The method NNQWC
(nearest-nucleus quantization without constraints)

$$W(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = V + V_c$$

$$V_c(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \sum_{i=1}^{N} \frac{n_i^2}{2\left|\vec{r}_i - \vec{R}_{n_i}\right|^2}$$

$$E = \min_{\vec{r}_1, \vec{r}_2, ..., \vec{r}_N} W(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$$

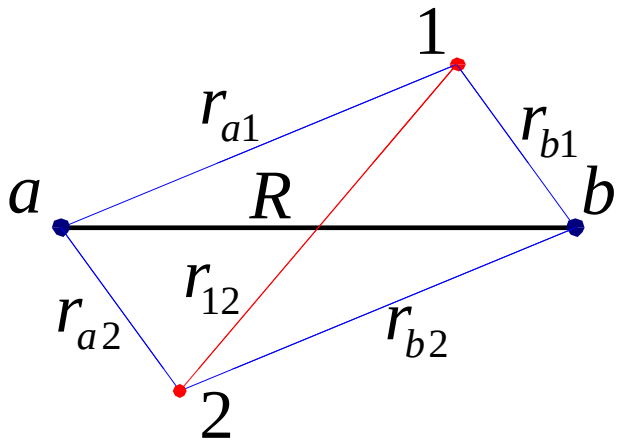
Hydrogen atom

$$N = 1 \qquad V = -\frac{1}{r}$$

$$V_{\mathrm{c}} = \frac{1}{2r^2}$$

$$E = \min_{r}\left(-\frac{1}{r} + \frac{1}{2r^2}\right) = -\frac{1}{2}$$

H_2 molecule



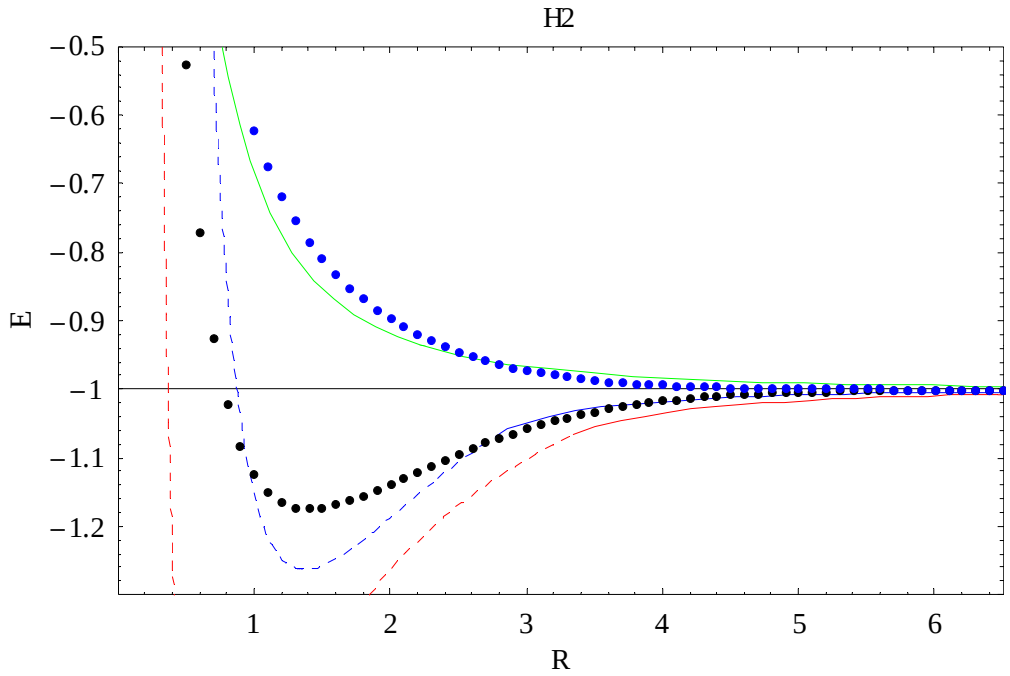
$$N = 2$$

$$V = -\frac{1}{r_{a1}} - \frac{1}{r_{b1}} - \frac{1}{r_{a2}} - \frac{1}{r_{b2}} + \frac{1}{r_{12}} + \frac{1}{R}$$

