Appendix 1

Long-Range Corrections for BFW Potential

In this appendix we give the analytic derivation of the long-range corrections for the BFW potential [Bar71, see also Chapter 2], more precisely for the two-body pressure and energy assuming the pair distribution $g(r)$ function equals unity over the cut-off. In the cases of the krypton and xenon potentials [Bar74, see also Chapter 2], the procedure is similar.

The two-body energy in terms of $g(r)$ may be expressed as [All87, see also Eq. (2.102)]:

$$E^{2b} = 2\pi N\rho \int_0^\infty g(r)u^{2b} r^2 dr . \quad (A1.1)$$

With a simulation cut-off $r_c$ and assuming $g(r)$ can be approximated by unity after the cut-off (see for example Figure 4.13), the long-range corrections for the energy can be written as:

$$E_{lrc}^{2b} = 2\pi N\rho \int_{r_c}^\infty u^{2b} r^2 dr . \quad (A1.2)$$

Substituting the BWF potential in Eq. (A1.2) gives:
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\[ E_{irc}^{2h} = 2\pi N p \int_{r_m}^{\infty} r_m^3 e^{\left[ \sum_{i=0}^{\infty} A_i (x - 1)^i \exp[\alpha(1 - x)] - \sum_{j=0}^{\infty} C_{2j+6} x^{2j+6} \right]} x^2 \, dx \] \quad (A1.3)

where \( x = \frac{r}{r_m} \) and \( r_m \) is the value where the potential is a minimum. To solve the integral in Eq. (A1.3) we have to solve each term. Consider the following terms:

\[
\begin{aligned}
\int_{r_e}^{\infty} x^2 \sum_{i=0}^{5} A_i (x - 1)^i \exp[\alpha(1 - x)] \, dx &= \\
\int_{r_e}^{\infty} x^2 A_0 \exp[\alpha(1 - x)] \, dx + \int_{r_e}^{\infty} x^2 A_1 (x - 1) \exp[\alpha(1 - x)] \, dx + \\
\int_{r_e}^{\infty} x^2 A_2 (x - 1)^2 \exp[\alpha(1 - x)] \, dx + \int_{r_e}^{\infty} x^2 A_3 (x - 1)^3 \exp[\alpha(1 - x)] \, dx + \\
\int_{r_e}^{\infty} x^2 A_4 (x - 1)^4 \exp[\alpha(1 - x)] \, dx + \int_{r_e}^{\infty} x^2 A_5 (x - 1)^5 \exp[\alpha(1 - x)] \, dx &= I_0 + I_1 + I_2 + I_3 + I_4 + I_5 \\
\end{aligned}
\]

where:

\[ I_0 = A_0 \int_{r_e}^{\infty} x^2 \exp[\alpha(1 - x)] \, dx \] \quad (A1.5)

\[ I_1 = A_1 \int_{r_e}^{\infty} (x^3 - x^2) \exp[\alpha(1 - x)] \, dx \] \quad (A1.6)
\[ I_2 = A_2 \int_{r_s/r_m}^{\infty} (x^4 - 2x^3 + x^2) \exp[\alpha(1-x)]dx \quad (A1.7) \]

\[ I_3 = A_3 \int_{r_s/r_m}^{\infty} (x^5 - 3x^4 + 3x^3 - x^2) \exp[\alpha(1-x)]dx \quad (A1.8) \]

\[ I_4 = A_4 \int_{r_s/r_m}^{\infty} (x^6 - 4x^5 + 6x^4 - 4x^3 + x^2) \exp[\alpha(1-x)]dx \quad (A1.9) \]

\[ I_5 = A_5 \int_{r_s/r_m}^{\infty} (x^7 - 5x^6 + 10x^5 - 10x^4 + 5x^3 - x^2) \exp[\alpha(1-x)]dx \quad (A1.10) \]

Now consider the following integrals:

\[ < 0 >= \int x \exp[\alpha(1-x)]dx = -\frac{1}{\alpha} \exp[\alpha(1-x)] + \text{const.} \quad (A1.11) \]

\[ < 1 >= \int x \exp[\alpha(1-x)]dx = \frac{1}{\alpha} \left\{ -x \exp[\alpha(1-x)] + < 0 > \right\} + \text{const.} \quad (A1.12) \]

\[ < 2 >= \int x^2 \exp[\alpha(1-x)]dx = \frac{1}{\alpha} \left\{ -x^2 \exp[\alpha(1-x)] + 2 < 1 > \right\} + \text{const.} \quad (A1.13) \]

\[ < 3 >= \int x^3 \exp[\alpha(1-x)]dx = \frac{1}{\alpha} \left\{ -x^3 \exp[\alpha(1-x)] + 3 < 2 > \right\} + \text{const.} \quad (A1.14) \]

