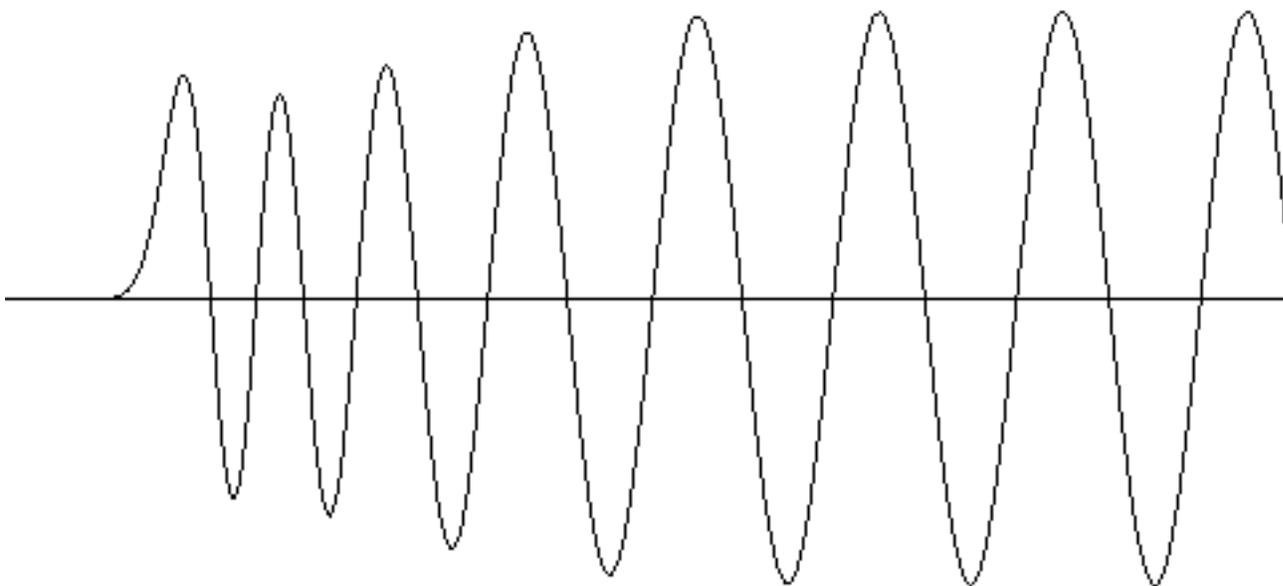


Here are lots of quantum mechanics questions from previous exams that would be fair game this year:

5. (2 min) What is a quantum-mechanical wave function a function of (*i.e.* what are its **independent variables** and **how many** are there)?
6. (4 min) **List** the conditions a wave function must satisfy in order to solve the Schrödinger equation.
7. (6 min) Suppose $\cos(ax)$ solves the Schrödinger Equation for a particle in one dimension.
 - a) From $\cos(ax)$ determine mathematically the kinetic energy as a function of position.
 - b) Explain mathematically how the total energy varies with $1/a$, the wavelength of the function.
4. (2 min) Formulae for the wave function of H-like atoms look very complicated because of all the constants that appear in order to give proper scaling. For what purpose does one need to scale the wave functions?

8. The curve below is Ψ , a solution to the Schrödinger equation for a familiar type of potential energy function. The horizontal line is at a Ψ value of 0. The function continues to the right as a sine wave.

