The complete time independent Schrodinger equation

The TISE is formed by mapping the classical hamiltonian onto a hamiltonian operator **H**. All that needs to be done is to replace momentum variables with momentum operators according to the rule:

$p_x \rightarrow (h/2\pi i)\partial/\partial x$ etc

This gives

$$\mathbf{H} = -(h^2/8\pi^2 M)\,(\partial^2/\partial x_1{}^2 + \partial^2/\partial y_1{}^2 + \partial^2/\partial z_1{}^2 + \partial^2/\partial x_2{}^2 + \partial^2/\partial y_2{}^2 + \partial^2/\partial z_2{}^2)$$
$$-(h^2/8\pi^2 m)\,(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + \mathrm{V}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}).$$

The complete TISE is then

$$\mathbf{H}\ \psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}) = E_{tot}\ \psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r})$$

where ψ is the wave function of the three body problem and E_{tot} is the total energy of the system.

The complete model cannot be solved exactly, so approximations must be found.

The Born Oppenheimer model

The important simplification introduced by Born and Oppenheimer in 1927 is based on the physical fact that each proton is almost 2000 times more massive than the electron. In the classical model they would therefore move much slower than the electron - they are effectively stationary. The masses appear in the denominators of the momentum operators so, roughly speaking, the quantum mechanical analogue of this effective classical picture will be to let $M \rightarrow \infty$ so that the proton momentum terms disappear. This will hopefully make the problem more tractable.

The proton coordinates will still appear in the potential energy terms but since $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ commute with the electron kinetic energy operator, they act like ordinary numbers. In 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 $|\boldsymbol{r}_1 - \boldsymbol{r}_2| = R$.

The proton-proton electrostatic energy $E_{pp} = (e^2/4\pi\varepsilon_0)/R$ does not depend on $\boldsymbol{r}$ and can be subtracted from the reduced one-body Schrodinger equation. Hence the BOpp model of the H_2^+ ion, with proton momentum terms set to zero is:

$$-(h^2/8\pi^2 m)\,(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2)\ \psi_e(\boldsymbol{r}) - (e^2/4\pi\varepsilon_0)(|\boldsymbol{r}_1 - \boldsymbol{r}|^{-1} + |\boldsymbol{r}_2 - \boldsymbol{r}|^{-1})\ \psi_e(\boldsymbol{r})$$
$$= E_e\ \psi_e(\boldsymbol{r})$$