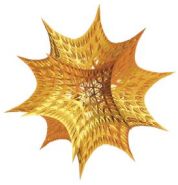

Mathematica Exercise: Linear Variational Theory

Physical Chemistry I
Fall 2005
M. Francl

Using as a basis set the first two solutions to the particle in a box problem, find the variational energy for a box with an oscillating floor. So:

$$V(x) = \sin^2 \frac{4\pi x}{a} \quad \text{and so} \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sin^2 \frac{4\pi x}{a}$$

$$f_1(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{\pi x}{a}$$

$$f_2(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{2\pi x}{a}$$

Use linear variation theory to find an estimate for the energy of the ground and excited states. Sketch the energy levels for the particle in a box with a flat floor and put the solutions for the oscillating floor on the diagram. What happens?

The Culture of Chemistry

Weird Words of Science:

quantophrenic

A term used for an obsession with and exaggerated reliance upon mathematical methods or results. (Source Oxford English Dictionary). For a long time, chemists considered quantum theorists (of which I am one) to be quantophrenics. The following quote summed it up well: "Every attempt to employ mathematical methods in the study of chemical questions must be considered profoundly irrational and contrary to the spirit of chemistry. If mathematical analysis should ever hold a prominent place in chemistry - an aberration which is happily almost impossible - it would occasion a rapid and widespread degeneration of that science." Auguste Comte, Cours de Philosophie Positive, 1830. Fortunately, quantum chemists persisted, and the methods they developed to treat chemical systems have become powerful tools for chemists in many areas.