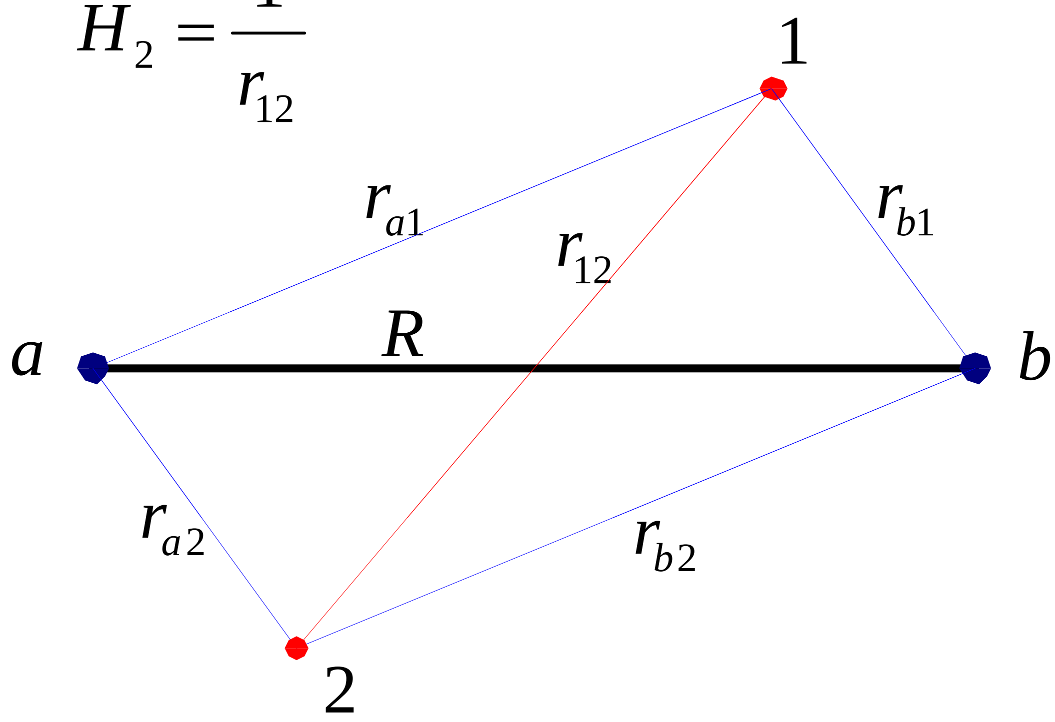
Schrodinger equation (no approximations)

$$H\,\Psi(\vec{r}_1,\vec{r}_2) = E\,\Psi(\vec{r}_1,\vec{r}_2), \quad H = H_0 + H_1 + H_2$$

$$H_0 = \frac{1}{R}, \qquad H_1 = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_{a1}} - \frac{1}{r_{b1}} - \frac{1}{r_{a2}} - \frac{1}{r_{b2}}$$

$$H_2 = \frac{1}{r_{12}}$$



“Bohr – D” approach

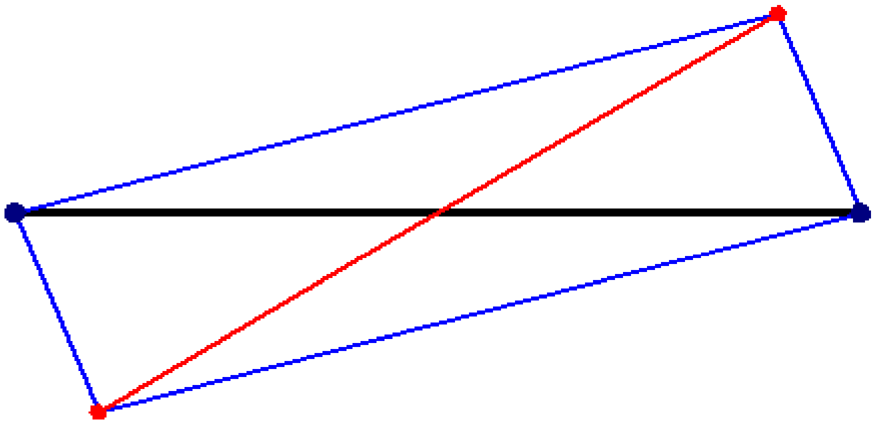
$$E = \min_{\vec{r}_1, \vec{r}_2} \left[\mathscr{H}_0 + \mathscr{H}_1(\vec{r}_1, \vec{r}_2) + \mathscr{H}_2(\vec{r}_1, \vec{r}_2) \right]$$

