2 Exact Solutions to the Schrödinger Equation ?

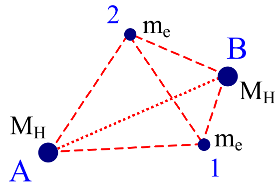
" *All we have to do is to solve the Schrödinger equation ....* "

If only it were this simple !

To illustrate how difficult it is consider the H_2 molecule : this consists of just two protons (A,B) and two electrons (1,2).

The Schrödinger equation is deceptively simple,

$$\hat{H}\Psi = E\Psi$$



but even in this case the $\hat{H}$ is an operator of a relatively complex form, containing kinetic energy (KE) terms for each of the four particles and potential energy (PE) terms for each of the six electrostatic pairwise interactions. More specifically:

$$\hat{H} = \frac{-\hbar^2}{2M_H}\left(\nabla_A^2 + \nabla_B^2\right)$$ - KE of nuclei A and B

$$+ \frac{-\hbar^2}{2m_e}\left(\nabla_1^2 + \nabla_2^2\right)$$ - KE of electrons 1 and 2

$$+ \frac{e^2}{4\pi\varepsilon_0 R_{AB}}$$ - Internuclear electrostatic PE (repulsive)

$$+ \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$ - Interelectronic electrostatic PE (repulsive)

$$- \left(\frac{e^2}{4\pi\varepsilon_0 r_{1A}} + \frac{e^2}{4\pi\varepsilon_0 r_{1B}} + \frac{e^2}{4\pi\varepsilon_0 r_{2A}} + \frac{e^2}{4\pi\varepsilon_0 r_{2B}}\right)$$ - Electron-nuclear PE terms (attractive)

\+ other terms (spin-orbit coupling etc.)

Neglect initially

where : KE = kinetic energy ; PE = potential energy ; $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

ε_o - vacuum permittivity constant.

If the Hamiltonian is this complex for H_2 , then imagine what it is like for a more complex molecule containing several atoms and many electrons !

To make any progress, we need to simplify the problem.