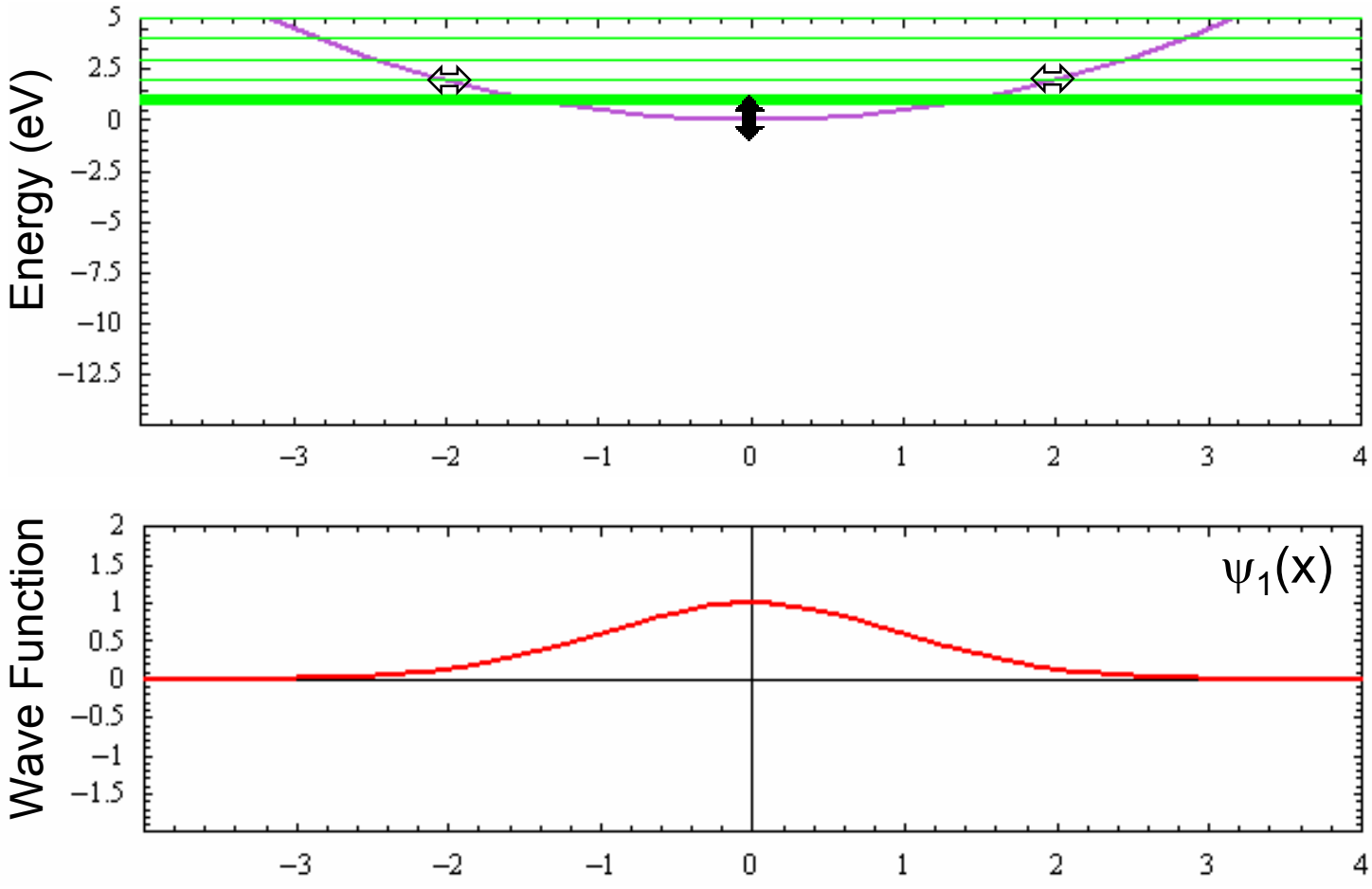
Quantum Bound States

File Developer Help

One Well | Double Well | Many Wells

– Total Energy – Potential Energy

Superposition... Configure Energy...



