Instructions for Getting Started with
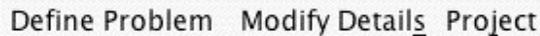## *Erwin Meets Goldilocks*

The purpose of these instructions is to tell you what the buttons on this version of the program do. **What** is being done is explained in the write up on the web site on the previous version of the program. If you want to learn from this exercise, you must read about what you are doing.

In your Java-enabled browser access the following URL:

https://webspace.yale.edu/chem125_f06/125/quantum/JavaErwin/JavaIntro.html
(at the bottom of that page you can download a stand-alone JAR file)

Java launches and a working window titled "Erwin Meets Goldilocks" appears.
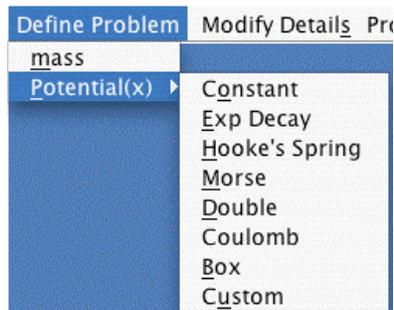
At the upper left are three menus:

The first, **Define Problem**, is used to set up the problem (naturally)

The second, **Modify Details**, is used when the program give nonsensical results because of it is using steps that are too big in tracing the curves.
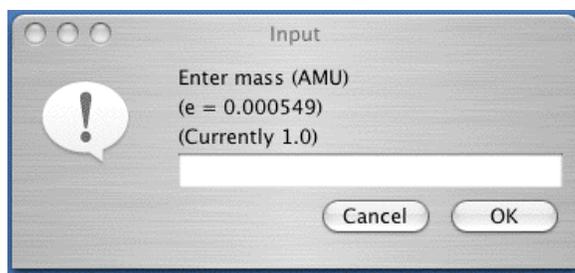
The third, **Project** is used to quit the current problem with the option to save it, or to resume a previously saved problem.

Click **Define Problem** to get the following menu (and submenu when cursor is on **Potential(x)**):

Remember that the problem (for one particle in one dimension) is defined by the mass of the particle and by its potential energy as a function of position.
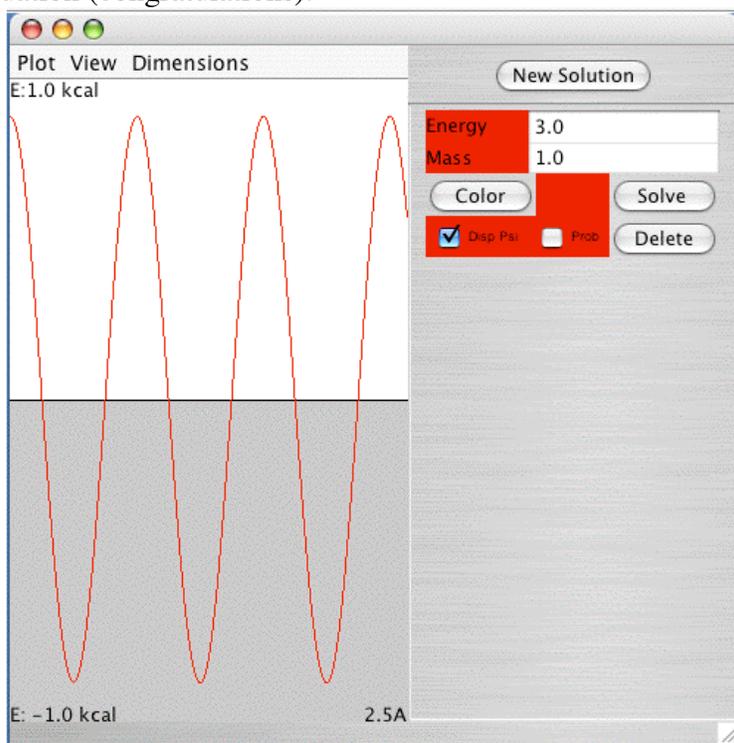
Click **mass** to get the following window:

Input

Enter mass (AMU)
(e = 0.000549)
(Currently 1.0)

Cancel   OK

For the present we can click **OK** to accept the default of 1 atomic mass unit (a hydrogen atom or proton) for the mass. Subsequently we may change the mass by returning to this window, but to learn the program it's best to start with 1 amu.

