Note on Potential Cutoffs

Suppose you have a general pair potential $u(r)$.

1. In HW#2, you implemented

$$u(r) = u(r) \text{ for all } r,$$

where there is no cutoff. The pair force is given by

$$F = -\frac{\partial u(r)}{\partial r} \text{ for all } r.$$

2. The truncated, shifted potential with a cutoff at R_c is given by

$$\begin{aligned} u_{c2}(r) = &\quad u(r) - u(R_c) &\quad &\text{for } r \le R_c \\ = &\quad 0 &\quad &\text{for } r > R_c. \end{aligned}$$

This potential gives a continuous energy at the cutoff, but not a continuous force. The force is given by

$$\begin{aligned} F_{c2} = &\quad -\frac{\partial u(r)}{\partial r} &\quad &\text{for } r \le R_c \\ = &\quad 0 &\quad &\text{for } r > R_c. \end{aligned}$$

3. To obtain a continuous energy and force, one can implement

$$\begin{aligned} u_{c3}(r) = &\quad u(r) - u(R_c) - (r - R_c)\frac{\partial u(r)}{\partial r}\bigg|_{R_c} &\quad &\text{for } r \le R_c \\ = &\quad 0 &\quad &\text{for } r > R_c \end{aligned}$$

for which the force is

$$\begin{aligned} F_{c3} = &\quad -\frac{\partial u(r)}{\partial r} + \frac{\partial u(r)}{\partial r}\bigg|_{R_c} &\quad &\text{for } r \le R_c \\ = &\quad 0 &\quad &\text{for } r > R_c. \end{aligned}$$