Potential Well:

Harmonic Oscillator

Display:

- (•) Wave Function
- ( ) Probability Density

Wave function view:

- [x] Real part
- [ ] Imaginary Part
- [ ] Magnitude
- [ ] Phase

Particle Mass:

m_e $10m_e$

Time: 0.00 fs

Play Pause Step

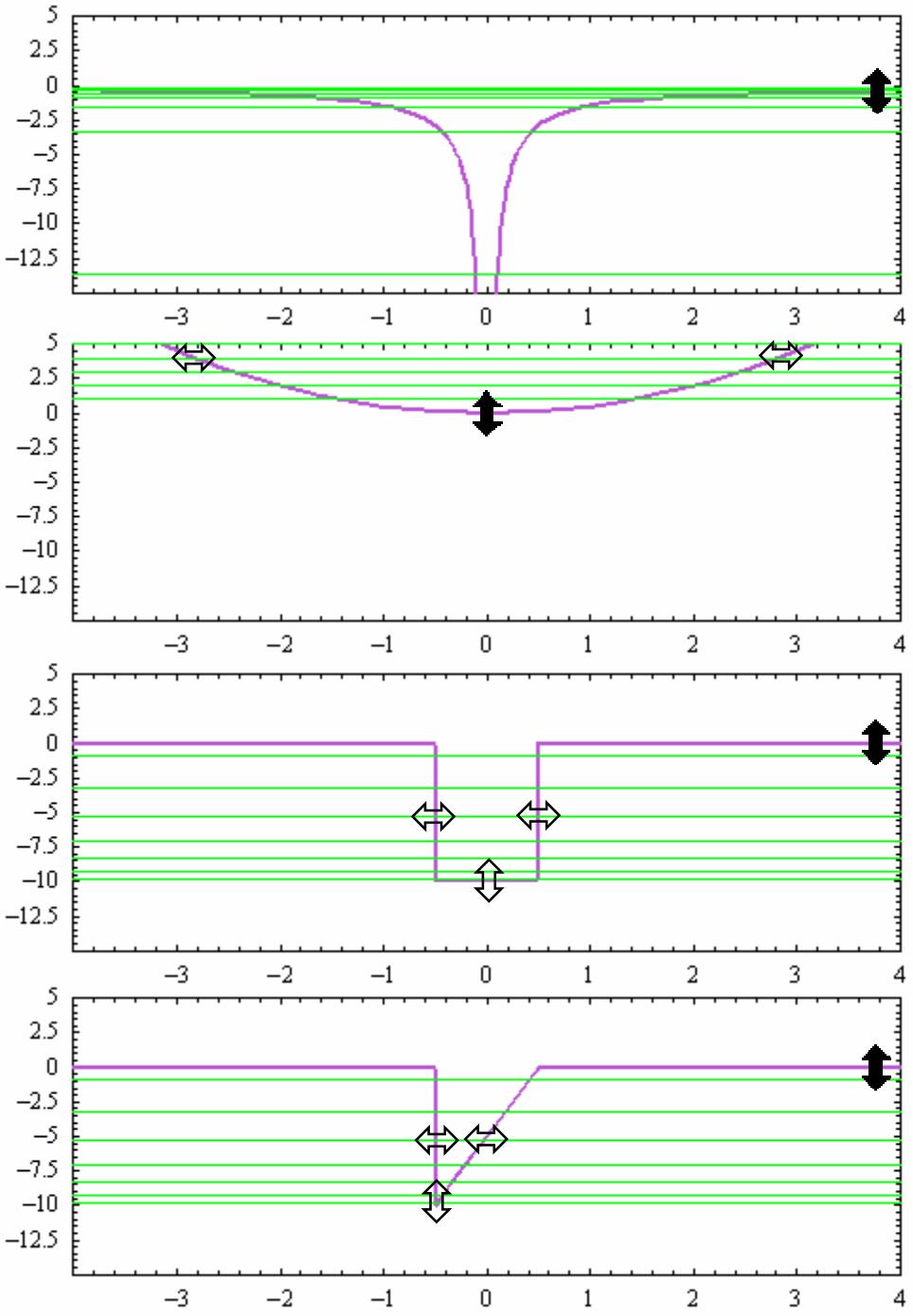
Reset All

Help!