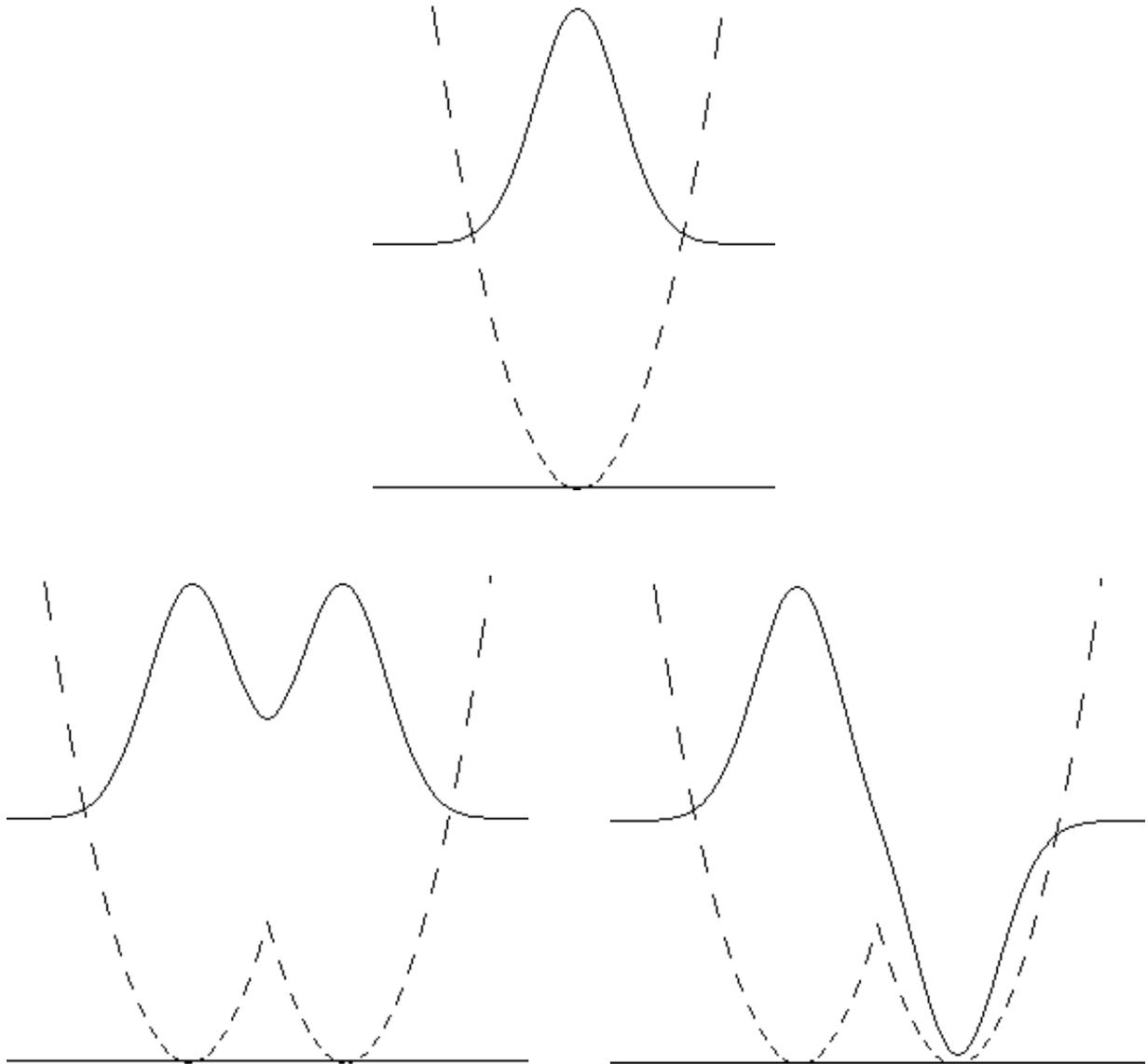
A. (8 minutes) Complete the lower graph by adding a potential energy function that would give this Ψ for the total energy shown. In a few words explain how key features of the energy plot are reflected in features of Ψ .



B. (1.5 minute) Name the potential function and say what chemical phenomenon it could represent.

C. (3 minutes) Could other acceptable Ψ functions be found with any old nearby energy? Explain.

9. Below are shown three potential energy functions (as dashed lines) and three superimposed wave functions (as solid lines) that are solutions of the corresponding one-dimensional Schrödinger equations (mass = 1 in each case). Each half of the two double minimum potentials is identical to a corresponding portion of the single minimum potential (which is for a single bond "harmonic oscillator"). Obviously there is a crude resemblance in shape between a portion of the first wave function and the left half of each of the others.



