Toy model of a covalent bond

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What is a covalent bond?

A **covalent bond** is a chemical bond that involves the sharing of electron pairs between atoms. The stable balance of attractive and repulsive forces between atoms when they share electrons is known as covalent bonding. For many molecules, the sharing of electrons allows each atom to attain the equivalent of a full outer shell, corresponding to a stable electronic configuration.
http://en.wikipedia.org/wiki/Covalent_bond

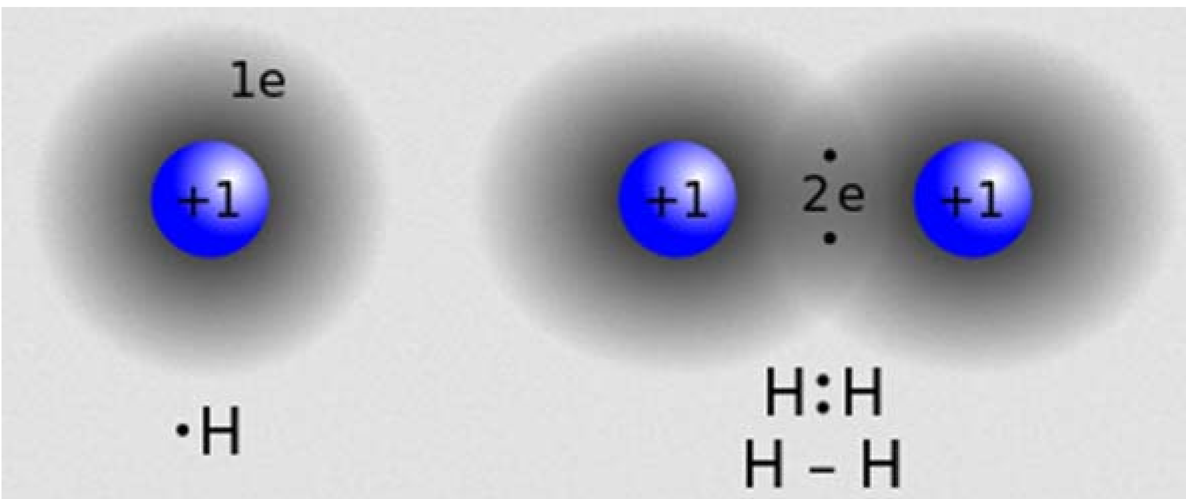

Fig. A covalent bond forming H_2 (right) where two hydrogen atoms share the two electrons.

In order to show how covalent bonding works, we discuss a one-dimensional toy model which is not at all realistic but it is analytically tractable. We consider a particle of mass *m* that moves along the *x* axis in an attractive double-delta potential. Here we discuss the eigenvalue (the bound state) problem for the Schrödinger equation for the attractive double-delta potential,

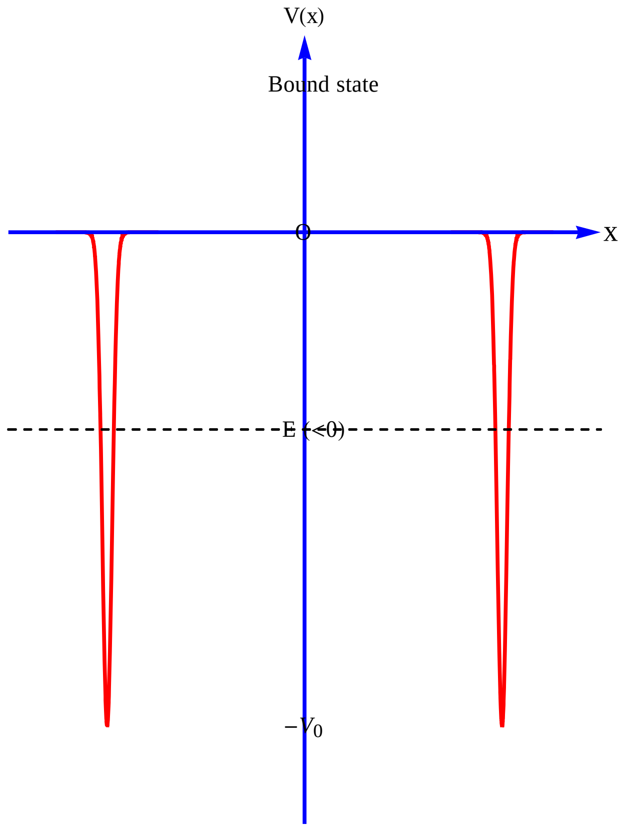

Fig. $V(x) = -V_0[\delta(x-a) + \delta(x+a)]$; attractive Dirac delta-type potential.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - V_0[\delta(x-a) + \delta(x+a)]\psi(x) = E\psi(x) = -\frac{\hbar^2 k^2}{2m}\psi(x)$$

where the potential energy is an even function of *x*,

$$V(x) = -V_0[\delta(x-a) + \delta(x+a)],$$

and the energy is given by

$$E = -\frac{\hbar^2 k^2}{2m} \ (<0),$$

for the bound state. Then we get

$$(\frac{d^2}{dx^2} - k^2)\psi(x) = -2\alpha[\delta(x-a) + \delta(x+a)]\psi(x),$$

where

$$\alpha = \frac{mV_0}{\hbar^2}.$$

We note that the wave function $\psi(x)$ is either an even function or an odd function of x.