Now go the the **DefineProblem/Potential(x)** menu and select **Constant** to get the following window, in which you just click the **Create** button. Obviously you'll later choose a more interesting potential which will require choosing some setup parameters.

A Problem window appears with a **New Solution** button in the upper right. **Click it**, **enter 3** in the input total energy window that pops up (the units are old fashioned kilocalories per mole, which are favored by most American organic chemists), and click the **OK** button. The following window appears showing that you have solved the Schrödinger Equation (congratulations):

Plot View Dimensions
E:1.0 kcal

New Solution

Energy   3.0
Mass   1.0

Color   Solve

☑ Disp Psi   ☐ Prob   Delete

E: –1.0 kcal   2.5A

The window may be resized (within the limits of the pre-defined blue field) by dragging at the lower right corner.

It consists of **two fields**. The **left half** is a superposition of **two graphs**, one of them the selected Potential as a function of x, the other Psi as a function of x.

The **horizontal x-axis** is common to the two graphs. It extends from 0 at the left to 2.5Å units at the right (See number in lower right corner of the graph). The right limit may be extended – or contracted - through **Dimensions/Distance** in the graph header).

One vertical axis is **Energy**. The boundary between the gray area and the white top plots the potential energy as a function of x. It's not very exciting, because we selected constant potential energy.

> (The gray color is adjustable through **View/Potential Fill Color**. If you prefer you may make the fill color white and draw the potential function as a line by selecting from **View/Potential Border Color**, but at the beginning using a fill color may help you keep from confusing the potential energy plot – part of the question - with psi plots – the answers)

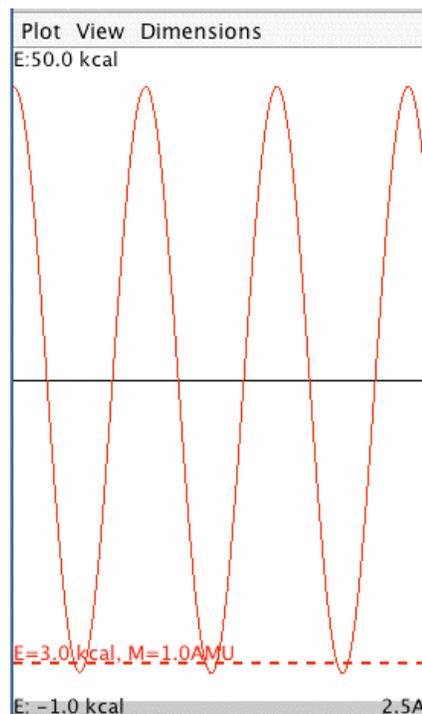The default position for zero is the center of the screen on an energy scale that goes from –1 to +1 kcal/mole. **Dimensions/Energy/Max** and **Dimensions/Energy/Min** allow you to adjust these limits. Why not make the maximum 50, and then click **View/Total Energy Line** to get this rescaled energy graph (note that the red psi curve is unchanged).

The white/gray boundary is still at 0, but the energy scale now extends to 50 kcal/mole, which allows plotting the horizontal dashed red line to show the total energy you selected (3 kcal/mole). This **total energy line** is labeled with the value of the energy and the mass you selected (1.0 amu).

So much for the potential and total energy plots.

