PERTURBATION THEORY AND THE VARIATIONAL PRINCIPLE

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.5.

A simple application of the variational principle is that the first order correction to the energy given by perturbation theory provides an upper bound on the effect of the perturbation hamiltonian H'. The first order perturbation is given by

$$E_{01} = \left\langle 00 \middle| H' \middle| 00 \right\rangle \tag{1}$$

where $|00\rangle$ is the unperturbed ground state wave function. According to the variational principle, $E_{01} \geq E_0'$ where E_0' is the ground state of H'. Therefore E_{01} can never underestimate the correction due to H' in the ground state.

Second-order perturbation theory says that the second-order correction to the ground state E_{02} is

$$E_{02} = \sum_{j \neq 0} \frac{\left|\langle j0| H' |00\rangle\right|^2}{E_{00} - E_{j0}} \tag{2}$$

Since the first order correction always overestimates the energy (unless it hits it bang on, in which case the second order correction will be zero), we would expect the second order correction to be negative in order to peg back the overestimate from the first order result. From the formula, this is always true, since $E_{00} < E_{j0}$ for all $j \neq 0$ (assuming non-degenerate states).