$$V_c = \frac{1}{2r_{a1}^2} + \frac{1}{2r_{b2}^2}$$

$$E = \min_{\vec{r}_1, \vec{r}_2} \left(V + V_c \right)$$

Results for H_2 molecule



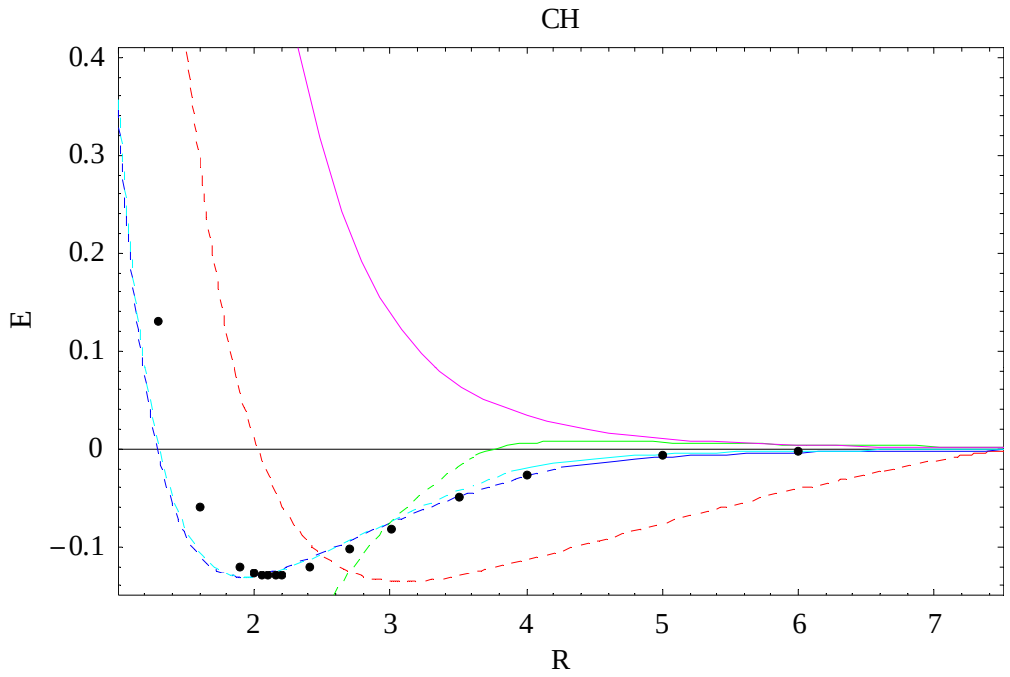
Dots – singlet and triplet (exact)

