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 $E_{+/-}$. All this has been accomplished for a particular model parameter R. The whole variational process is repeated for other values of R in order to build up a functional dependence $E_{+/-}(R)$. As quantum systems tend to minimise their total energy through radiation, the total energy $E_{+/-} + E_{pp}$ must be minimised with respect to R. The results for the total energy are shown below:

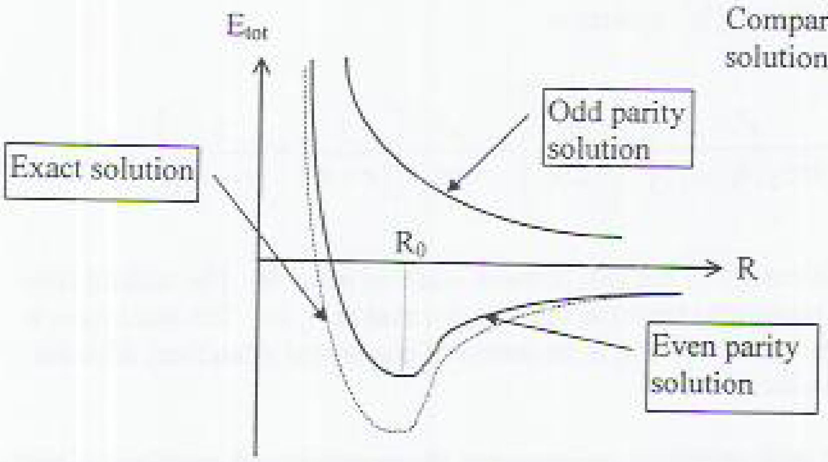

Figure 4

Comparison of exact and variational solutions to BOpp model

The even parity solution gives lower energies than the odd parity solution for any R and predicts an optimum value of R, the proton-proton separation, where E_{tot} is lowest. This is marked R_0 on Figure 3. The odd parity solution does not provide any binding. There is little electron charge density between the protons in this odd parity solution, and none at all at $r = 0$, so the protons will experience almost the full repulsive force between them. The even parity solution, however, does have appreciable negative charge density between the protons leading to stability for some values of R. The protons are attracted to the central negative charge density, and this overcomes repulsion. The even parity solution also matches the exact solution to the BOpp model, marked by the dashed line in Figure 3.

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.

Conclusions

There is good agreement between the variational solution to the Born Oppenheimer approximation and experimental results. The solution provides a picture of binding in H_2^+: each proton is attracted towards the concentration of negative charge between them, and this overcomes their mutual repulsion.