A commonly used potential energy function to describe the interaction between two atoms is the Lennard-Jones 6,12 potential

\[
U(r) = U_0 \left[ (r_0 / r)^{12} - 2(r_0 / r)^6 \right]; \quad r > 0 .
\]

where \( r \) is the distance between the atoms. Let \( m \) denote the effective mass of the system of two atoms.

a) Determine the value of \( r \) such that the potential energy is minimum.

b) Determine the value of the second derivative of the potential energy at the minimum of the potential.

c) Find the angular frequency of small oscillations about the stable equilibrium position for two identical atoms bound to each other by the Lennard-Jones interaction.

Solution:

The equilibrium points are found by setting the first derivative of the potential energy equal to zero,

\[
0 = \frac{dU}{dr} = U_0 \left[ -12r_0^{12}r^{-13} + 12r_0^6r^{-7} \right].
\]

Therefore the equilibrium point is located at \( r = r_0 \).

The second derivative of the potential energy is

\[
\frac{d^2U}{dr^2} = U_0 \left[ +12(13)r_0^{12}r^{-14} - 12(7)r_0^6r^{-8} \right].
\]

Evaluating this at \( r = r_0 \) yields

\[
\frac{d^2U}{dr^2}(r_0) = 72U_0r_0^{-2}
\]

The angular frequency of small oscillation is therefore
$$\omega_0 = \sqrt{\frac{d^2U}{dr^2}(r_0)} / m = \sqrt{\frac{72U_0}{mr_0^2}}.$$