Java Application Window

Potential Wells

- Coulomb:
  $U(x) = -ke^2/|x|$
- Harmonic Oscillator
  $U(x) = \frac{1}{2}m\omega^2x^2$
- Square well
  $U(x) = 0$ if $|x| \geq a/2$
  $-U_0$ if $|x| < a/2$
- Asymmetric well
  $U(x) = 0$ if $|x| \geq a/2$
  $-U_0(x-\frac{1}{2})$ if $|x| < a/2$



Handles on potential wells

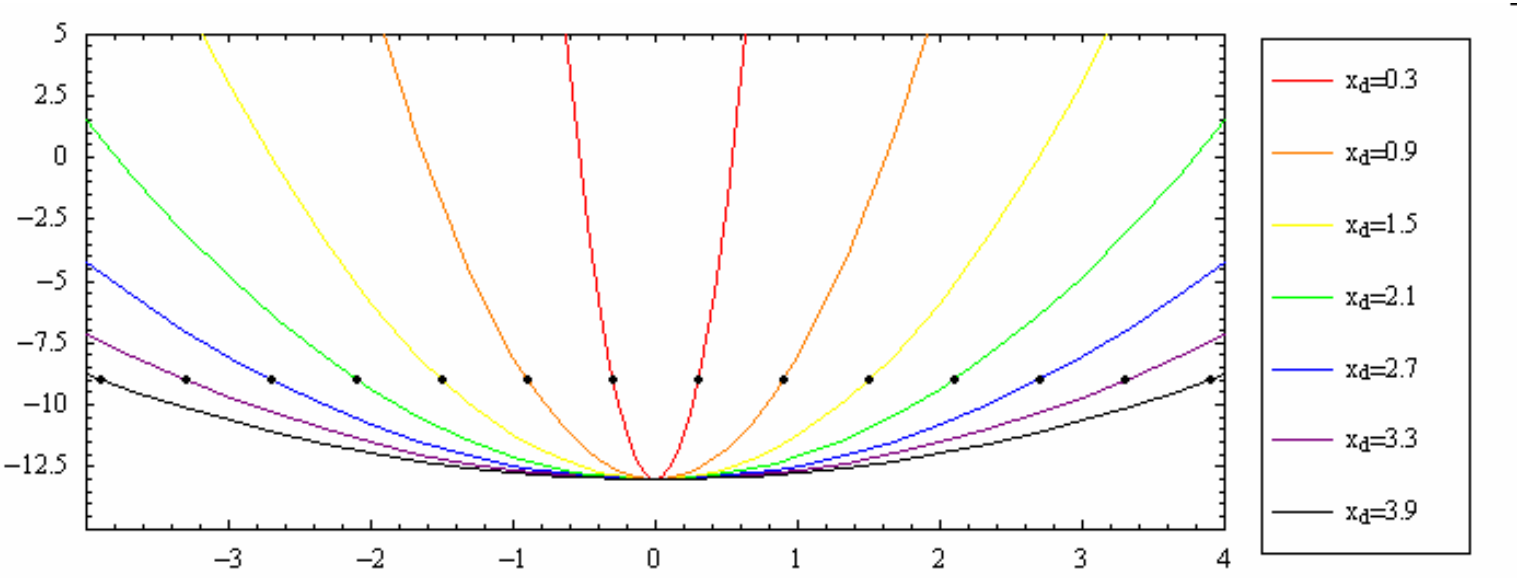
- Solid arrows change offset, i.e. move entire potential well up and down.
- Because Coulomb potential set by properties of H atom, width and depth not adjustable by handles.
- Vertical arrows on square/asymmetric wells change depth U_0. In graphs shown on previous slide, U_0=10eV.
- Horizontal arrows on square/asymmetric wells are linked so that mousing over one highlights both. Moving them changes width a. In graphs shown on previous slide, a=1nm. Well is always centered at 0nm.
- Horizontal arrows on harmonic oscillator are linked as for other wells and change ω. Large $\omega \Rightarrow$ narrower well, small $\omega \Rightarrow$ wider well. Note that width of well will also change if you change particle mass.

