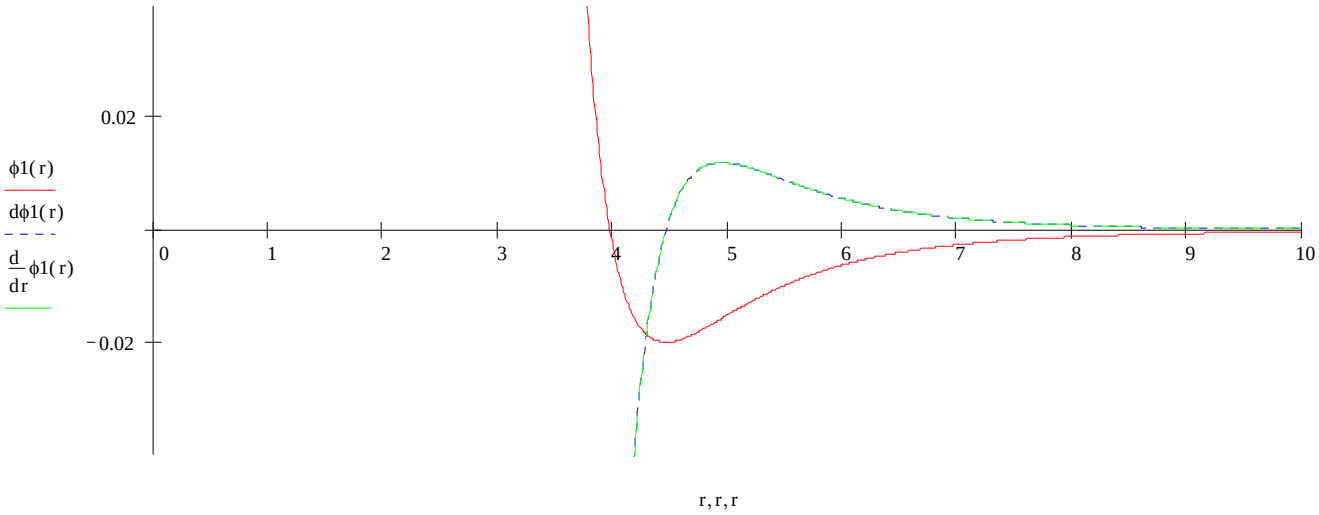
$r := 0.01, 0.02 .. 10$

Lennard-Jones potential

$\varepsilon := 0.01997$ $\sigma := 3.98$ $\phi 1(r) := 4 \cdot \varepsilon \cdot \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$ $d\phi 1(r) := -24 \cdot \frac{\varepsilon}{r} \cdot \left[2 \cdot \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$ OptDist: $2^{\left(\frac{1}{6}\right)} \cdot \sigma = 4.467$