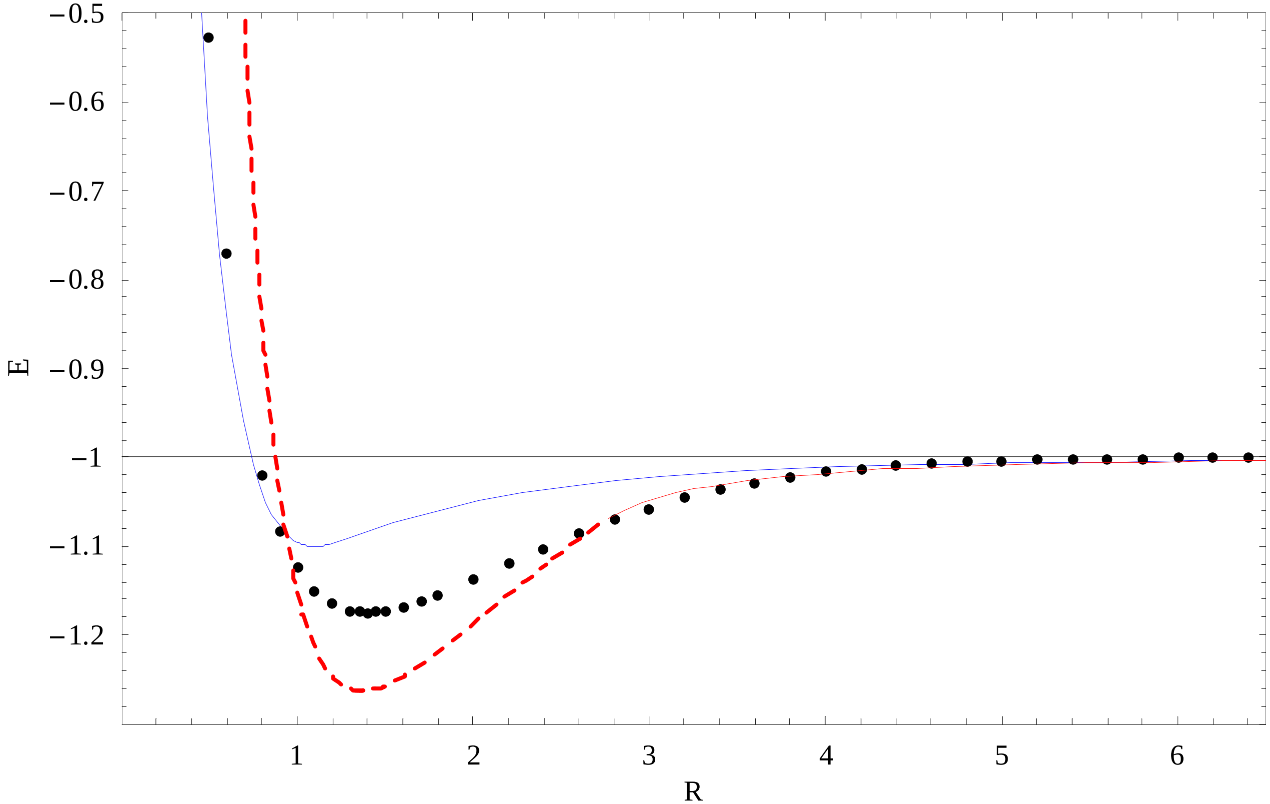
$$\mathscr{H}_0 = \frac{1}{R}$$

$$\mathscr{H}_1 = \frac{1}{2r_{a1}^2} + \frac{1}{2r_{b2}^2} - \frac{1}{r_{a1}} - \frac{1}{r_{b1}} - \frac{1}{r_{a2}} - \frac{1}{r_{b2}}$$

$$\mathscr{H}_2 = \frac{1}{r_{12}}$$

“Bohr – *D*” results





Variational (HL) approach

$$E = \min_{\alpha,\beta} W(\alpha,\beta), \qquad W(\alpha,\beta) = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\Psi_{\alpha,\beta}(\vec{r}_1,\vec{r}_2) = \exp(-\alpha|\vec{r}_1|)\exp(-\beta|\vec{r}_2 - \vec{R}|) + \exp(-\alpha|\vec{r}_2|)\exp(-\beta|\vec{r}_1 - \vec{R}|)$$