Harmonic oscillator width

- Choose the vertical position of the width arrows to be some fixed distance V_0 from the bottom of the well, so the position on the graph is $V_0 + C$, where C is the offset.
- $V_0 = 4$ looks like a reasonable valuable, but you may not want to hard code it, just in case.
- The horizontal position of the arrows is then given by the solution to the equation $V_0 = \frac{1}{2}m\omega^2 x_d^2$, or $x_d = \pm\sqrt{(2V_0/m\omega^2)}$.
- In the "Configure energy" dialogue, instead of a width slider, there should be an "angular frequency" slider that controls ω.
- There are thus three linked controls for m, ω, and x_d, related by the above equations. Changing ω should change x_d and vice versa, without affecting m. Changing m should change x_d, without affecting ω.
- The range for ω should be $1\text{x}10^{15}$ s^{-1} to $15\text{x}10^{15}$ s^{-1}.
- To avoid making ω or m go off scale, the allowed range for x_d will need to be a function of m. This range will determined from the value of m and the range for ω using the equation above. My calculations give 0.267 to 4 nm when $m=m_e$, and 0.0843 to 1.26 nm when $m=10m_e$.

Harmonic oscillator width

- Here are some samples of harmonic oscillator potentials with various values of x_d.
- The dots are located where arrows would be.



- In this picture, V0 = 4 eV, $m=m_e$, offset = -13 eV.

Choosing Energy Eigenstate

- Each energy eigenstate (green lines) has a different wave function associated with it. User needs to be able to select which wave function is displayed by selecting eigenstate. See falstad.com/qm1d/ for an example.
- If you mouse over any of the energy eigenstate lines, it should turn gray and a thin gray wave function corresponding to that eigenstate should also appear in the wave function graph.
- If you click on eigenstate in energy graph then eigenstate should change color and the corresponding wave function should appear in the wave function graph.

Wave function & Probability Density

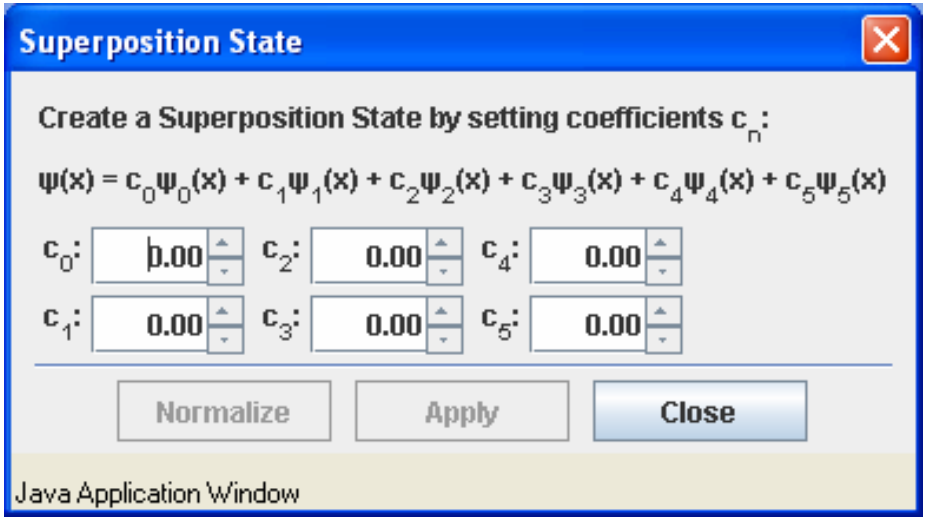
- Wave function and Probability density display options show graphs identical to corresponding graphs in QT, but only one at a time.
- Options for wave function display look the same as in QT. We may as well keep them enabled if probability density is selected to emphasize that it is purely real. Thus, in probability density mode, “real part” and “magnitude” will show the same thing in different colors (red/black), and checking “imaginary part” or “phase” will do nothing (since there is no imaginary part or phase).
- Bottom graph will take up about a third of the space (same size as in QT) and energy graph will take up 2/3.

Configure Energy Dialogue

Non-modal dialogue box containing the following sliders:

- “Offset” available for all wells, range = -15 to +5 eV, default = 0 eV.
- “Width” available only for square and asymmetric wells, range = 0.1 to 8 nm for single well, 0.1 to 3nm for double wells, 0.1 to 1 nm for multiple wells, default = 1 nm.
- “Depth” available only for square and asymmetric wells, range = 0 to 20 eV, default = 10eV
- “Angular Frequency ω” available only for harmonic oscillator, 1×10^{15} to 15×10^{15} s^{-1}, default = 2×10^{15} s^{-1}.
- “Spacing” available only for double and multiple wells, range = 0.3 to 4 nm, default = 1.2 nm.