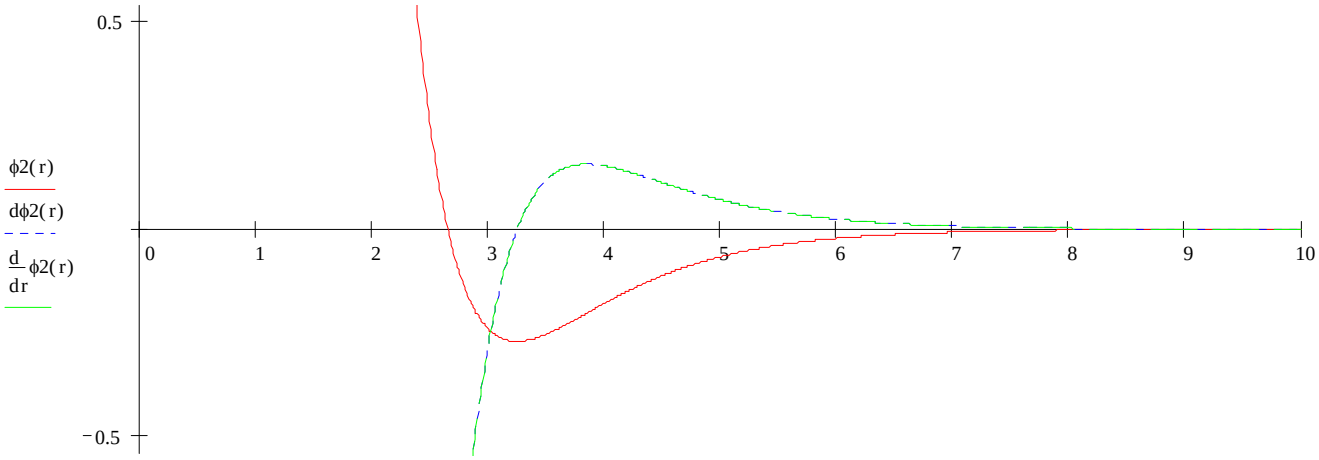


r, r, r

Morse potential

$\varepsilon := 0.2703$ $\alpha := 1.1646$ $\sigma := 3.253$ OptDist: σ

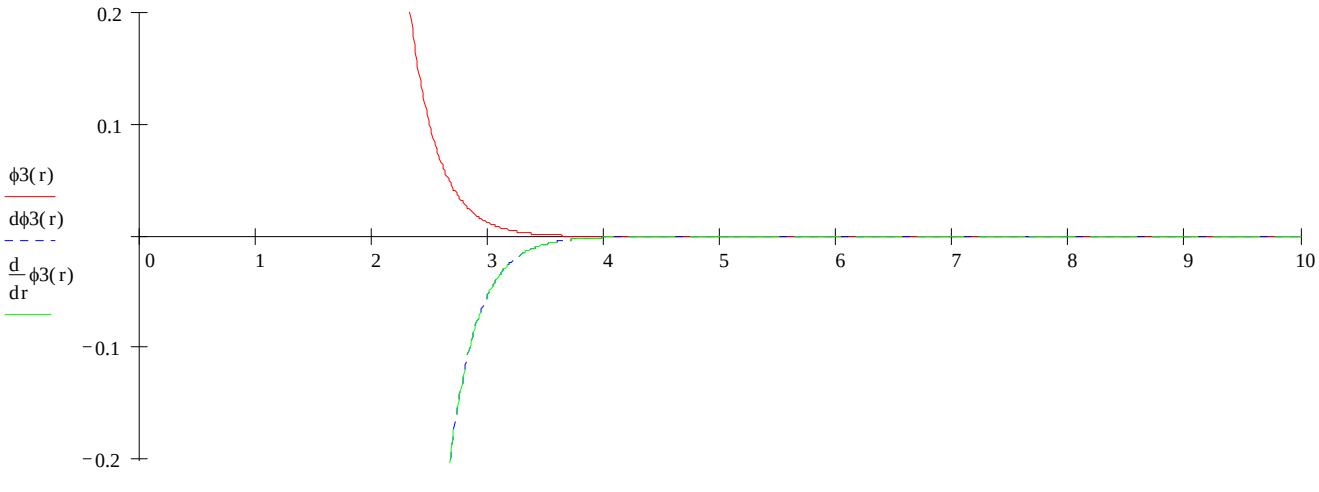
$\phi 2(r) := \varepsilon \cdot (\exp(-2 \cdot \alpha \cdot (r - \sigma)) - 2 \cdot \exp(-\alpha \cdot (r - \sigma)))$ $d\phi 2(r) := \varepsilon \cdot (-2 \cdot \alpha \cdot \exp(-2 \cdot \alpha \cdot (r - \sigma)) + 2 \cdot \alpha \cdot \exp(-\alpha \cdot (r - \sigma)))$



r, r, r

Born-Mayer potential

$\varepsilon := 0.1004$ $\rho := 10.34$ $\sigma := 2.5$ $\phi 3(r) := \varepsilon \cdot \exp\left(-\rho \cdot \frac{r - \sigma}{\sigma} \right)$ $d\phi 3(r) := -\varepsilon \cdot \frac{\rho}{\sigma} \cdot \exp\left[-\rho \cdot \frac{(r - \sigma)}{\sigma} \right]$



r, r, r