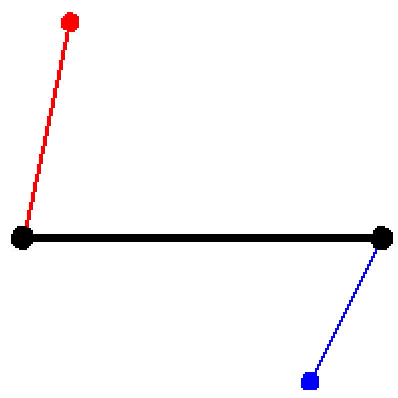
$$W = W_0 + W_1 + W_2, \qquad W_0 = \frac{1}{R}$$

$$W_1(\alpha,\beta) = \frac{\langle \Psi | H_1 | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \qquad W_2(\alpha,\beta) = \frac{\langle \Psi | \frac{1}{r_{12}} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

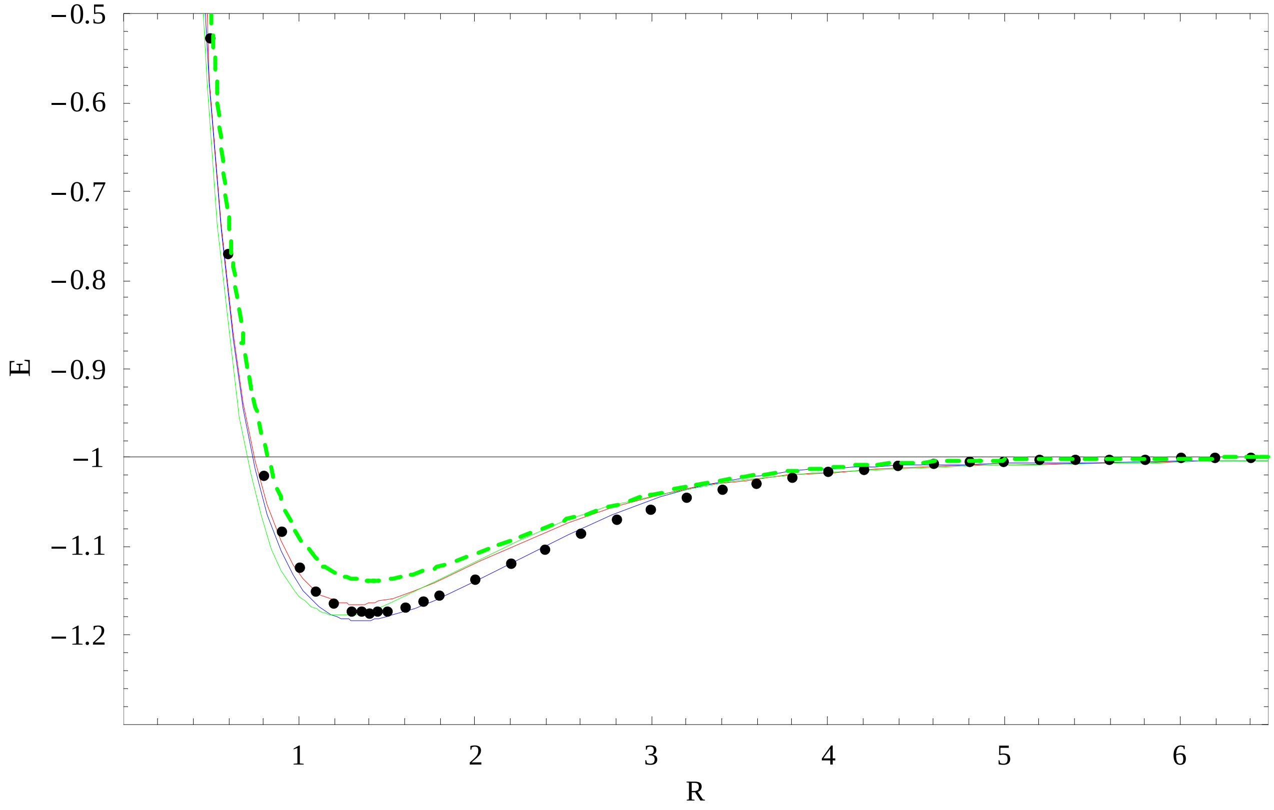
Hybrid variational – Bohr approach

