

**Chemistry 3890**  
**Problem Set 11**  
**Fall 2011**

A “grade it yourself” problem set.  
Solutions will be posted after the last week of class.

LAST REVISED: November 28, 2011

Approximations are the most precious fruits of theory.

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**Problem 1** Use first-order perturbation theory to estimate the first three energy levels for the perturbed HO,  $V(x) = \frac{1}{2}\omega^2x^2 + \beta x^4$ .

Compare your answers with those obtained numerically in PS 6, problem 3 (set  $m = \hbar = \omega = 1$ ,  $\beta = 0.06$ ).

**Problem 2** Use the variational approach to determine an approximate expression for the ground state energy for the linear potential  $V(x) = \alpha \text{Abs}[x]$ . Use a (normalized) trial function of the form

$$\psi_\beta = N_\beta e^{-\beta^2 x^2} \quad (1)$$

where  $N_\beta$  is a normalization constant. (The use of  $\beta^2$  in the exponent makes the minimization with respect to  $\beta$  easier.)

Using a suitable trial function for the first excited state (HINT: this function should be *odd* under  $x \rightarrow -x$ ), derive an estimate for the first excited state energy.

Compare your variational estimates to the numerical answers you obtained in PS 6, problem 2 (set  $m = \hbar = 1$ ,  $\alpha = 1/\sqrt{2}$ ).

Is the variational principle satisfied?

**Problem 3** Use the variational approach to determine an approximate ground state energy for the perturbed HO potential  $V(x) = \frac{1}{2}\omega^2x^2 + \beta x^4$ . Use a (normalized) trial function of the form

$$\psi_\alpha = N_\alpha e^{-\alpha x^2} \quad (2)$$

where  $N_\alpha$  is a normalization constant.

Your expression for the variational ground state energy for general  $\omega$  and  $\beta$  will be long and unwieldy, so it is not necessary to **Print** it. (Use the semicolon ; to suppress output.)

Find the numerical value of your estimate for  $m = \hbar = \omega = 1$ ,  $\beta = 0.06$ . Compare the value with that obtained in PS 6, problem 3.

Using a suitable trial function, derive an estimate for the first excited state energy. Again, compare your value with the numerical answers you obtained in PS6.

Is the variational principle satisfied?

