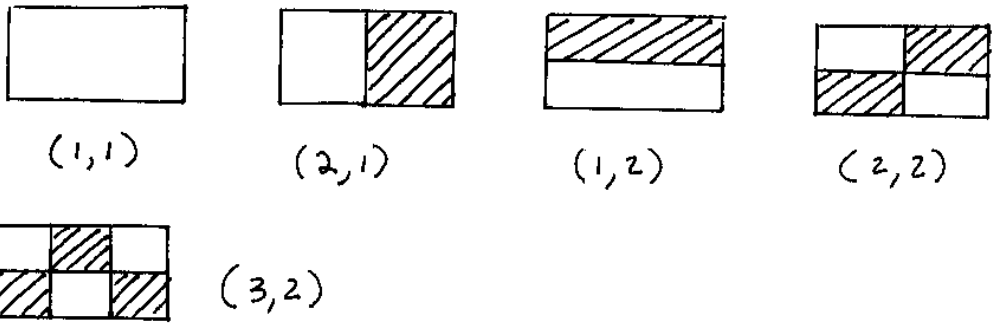
Chemistry 1410 HW #2 Spring 2001

1. Plot the wavefunctions of the 2-dimensional-particle-in-the-box problem with the (1,1) (1,2), (2,1) (2,2), (3,2) quantum #'s.



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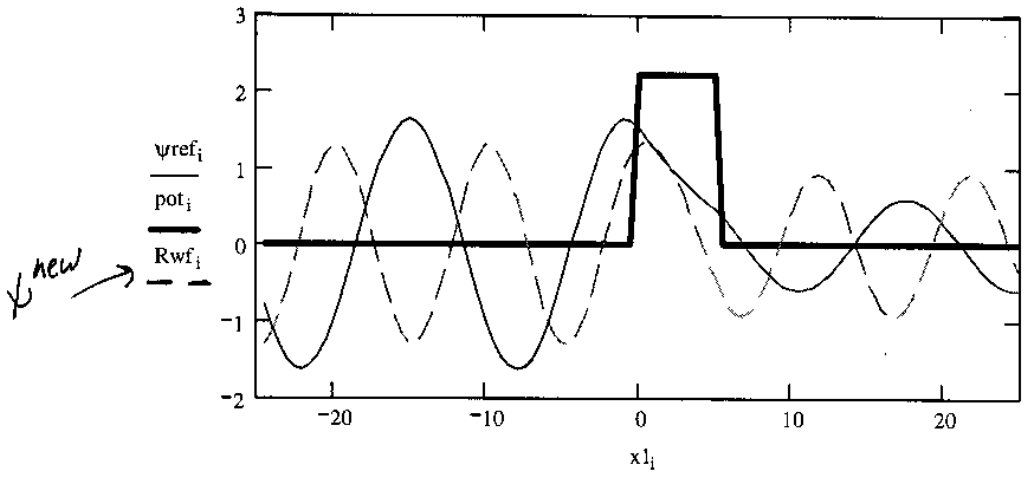
2. Results of calculations with the tunneling program.



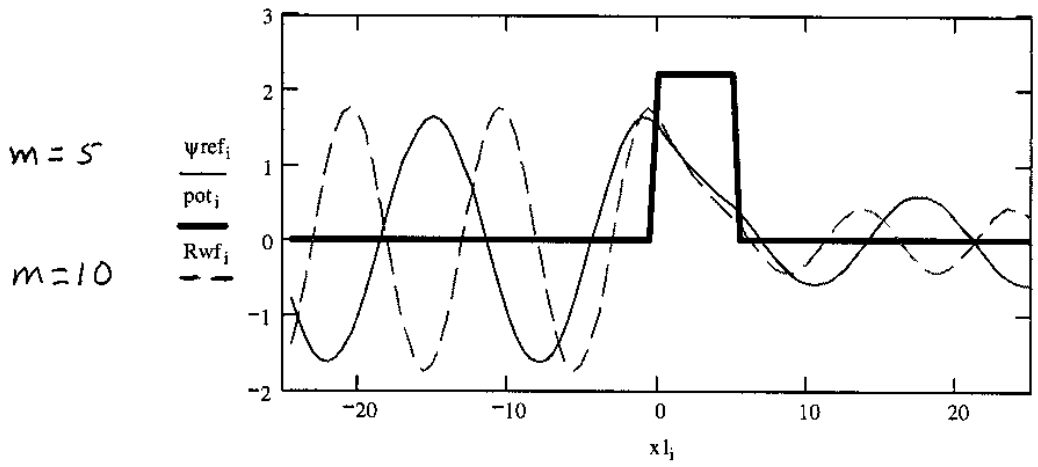
2x energy ⇒ higher probability of tunneling.

