The proton-proton electrostatic energy is added to give the BOpp approximation to the total energy.

As quantum systems tend to minimise their total energy through radiation, we must **minimise $E_{tot}(R)$** with respect to R (box 6).

The **output** (box 7) is the final Born Oppenheimer approximation to the total energy and proton-proton separation.

Results

The even parity solution gives lower total energies than the odd parity solution for any R. There is little electron charge density between the protons in the odd parity solution, and none at all at $r = 0$. The even parity solution, however, does have appreciable negative charge density between the protons.

Experiments give information on E_{tot} and R_0. The results for E_{tot} and R_0 are reasonable but can be improved by scaling the charge in the trial wavefunctions (this will increase the negative charge density between the protons). This leads to closer agreement to experiment, especially for R_0.

(**Comment:** An exact solution for the ground state of the BOpp model has in fact been found by other methods and there is a good match between this and ψ_+. This gives us confidence in the variational part of the calculation).

Conclusions

There is good agreement between the variational solution to the Born Oppenheimer approximation and experimental results. The even parity solution also goes some way to answering this mystery: how can this molecule exist if the two protons repel each other?

The answer is that the even parity solution has appreciable negative charge density between the protons. The protons are attracted to the central negative charge density, and this overcomes their mutual repulsion. By contrast, the odd parity solution has little probability density between the protons - falling to zero midway between them - so the protons feel almost the full Coulomb repulsion.

This picture of an effective attractive force due to an intermediate particle has been a very fruitful one in nuclear physics.