$$\frac{\psi_e(x)}{\psi_e(a)} = \begin{cases} e^{k(x+a)} & x < -a \\ \dfrac{\cosh(kx)}{\cosh[(ka)}, & -a < x < a \\ e^{-k(x-a)} & x > a \end{cases}$$

$$\frac{\psi_o(x)}{\psi_o(a)} = \begin{cases} -e^{k(x+a)} & x < -a \\ \dfrac{\sinh(kx)}{\sinh(ka)} & -a < x < a \\ e^{-k(x-a)} & x > a \end{cases}$$

Here we use the boundary condition:

$$\frac{d}{dx}\psi(x)\Big|_{a-0}^{a+0} = -2\alpha\psi(a),$$

for the even and odd function, respectively. Then we have

$2\alpha a = ka[1 + \tanh(ka)]$ for the even parity

$2\alpha a = ka[1 + \coth(ka)]$ for the odd parity

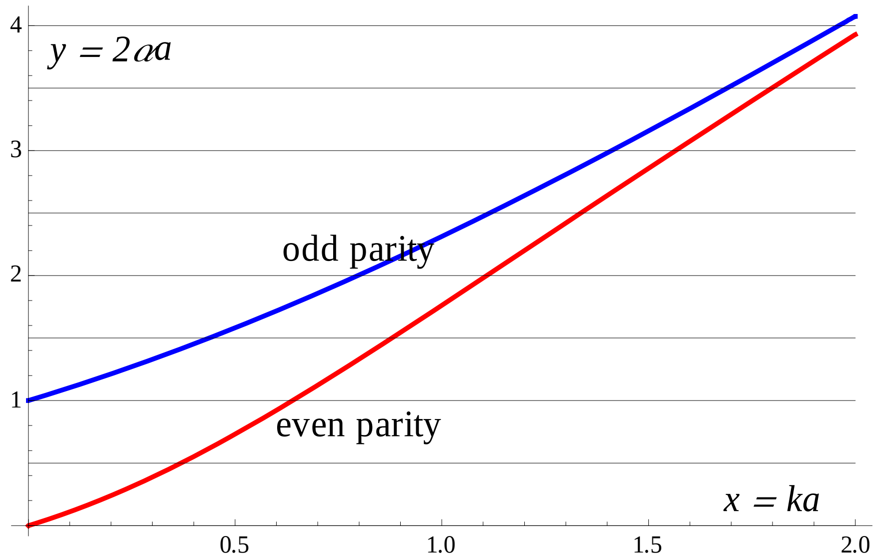

Fig. Plot of $y = 2a\alpha$ vs ka for the even parity and the odd parity.

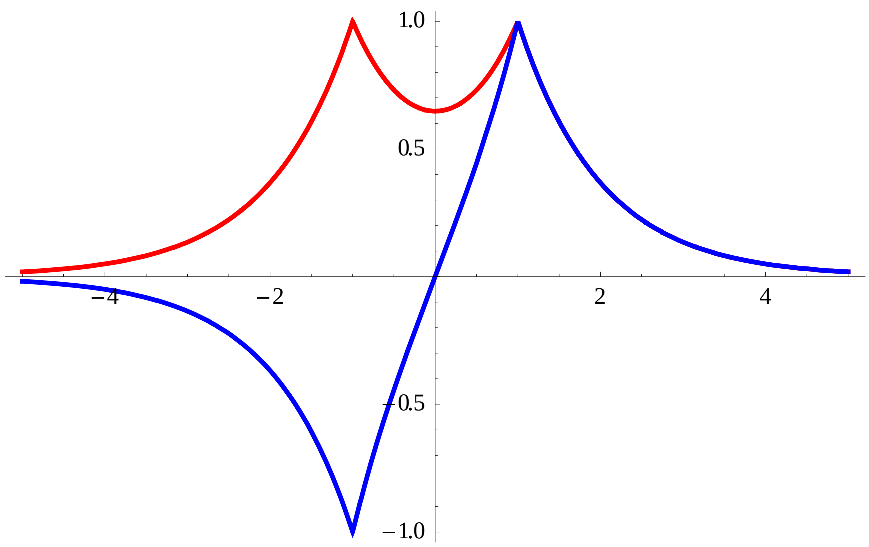

Fig. Even and odd function. k = 1. a = 1. y = 1.76159 for the even parity (red) and y = 2.31304 for the odd parity.