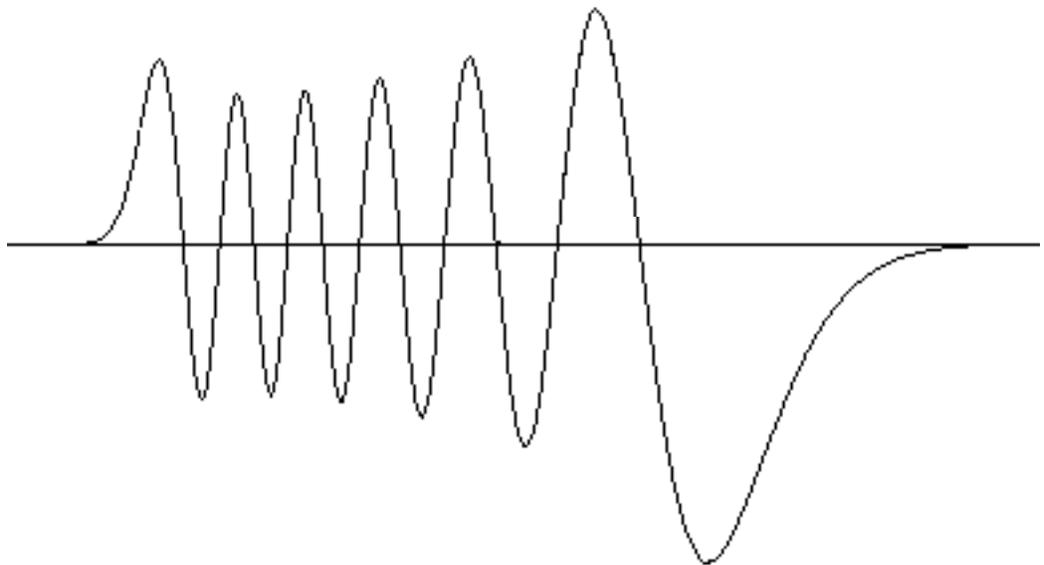
A. (3 minutes) On each potential energy diagram draw a horizontal line denoting the actual total energy. Explain in a few words, and by drawing on the diagrams, how you decided where to position each line.

B. (9 minutes) The three total energies for the wave functions on the previous page are 3.83, 4.15, and 4.39 kcal/mole, but not necessarily in that order. Label each diagram with the proper total energy, and explain below in a few words how you decided which is which. [Hint: one approach would be to draw vertical lines bisecting each double-minimum diagram and compare ψ functions in the left half with each half with each

C. (2 minutes, a challenging question for small credit. Make sure you've completed the rest of the exam before doing this one.) Explain why the existence of the second minimum alters the shape of the wave function (and thus the energy) in the first minimum.

6. (4 min) Write Schrödinger's formulation of the **kinetic energy of one particle in one dimension**.

7. (11 min) Below is a **wave function (Ψ)** that solves the Schrodinger equation for a particle governed by a familiar potential energy function. The horizontal line corresponds to $\Psi = 0$.



- a) Carefully draw a second graph on top of the figure to show the **potential energy curve** for this system. Reuse the horizontal $\Psi = 0$ line, this time to denote the **total energy** for this wave function
- b) Label (as A, B, C, D, E) the **five regions** in the figure that you consider to be the most interesting. Explain below what causes the shape of the wave function in each of these regions.

A:

B:

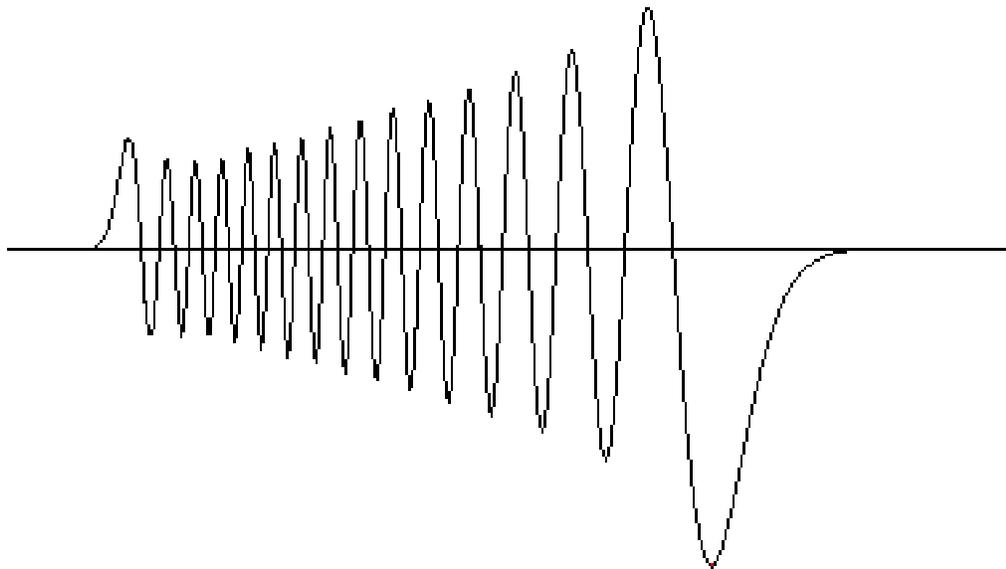
C:

D:

E:

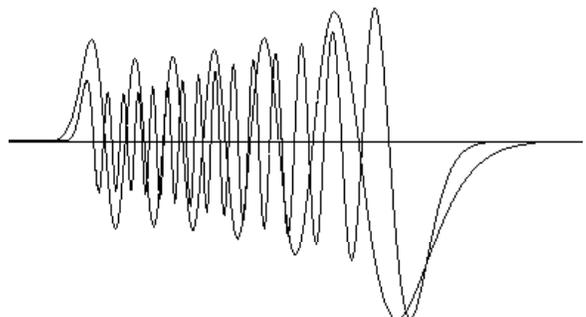
8. (3 min) Is the energy of this wave function in Question 7 quantized? That is, would a very slightly altered energy also yield a satisfactory wave function? Explain your thinking.

9. (3 min) The wave function below is a solution to the Schödinger equation for exactly the **same potential energy curve** as the one in Question 7, and it has exactly the **same total energy**. What must have changed? Explain.



10. (1 min) **Don't waste time on this** unless you have completed the rest of the rest of the exam.

The small figure at the right is an overlay of the wave function of Question 7 with that of Question 9. Explain why the latter does not extend as far to right or left as the former and what this teaches about tunnelling.