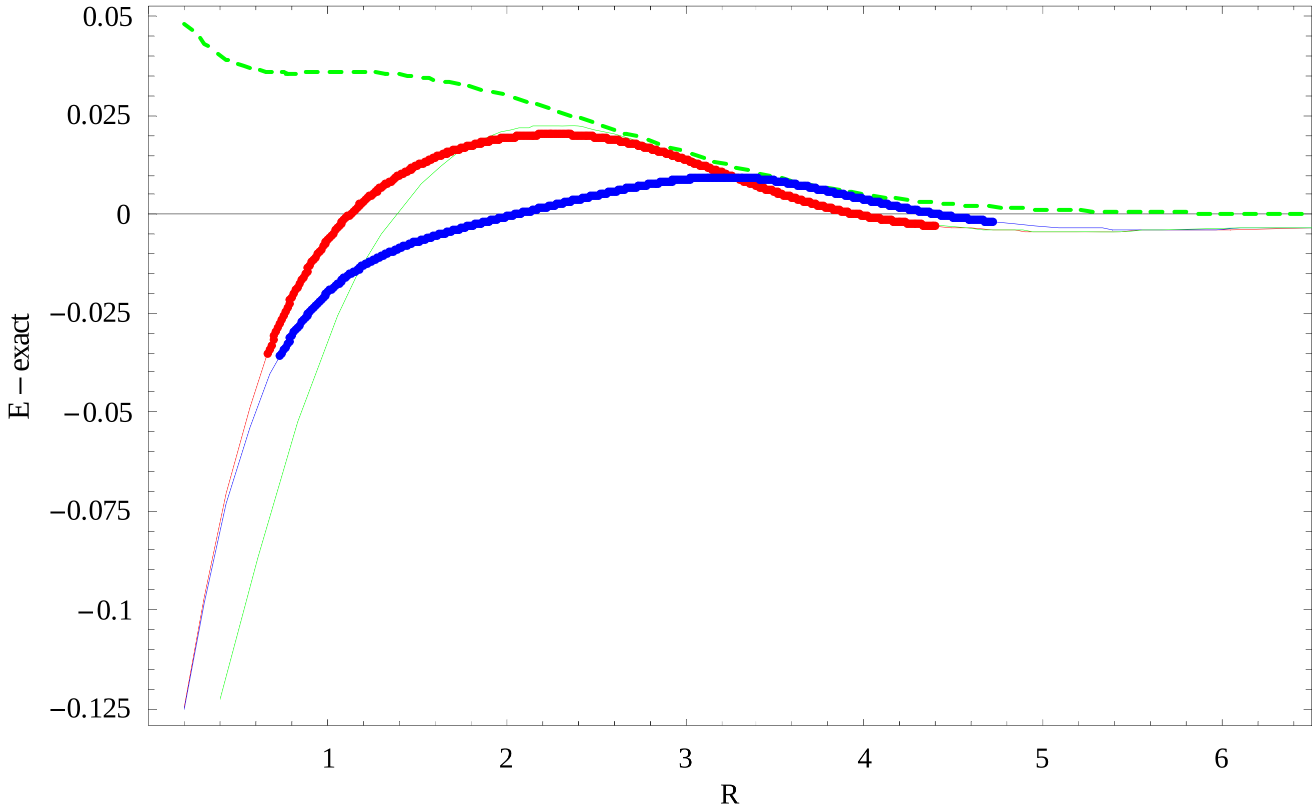
$$E = \min_{\vec{r}_1, \vec{r}_2} \left[\mathcal{H}_0 + \mathcal{H}_1(\vec{r}_1, \vec{r}_2) + \mathcal{H}_2(\vec{r}_1, \vec{r}_2) \right],$$

$$W_1\left(\frac{1}{|\vec{r}_1|}, \frac{1}{|\vec{r}_2 - \vec{R}|}\right) = \mathcal{H}_1(\vec{r}_1, \vec{r}_2)$$



Results




0.05
0.025
0
−0.025
−0.05
−0.075
−0.1
−0.125
E − exact
1
2
3
4
5
6
R