Superposition Dialogue



- The number of coefficients shown is equal to the number of bound states in the well, up to a max of 6.
- If only one eigenstate is selected, as it would be before using superposition dialogue, the coefficient corresponding to that dialogue is set to 1, all others to zero.
- Wave function for superposition state given by equation at left.
- If the user hits “apply” or “close” and the coefficients are not normalized, a dialogue box should come up that says, “The coefficients must be normalized so that $c_1^2 + c_2^2 + c_3^2 + c_4^2 + \ldots = 1$. Do you want the coefficients to be normalized automatically?”

Units and Scales

- Throughout this simulation, the units are:
  - Energy – eV
  - Distance – nm
  - Time – fs
  - Mass – eV/c^2
- To give correct units, the constants used in equations should be:
  - $\hbar$ = 0.658 (eV fs)
  - ke^2 = 1.44 (eV nm)
  - Slider changes mass within range of 5.68 (electron mass) to 56.8.
- For all energy graphs, the scale should be -4 to +4 nm and -15 to +5eV. There are no zoom buttons; the scale can't be changed. Wave function and probability graphs have the same horizontal scale. Set the vertical scales to -2 to +2 for wave function graph and 0 to 4 for probability graph for now, but make these easy to change.

Miscellaneous

- The stopwatch is always on. Clock resolution should be the same as in QT (for now).
- There is no “restart” button.
- The legend in the corner of the wave function/probability density graph should say “$\psi_n(x)$” for wave function, or “$|\psi_n(x)|^2$” for probability, where n is the number of the selected eigenstate.
- The wave function/probability density displayed depends on which eigenstate is selected.
- The positions of energy eigenstate lines and the shape of wave function/probability density are functions of which potential is selected, the width, depth, and spacing of the potential, and the particle mass. These are determined by solving time-independent Schrodinger equation.
- Changing mass will affect the shape of harmonic oscillator potential, but not any other potential well shapes.

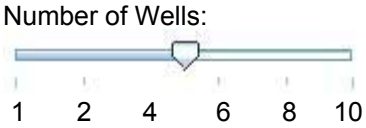
Defaults

- Potential Well – Square Well
- Display – Wave function
- Wave function view – Real part
- Particle mass – electron mass m_e

Two Well Panel

- This panel will have the same functionality as the one well panel, but instead of a single well centered at the origin, there will be two wells equidistant on either side of the origin.
- The only allowed potential wells will be Coulomb and Square.
- The user will still be able to change the depth and width of the wells as in the One Well panel. The depth and width of the two wells should be linked so that they cannot be changed independently.
- To avoid clutter we could get rid of the solid arrow that shifts the whole well up and down in this panel.
- The only new functionality will be to change the spacing between the wells. In the next slide this is implemented by two linked arrows attached to dotted lines through the middle of the wells. This is on the verge of being too cluttered, so we may consider a slider instead.

Many Wells Panel



- This panel will be similar to the Two Wells panel but will include a slider on the control panel that allows the user to change the number of wells to any integer from 1 to 10.
- Again the user should be able to control the depth, width and spacing between the wells (as a whole, not of each well independently).
- If we use the same user interface for depth width and spacing as in previous panel, it will get very cluttered. Should we use sliders instead?