The red curve is psi that solves Schrödinger's Equation for this problem. It happens to be a cosine wave with a certain wavelength. The horizontal black line in the center of the screen shows the **zero** of the psi plot (it can be removed using **View/Axis**, but I wouldn't recommend removing it, unless maybe you want to see the potential graph with no trace of the psi plot). Obviously the value of psi is positive above this line, and negative below. The psi **scale** is arbitrary and adjusted by the program to make psi pretty much fill the screen.
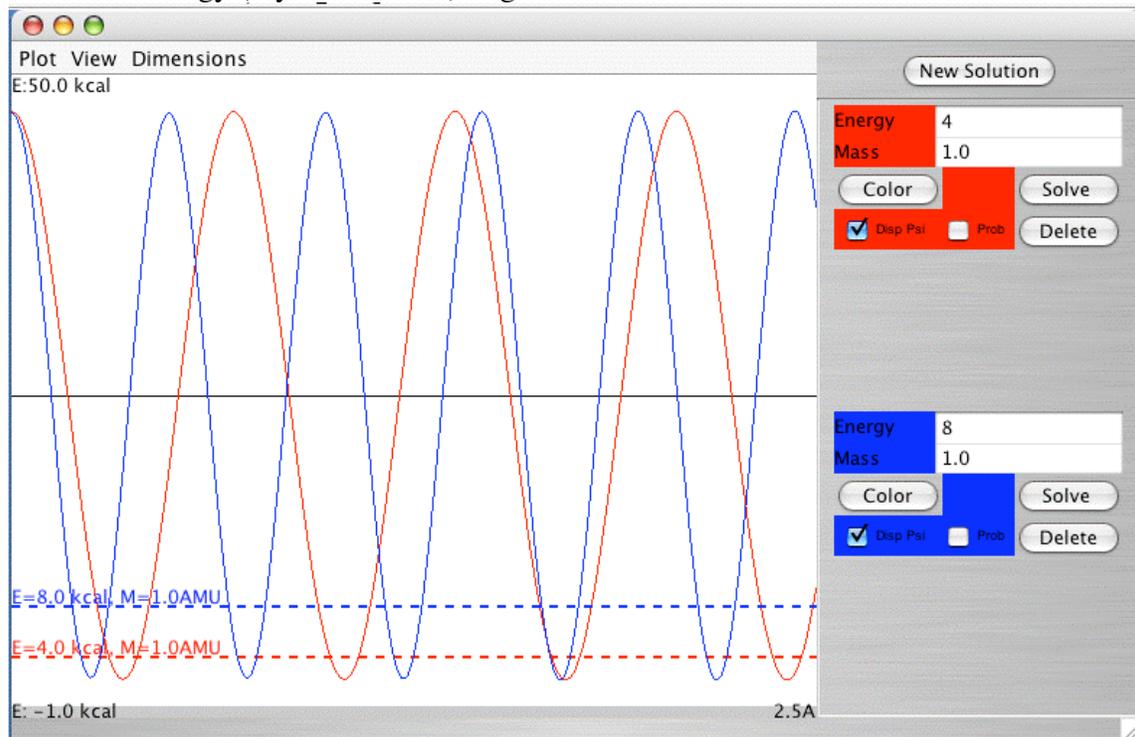
The **Right Half** of the window shows the parameters on which the psi plot is based. The mass you selected to set up the problem and the energy you guessed as a possible total energy.

You may change the tentative energy and press return to see how psi changes. DON'T PRESS THE SOLVE BUTTON NOW (it is for use with other potentials). Make the energy 4 and see what happens.

An alternate possibility is to make a separate curve for the new energy, so you can compare directly with the old one. To do this press the **New Solution** button and enter a different energy (say 8 kcal/mole) to get:

The other buttons allow changing the color of a psi plot (and its total energy dashed line), to delete a psi plot, and to plot the square of psi as well as, or in place of psi itself.

I believe this is enough to get you started properly. I will provide more instruction on the various potentials, and on using the **Solve** button later. You can probably work it out for yourself, but don't use it until you have had considerable experience at guessing energies to obtain psi functions that remain finite. The point is to learn, not just to find an answer.

Printing may not be available in the applet version, but is available in the stand alone JAR application.

Good luck, and thanks to **Tom Gniadek**, who has prepared this program for us.