



Figure 1: The Jagla ramp potential

In my code I have chosen to use the formulation of the Jagla potential given by [1]. The equations for Fig. (1) are

$$U(r) = \begin{cases} \infty, & r < \lambda_0, \\ m_1 r + b_1, & \lambda_0 < r \leq \lambda_1, \\ m_2 r + b_2, & \lambda_1 < r \leq \lambda_2, \\ 0, & r > \lambda_2, \end{cases} \quad (1)$$

where

$$m_1 = \frac{\varepsilon_2 - \varepsilon_1}{\lambda_1 - \lambda_0}, \quad (2)$$

$$b_1 = \varepsilon_2 - \frac{\varepsilon_2 - \varepsilon_1}{\lambda_1 - \lambda_0} \lambda_1, \quad (3)$$

$$m_2 = \frac{-\varepsilon_2}{\lambda_2 - \lambda_1}, \quad (4)$$

$$b_2 = \varepsilon_2 + \frac{\varepsilon_2}{\lambda_2 - \lambda_1} \lambda_1. \quad (5)$$

This definition maps directly onto the parameters from [2] in the following way:

$$\lambda_0 = a, \tag{6}$$

$$\lambda_1 = b, \tag{7}$$

$$\lambda_2 = c, \tag{8}$$

$$\varepsilon_1 = U_R, \tag{9}$$

$$\varepsilon_2 = U_A, \tag{10}$$

$$\tag{11}$$

Furthermore, the parameters map to the original definition of the potential given in [3] with:

$$\gamma = -\frac{\lambda_2 - \lambda_0}{\lambda_2 - \lambda_1} \varepsilon_2, \tag{12}$$

$$\epsilon = -\frac{\lambda_0 - \lambda_2}{\lambda_1 - \lambda_2} \varepsilon_2 + \varepsilon_1, \tag{13}$$

$$r_0 = \lambda_0, \tag{14}$$

$$r_1 = \lambda_1, \tag{15}$$

$$r_2 = \lambda_2. \tag{16}$$

$$\tag{17}$$

References

- [1] Benavides, A.; Cervantes, L.; Torres, J. *Journal of Physical Chemistry C* **2007**, *111*, 16006–16012.
- [2] Buldyrev, S.; Kumar, P.; Debenedetti, P.; Rossky, P.; Stanley, H. *Proceedings of the National Academy of Sciences* **2007**, *104*(51), 20177.
- [3] Jagla, E. *Physical Review E* **2001**, *63*(6), 61501.