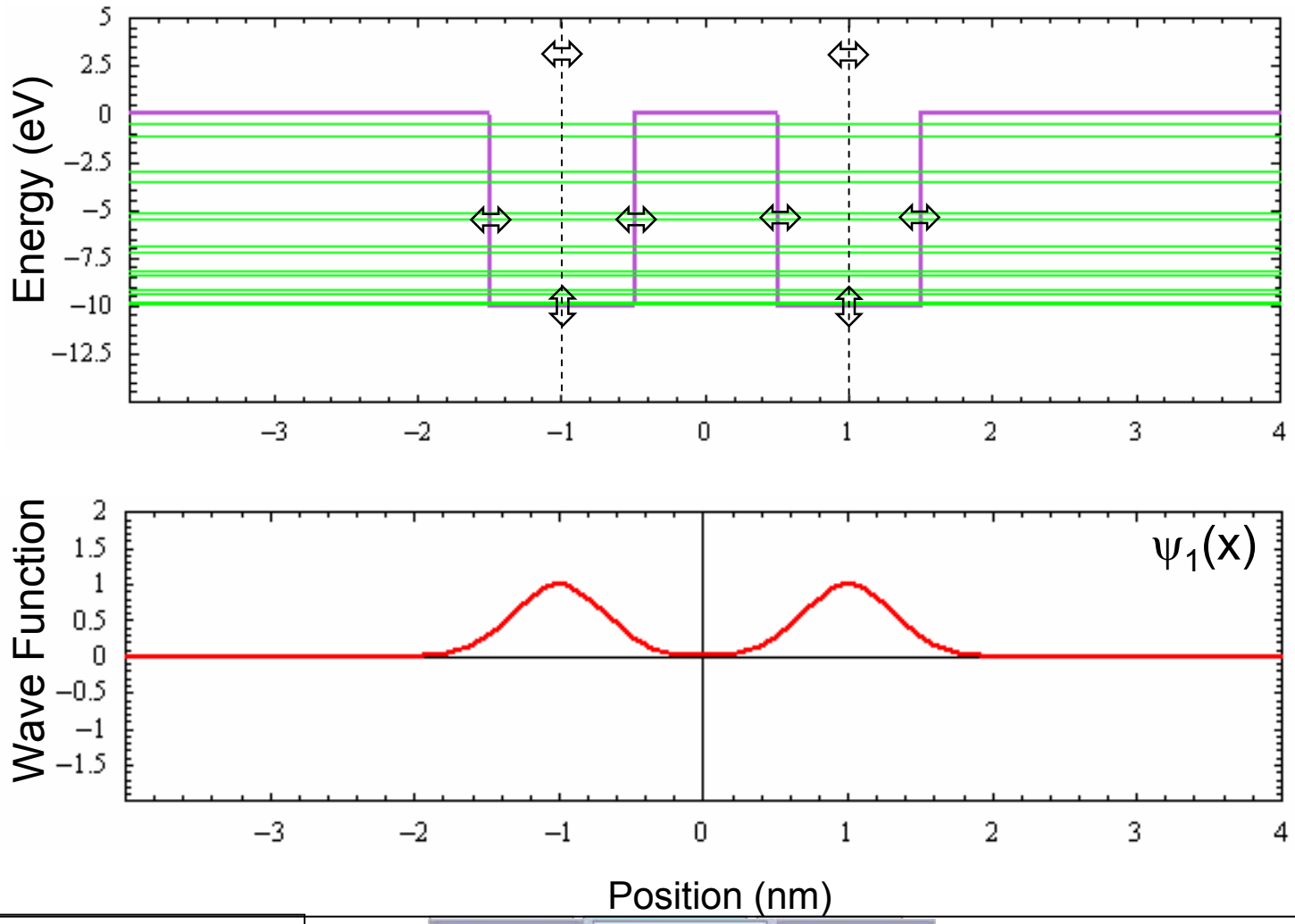
Quantum Bound States

File Developer Help

One Well | Double Well | Many Wells

– Total Energy – Potential Energy

Superposition... Configure Energy...



Potential Well:

Square Well

Display:

- ⊙ Wave Function
- ○ Probability Density

Wave function view:

- ☒ Real part
- ☐ Imaginary Part
- ☐ Magnitude
- ☐ Phase

Particle Mass:

m_e $10m_e$

Time: 0.00 fs

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Help!

Java Application Window

Formulae for Multiple Potential Wells

- Coulomb

$$U(x) = \sum_{i=1}^{N} \frac{-ke^2}{|x - x_i|}$$

- Square well

$$U(x) = \sum_{i=1}^{N} \begin{cases} -U_0 & \text{if } x \geq x_i - a/2 \text{ and } x \leq x_i + a/2, \\ 0 & \text{otherwise.} \end{cases}$$

- where x_i is the center of the i^{th} well and is given by $x_i = d\left(i - \frac{N+1}{2}\right)$ if N is the number of wells and d is the spacing between them.

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 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.