ψ^{ref} m = 5, width = 5, E = .008, Eover = 0.9

→ ψ^{new} m = 5, width = 5, E = .016, Eover = 1.8

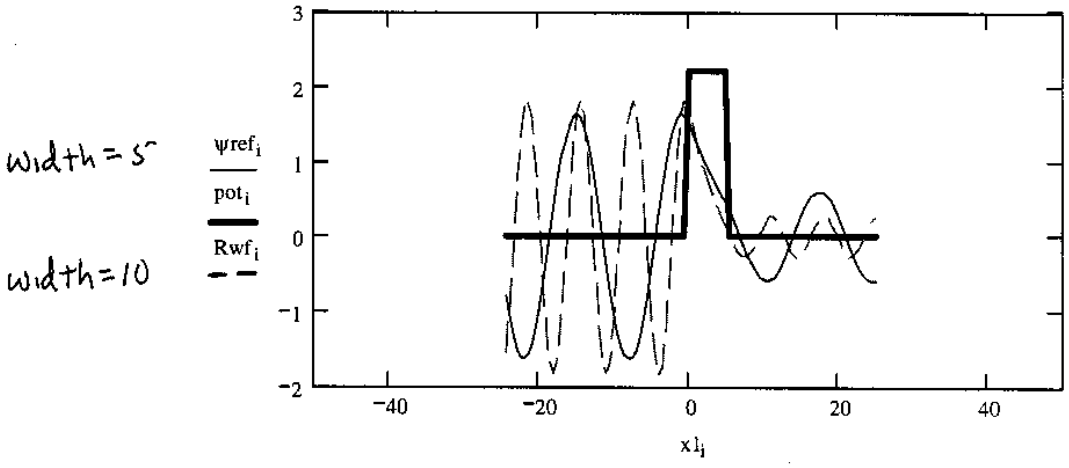
Note, Eover had to be changed to keep height const.

Here we plot the two wavefunctions together.



2x mass ⇒ decreased probability of tunneling

Here we plot the two wavefunctions together.



double width, decreased tunneling.

Note the program should really plot two different width barriers.

4. $\int_0^\infty e^{-x^2} dx \rightarrow \frac{1}{2}\sqrt{\pi}$

$\int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx \rightarrow 0$

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3. Particle-in-a-finite-box

Here is a web page that discuses the particle in a spherical box problem. Later I will post some links that give programs that one can use interactively or download.

http://www.colorado.edu/physics/phys3220/3220_fa97/notes/notes9_10/notes9_10_5.html

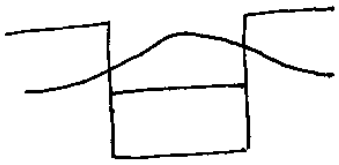
Here is a web page with an interactive program for studying the particle in a finite box problem.

http://webphysics.davidson.edu/faculty/dmb/SingleWells/Well2.html

There is a program on the qsad.bu.edu site that is appropriate for this problem.

Particle-in-finite-box problem

No matter what parameters you choose, you will find at least one bound level for this problem.



← ground state wave-function. Note the tunneling

particle-in-spherical box

The ground state wave function has no nodes and goes to zero at the boundary if the potential is infinite outside the box.