Green and red – one-dimensional configurations

$(x_2 = -x_1)$ and $(x_1 > 0,\ x_2 > 0)$

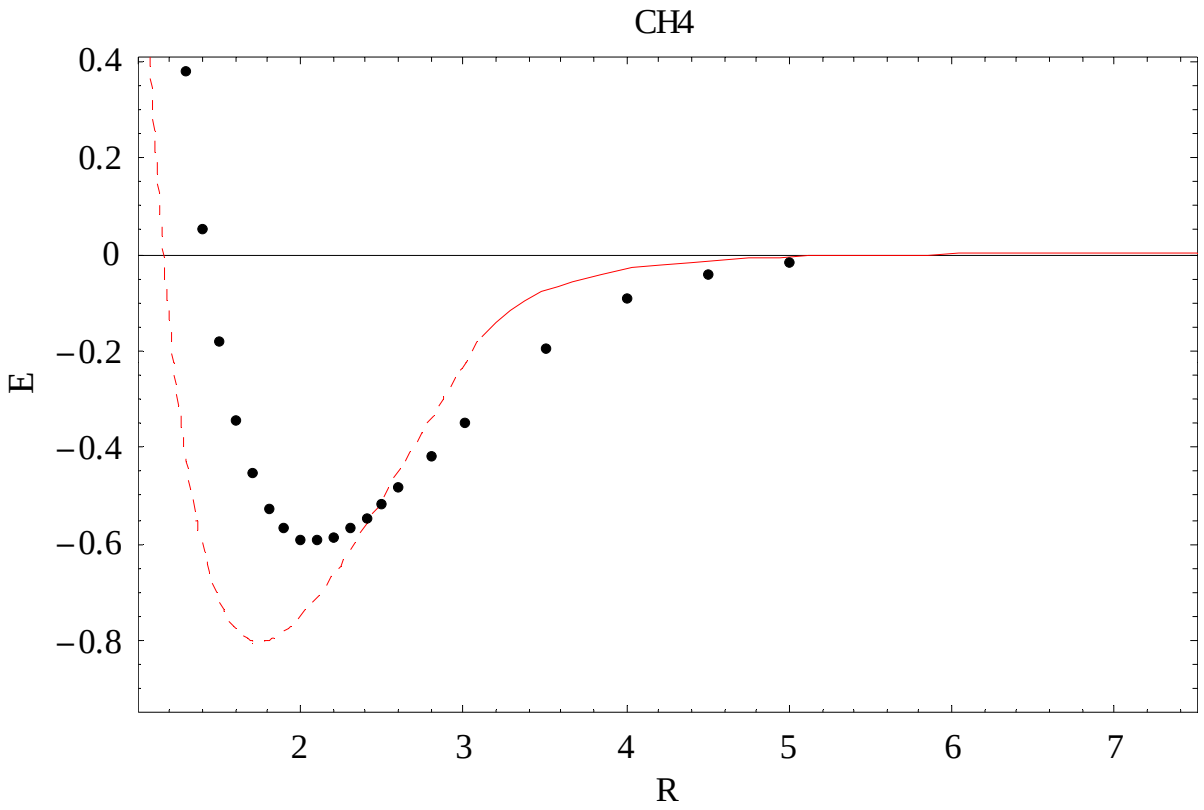
Blue – two-dimensional configuration

Results for CH molecule $N = 5$



Dots – exact
Red line - linear configuration
(unstable for R<7.2)
Blue and green lines - planar configurations
Cyan and magenta lines - 3-dimensional
tetrahedral configurations

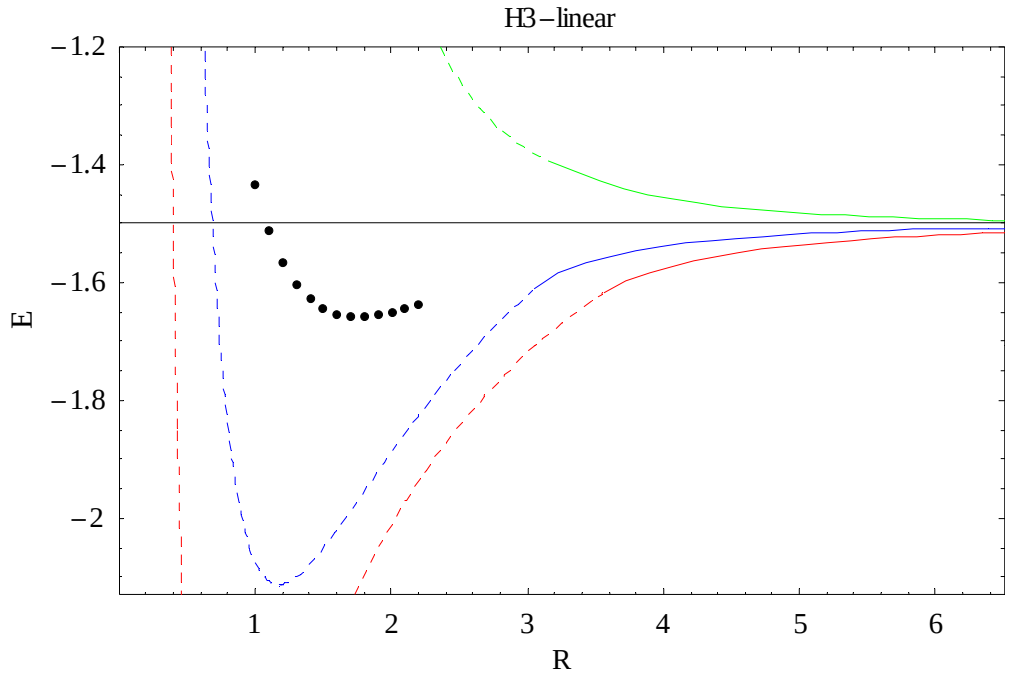
Results for CH_4 molecule $N = 8$



Totally symmetric
tetrahedron configuration of
electrons

Results for H_3 in linear configuration

$N = 3$



Dots –exact

Green and red – one-dimensional configurations

$(x_3 = -x_1,\ x_2 = 0)$ and $(x_1 > 0,\ x_2 > 0,\ x_3 > 0)$

Blue – two-dimensional configuration