[pex15] Young modulus for generalized Lennard-Jones potential

Consider a crystal with simple cubic structure and an interatomic potential of the form

$$U(r) = 4\epsilon_0 \left[\left(\frac{r_0}{r} \right)^{2m} - \left(\frac{r_0}{r} \right)^{m} \right]$$

with $m > 0$ and positive constants ϵ_0, r_0. This potential has a unique minimum at $r = a$, where a is now taken to be the lattice spacing. For $m = 6$ it is the familiar Lennard-Jones potential.
(a) Find a/r_0 as a function of m and the value $U(a)$ of the potential minimum.
The Young modulus is defined as the ratio, $Y = \sigma/e$, of tensile stress, $\sigma = F/A_0$, and tensile strain, $e = \Delta L/L_0$. In the situation at hand, we can set $F = k(r - a)$ with $k = (d^2U/dr^2)_a$, $A_0 = a^2$, $\Delta L = r - a$, $L_0 = a$.
(b) Show that for the potential $U(r)$ we thus obtain $Y = k/a$. Then evaluate k in terms of ϵ_0, a, m.

[adapted from Jones 2002]

Solution: