

# Nearest atom q. for H<sub>2</sub>

$$r_{a1} = r_{b2} = a, \quad r_{b1} = r_{a2} = b$$

$$E(a,b) = \left( \frac{1}{2a^2} - \frac{1}{a} - \frac{1}{b} \right) \times 2 + \frac{1}{r_{12}} + \frac{1}{R}$$

$$r_{12}^2 = 2a^2 + 2b^2 - R^2$$

$$\frac{\partial}{\partial a} E(a,b) = \frac{2}{a^2} - \frac{2}{a^3} - \frac{2a}{r_{12}^3}$$

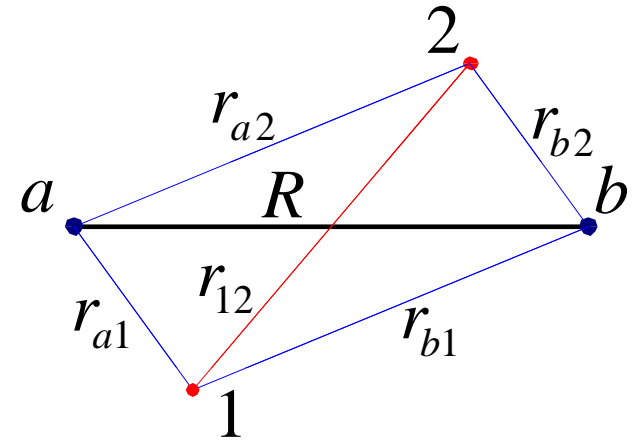
$$\frac{\partial}{\partial b} E(a,b) = \frac{2}{b^2} - \frac{2b}{r_{12}^3}$$

$$a^4 + r_{12}^3(1-a) = 0$$

$$b^3 - r_{12}^3 = 0$$

$$r_{12} = b$$

$$\begin{cases} 2a^2 + b^2 - R^2 = 0 \\ a^4 + b^3(1-a) = 0 \\ E = \frac{1}{a^2} - \frac{2}{a} - \frac{1}{b} \end{cases}$$



Eliminating  $b$  from the equations

$$b = \frac{a^2}{1 - 2a - a^2 E}$$

$$\left\{ \begin{array}{l} (2a^6 - R^2 a^4)E^2 + (8a^5 - 4a^4 - 4R^2 a^3 + 2R^2 a^2)E + \\ \quad 9a^4 - 8a^3 + 2a^2 - 4R^2 a^2 + 4R^2 a - R^2 = 0 \\ a^6 E^3 + (6a^5 - 3a^4)E^2 + (12a^4 - 12a^3 + 3a^2)E + \\ \quad 9a^3 - 13a^2 + 6a - 1 = 0 \end{array} \right.$$

Eliminating  $E$  from the equations

$$P(a, R) = a^6 [a(16 - 9a) - 8] + (12R^2 a^4 - 6R^4 a^2 + R^6)(1 - a)^2 = 0$$

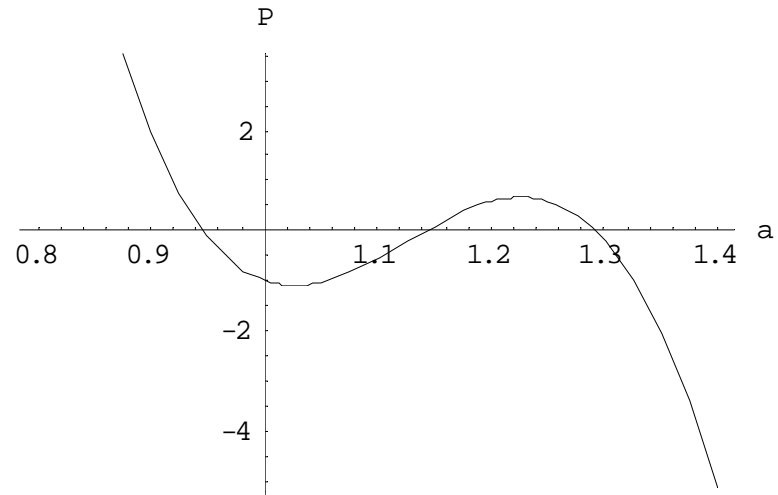
This equation implicitly defines a function  $a(R)$

Analytic continuation of the function  $a(R)$

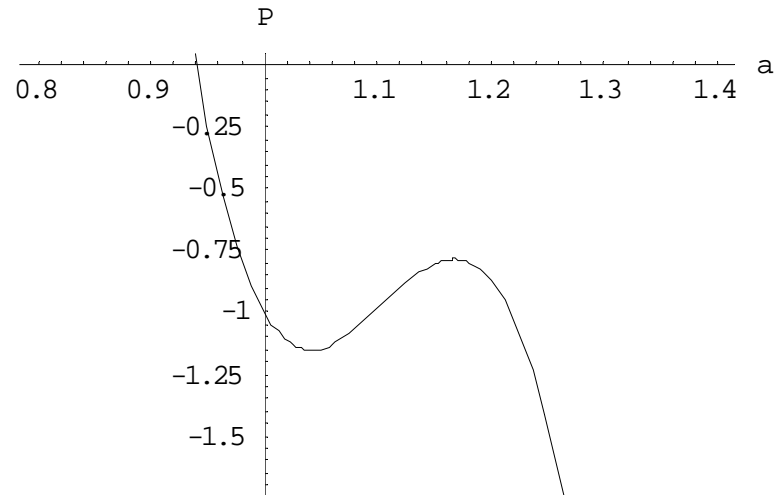
$R$	$a$
5	1.01
3	1.08
2.8	1.14
2.7	$1.19 \pm 0.10i$
2.6	$1.16 \pm 0.15i$
2.5	$1.13 \pm 0.18i$

$$P(a, R) = a^6[a(16 - 9a) - 8] + (12R^2a^4 - 6R^4a^2 + R^6)(1 - a)^2 = 0$$

$R = 2.8$



$R = 2.7$



Animated configuration (with change of  $R$ )

