Problem M23 (Materials and Structures)

The potential energy, U of a pair of atoms in a solid can be written as:

$$U = \frac{-A}{r^m} + \frac{B}{r^n}$$

where r is the separation of the atoms and A, B, m and n are positive constants. Indicate the physical significance of the two terms in this equation.

A material has a simple cubic unit cell with atoms placed at the corners of the cubes. Show that, when the material is stretched in a direction parallel to one of the cube edges, Young's modulus E is given by:

$$E = \frac{mnkT_M}{\Omega}$$

Where Ω is the mean atomic volume, k is Boltzmann's constant and T_M is the absolute melting temperature of the solid. You may assume that $U_0(r_0) = -kT_M$,where r0 is the equilibrium separation of a pair of atoms.