Simple approach to molecular bond

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A simple approach

Victor Weisskopf was known as a master of simple arguments that lead to surprisingly accurate estimates of physical quantities.

This will follow the reasoning in *Search for Simplicity: the molecular bond*, American Journal of Physics **53**(5), 1985, p.399–400

A copy of the original paper is on the course web area as:

`198505_WeisskopfBond.pdf`

Two H nuclei are a distance ρ apart.

When they are far apart compared to the Bohr radius a_B, the energy of the system is that of two isolated H atoms:

$$E = -2\text{Ry}, \text{ where } \rho \gg a_B.$$

where $\text{Ry} = me^4/2\hbar^2$ is the "Rydberg", the energy of one H atom, and $a_B = \hbar/me^2$.

When the atoms are far apart, the mutual attraction and repulsion between the pairs of electrons and protons cancel, leaving only the electronic E of each atom.

When $\rho \sim a_B$, what happens?

Consider the energy minus the repulsion energy of the proton:

$$E' = E - e^2/\rho$$

for extreme cases.

First, for large ρ we know that

$$E' = -2\mathrm{Ry} - e^2/\rho, \quad \rho \gg a_B.$$

Next, suppose we can push the two protons together: $\rho \to 0$.

As far as the electronic E is concerned, we just made a He atom, the two electrons are just attracted to a charge $2e$.

The electron-proton energy E' is known in this case:

$$E' = -5.7\text{Ry}, \quad \rho \to 0;$$

from the QM of the He atom.

Now we play simpleminded. How far away is large ρ?, Why not two* Bohr radii?, so pretend

$$E' = -2\text{Ry} - e^2/\rho \text{ for } \rho > 2a_B,$$

and we know

$$E' = -5.7\text{Ry at } \rho = 0.$$

How do we connect these values? Well, why not a straight line?

* $\frac{1}{2} = 0$ for large values of 2!

So we interpolate E' between $\rho = 0$ and $\rho = 2a_B$ with a linear function.

Then add e^2/ρ back to get the total E. This gives the graph:

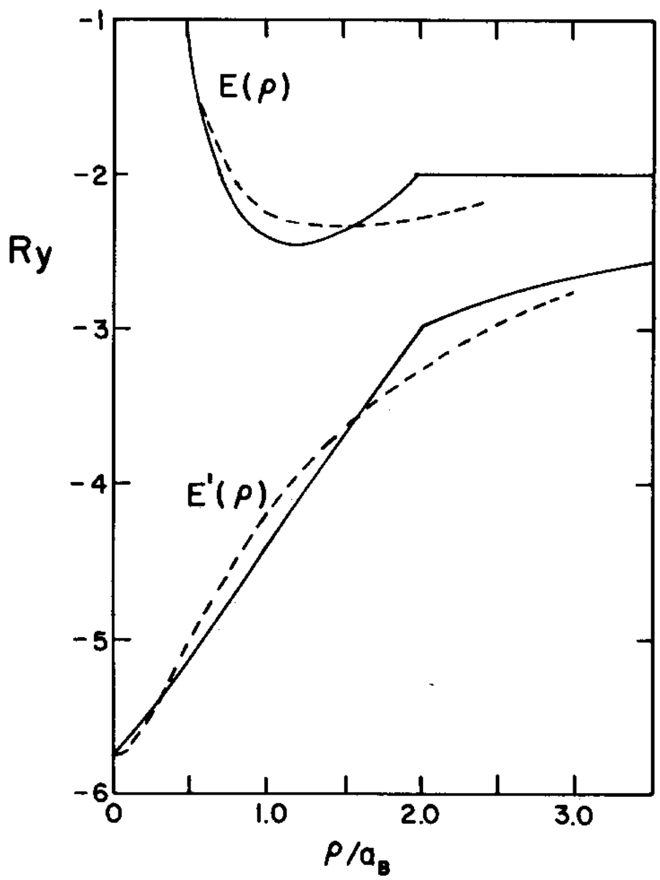

Fig. 1. Energy E of two hydrogen atoms as a function of the distance ρ between the nuclei. $E'(\rho) = E - e^2/\rho$. The energies are measured in Ry, the distance in units of a_B. The full curves are the approximate results, and the broken curves are the exact results.

This gives amazingly good results for such a simple approach.

The minimum of the potential is at

$$\rho_0 = 1.22a_B \text{ (actual is } 1.43a_B.)$$

The binding energy is

$$E(\rho_0) - E(\rho_\infty) = 0.42\text{Ry (actual } 0.34\text{Ry.)}$$

Exact (?) calculations using the Schrödinger equation are shown as dotted curves on the graph.

What's the physics?

1. The electrons spins must be opposite: the -5.7Ry value is for the *ground state* of He, if the spins are parallel, E will increase too much: no bonding.

2. At around $2a_B$ the electron clouds merge. Either electron is attracted by *both* nuclei. This is counteracted by the repulsion between the nuclei, but attraction wins out around $\rho \sim 1\frac{1}{2}a_B$, as long as the electrons have opposite spin.

So the molecular bond is an electrostatic effect, modified by the fermion state requirements of electrons.