MATH 261, Spring 2001 **Due Date:**____________ **Name(s):** ________________________

Honors Project 15: The Stretching Potential of a Chemical Bond

The stretching potential of a chemical bond is approximately described by the function

$$V(s) = D_e(1 - e^{-\alpha s})^2$$

where D_e is the energy required to break the bond, α is a parameter, and s is the coordinate that gives the displacement from the equilibrium bond length.

Problems:

1. Find a power series expansion of $V(s)$ about the equilibrium, $s = 0$, in terms of s through the s^8 term.
2. Compare this expansion with the potential for stretching a simple ("harmonic") spring
$$V_{spring}(s) = \frac{1}{2}ks^2.$$
3. The restoring force of a spring is $\frac{\partial V}{\partial s}$, and the force constant is $\frac{\partial^2 V}{\partial s^2}|_{s=0}$. What are the restoring forces and the force constants obtained from $V(s)$ and $V_{spring}(s)$? How and what does this tell you about α?
4. If the power series were truncated (as an approximation to $V(s)$), how far would you have to go to be sure that the asymmetry of $V(s)$ (plot it!) was present for small displacements about $s = 0$?

[A particular $V(s)$ is said to be symmetric about $s = 0$ if, for every choice of s, $V(s) = V(-s)$. It is asymmetric if this is not satisfied. For chemical bonds, $V(s)$ may be nearly symmetric for small displacements away from the equilibrium, but it has to be asymmetric overall because breaking a bond, i.e. $s > 0$, is different than compressing it, i.e. $s < 0$.]

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