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:

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

Where $W$ 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 $U_0(r_0) = WkT_M$, where $r_0$ is the equilibrium separation of a pair of atoms.