other words they are parameters of the model. Since only the separation of the protons can be physically significant, the single adjustable parameter of the model is in fact $|r_1 - r_2| = R$. The proton-proton electrostatic energy $E_{pp} = (e^2/4\pi\varepsilon_0)/R$ does not depend on r and can be subtracted from the reduced one-body Schrodinger equation.

The resulting hamiltonian is shown in box 3.

The BOpp TISE is

$$\mathbf{H}_e \psi_e = E_e \psi_e$$

$\psi_e(r)$ is the electron wave function and E_e is the energy of the electron. The BOpp approximation to the total energy is then $E_{tot} = E_e + E_{pp}$.

The Born Oppenheimer model now describes an electron moving in a double well potential,

$$V_e = -(e^2/4\pi\varepsilon_0)(|r_1 - r|^{-1} + |r_2 - r|^{-1})$$

V_e is not a central potential. This makes the model hard to solve, and we move on to the approximation scheme of box 4.

The **Variational solution for $\mathbf{E_e(R)}$** follows another sequence which is contained in box 4.

A sensible choice for ψ_t is important in variational methods, and in this case a superposition of 1s hydrogen wave functions is a good place to start. This is because when the electron is near to either proton, the system imitates a hydrogen atom and a free proton. Using ψ_1 and ψ_2 to denote 1s hydrogen wave functions centred on either proton then the variational choice is:

$$\psi_t = A\psi_1 + B\psi_2.$$

$E_{e,t}(A,B)$ is minimised at an extremum: $(\partial/\partial A)\, E_{e,t}(A,B) = (\partial/\partial B)\, E_{e,t}(A,B) = 0$. There are two solutions, $A = B$ or $A = -B$, a result which also follows from the symmetry of the system ($|A|^2 = |B|^2$). The two solutions have even (+) and odd parity (−):

$$\psi_+ = N_+ (\psi_1 + \psi_2)$$

and

$$\psi_- = N_- (\psi_1 - \psi_2)$$

$N_{+/-}$ normalise the solutions. The energies calculated at these extrema are $E_{+/-}$.
The process is looped for different values of the parameter R.