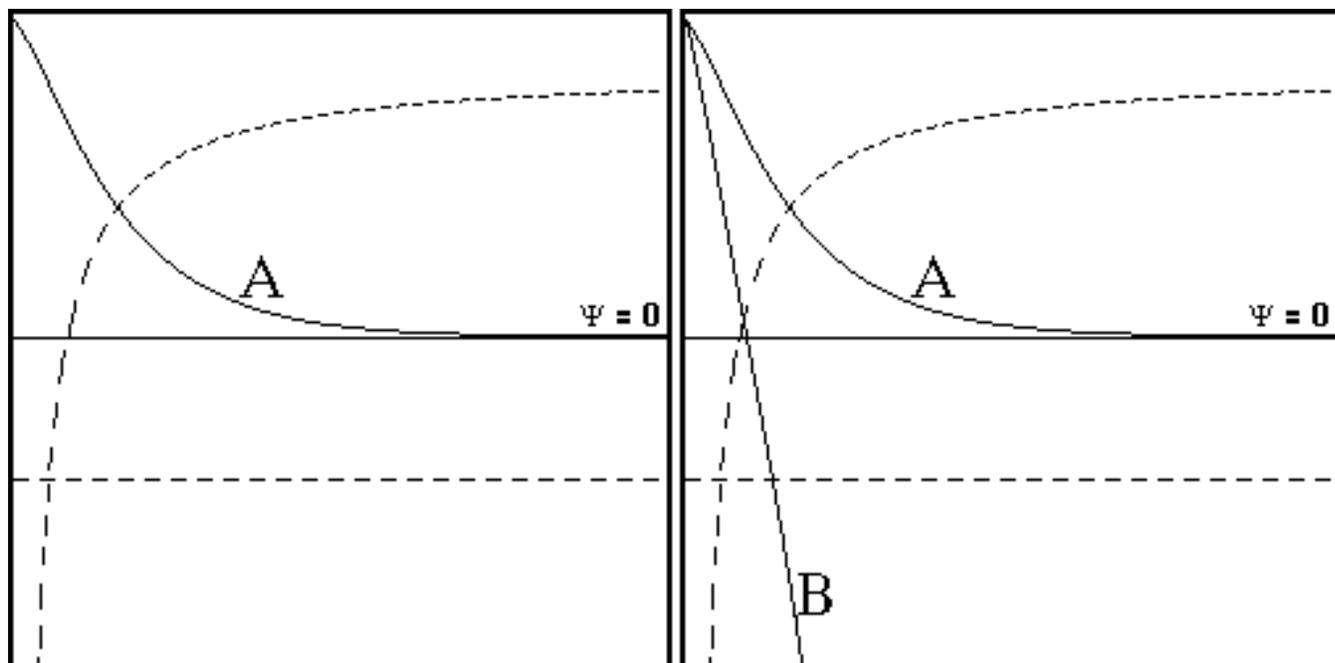


Thomson in Wonderland

5a. (3 min) Most people nowadays make fun of J. J. Thomson's "Plum Pudding" atom, but he proposed it for a good reason. Describe the model, and explain the relevance of Earnshaw's Theorem.

5b. (2 min) After Rutherford demonstrated that the nucleus was tiny, how did Thomson suggest accommodating Earnshaw's Theorem (in 1923)?

The diagrams show the Coulombic potential for a one-dimensional Hydrogen atom as a dashed curve, and, as solid curve "A", a wave function that solves Schrödinger's equation for the mass of an electron. The horizontal axis is the distance of the electron from the proton. The dashed horizontal line is the total energy for this wave function. The second diagram includes an unsatisfactory trial wavefunction, "B", which is plotted for the **SAME ENERGY**, but **TWICE the MASS**.



5c. (4 min) Use the quantum mechanical formula for kinetic energy to **explain** the way in which "B" differs from "A".

Thomson in Wonderland (continued)

- 5d.** (3 min) **Explain which direction** the total energy would need to be adjusted to generate a satisfactory nodeless wavefunction for the overweight electron. **Draw a new horizontal line** on the left diagram to indicate this new energy schematically (don't try to be quantitatively precise).
- 5e.** (3 min) **Explain** whether the nodeless wave for the heavier electron, with its new, proper energy would be **broader or narrower** than "A". [Hints: Think where its point of inflection would be, or how the wavelength for a constant-potential-energy particle changes with mass for constant total energy.]
- 5f.** (4 min) What might a helium atom (1 nucleus, 2 electrons) look like if the proton and the electron exchanged masses? That is, if the electron has a mass of 1 amu and the proton a mass of 0.000549 amu. [Think back to Thomson's atom]

1.
$$\Psi = \text{Const} \left(e^{-a_1 r_1} \right) \left(e^{a_2 r_2} \right) \left(x_3 e^{-a_3 r_3} \right)$$

- a) (2 min) What atomic or molecular system might the wavefunction above be written to describe?
- b) (6 min) Describe in words **each of the 3 expressions** (in parentheses), explaining **where it came from** and what the numerical **subscripts** mean.

$$\left(e^{-a_1 r_1} \right)$$

$$\left(e^{a_2 r_2} \right)$$

$$\left(x_3 e^{-a_3 r_3} \right)$$

- c) (2 min) What is fundamentally wrong with a wavefunction of this type?
- d) (5 min) Use this example to describe how one goes about modifying a wave function by the Self-Consistent-Field procedure without introducing any additional terms into the formula.