\[ < 4 >= \int x^4 \exp[\alpha(1-x)]dx = \frac{1}{\alpha} \left\{ -x^4 \exp[\alpha(1-x)] + 4 < 3 > \right\} + \text{const.} \quad (A1.15) \]
\[ < 5 > = \int x^5 \exp[\alpha(1 - x)] dx = \frac{1}{\alpha} \left\{ - x^5 \exp[\alpha(1 - x)] + 5 < 4 > \right\} + \text{const.} \]  
\quad (A1.16)

\[ < 6 > = \int x^6 \exp[\alpha(1 - x)] dx = \frac{1}{\alpha} \left\{ - x^6 \exp[\alpha(1 - x)] + 6 < 5 > \right\} + \text{const.} \]  
\quad (A1.17)

\[ < 7 > = \int x^7 \exp[\alpha(1 - x)] dx = \frac{1}{\alpha} \left\{ - x^7 \exp[\alpha(1 - x)] + 7 < 6 > \right\} + \text{const.} \]  
\quad (A1.18)

Using these expressions and the following relations:

\[ R = \frac{r_c}{r_m} \quad ; \quad Q = \frac{1}{\alpha} \exp \left[ \alpha \left( 1 - \frac{r_c}{r_m} \right) \right]. \]  
\quad (A1.19)

we can solve the following integrals as:

\[ < 0 >' = \int_{\frac{r_c}{r_m}}^{\infty} \exp[\alpha(1 - x)] dx = Q \]  
\quad (A1.20)

\[ < 1 >' = \int_{\frac{r_c}{r_m}}^{\infty} x \exp[\alpha(1 - x)] dx = -\frac{1}{\alpha} \left\{ - \frac{r_c}{r_m} \exp \left[ \alpha \left( 1 - \frac{r_c}{r_m} \right) \right] + < 0 >' \right\} = Q \left( R - \frac{1}{\alpha} \right) \]  
\quad (A1.21)
\[< 2 >' = \int_{r_c/r_m}^{\infty} x^2 \exp[\alpha(1-x)] \, dx = \frac{1}{\alpha} \left\{ -\left( \frac{r_c}{r_m} \right)^2 \exp \left[ \alpha \left(1 - \frac{r_c}{r_m} \right) \right] + 2 < 1 >' \right\} = (A1.22)\]

\[Q \left[ R^2 - \frac{2}{\alpha} R + \frac{2}{\alpha^2} \right] \]

\[< 3 >' = \int_{r_c/r_m}^{\infty} x^3 \exp[\alpha(1-x)] \, dx = \frac{1}{\alpha} \left\{ -\left( \frac{r_c}{r_m} \right)^3 \exp \left[ \alpha \left(1 - \frac{r_c}{r_m} \right) \right] + 3 < 2 >' \right\} = (A1.23)\]

\[Q \left[ R^3 - \frac{3}{\alpha} R^2 + \frac{6}{\alpha^2} R - \frac{6}{\alpha^3} \right] \]

\[< 4 >' = \int_{r_c/r_m}^{\infty} x^4 \exp[\alpha(1-x)] \, dx = \frac{1}{\alpha} \left\{ -\left( \frac{r_c}{r_m} \right)^4 \exp \left[ \alpha \left(1 - \frac{r_c}{r_m} \right) \right] + 4 < 3 >' \right\} = (A1.24)\]

\[Q \left[ R^4 - \frac{4}{\alpha} R^3 + \frac{12}{\alpha^2} R^2 - \frac{24}{\alpha^3} R + \frac{24}{\alpha^4} \right] \]

\[< 5 >' = \int_{r_c/r_m}^{\infty} x^5 \exp[\alpha(1-x)] \, dx = \frac{1}{\alpha} \left\{ -\left( \frac{r_c}{r_m} \right)^5 \exp \left[ \alpha \left(1 - \frac{r_c}{r_m} \right) \right] + 5 < 4 >' \right\} = (A1.25)\]

\[Q \left[ R^5 - \frac{5}{\alpha} R^4 + \frac{20}{\alpha^2} R^3 - \frac{60}{\alpha^3} R^2 + \frac{120}{\alpha^4} R - \frac{120}{\alpha^5} \right] \]

\[< 6 >' = \int_{r_c/r_m}^{\infty} x^6 \exp[\alpha(1-x)] \, dx = \frac{1}{\alpha} \left\{ -\left( \frac{r_c}{r_m} \right)^6 \exp \left[ \alpha \left(1 - \frac{r_c}{r_m} \right) \right] + 6 < 5 >' \right\} = (A1.26)\]

\[Q \left[ R^6 - \frac{6}{\alpha} R^5 + \frac{30}{\alpha^2} R^4 - \frac{120}{\alpha^3} R^3 + \frac{360}{\alpha^4} R^2 - \frac{720}{\alpha^5} R + \frac{720}{\alpha^6} \right] \]
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\[
< 7 > = \int_{r_m}^{\infty} \left[ \frac{1}{\alpha} \left( \frac{r_c}{r_m^2} \right) \exp \left[ \alpha \left( 1 - \frac{r_c}{r_m} \right) \right] + 7 < 6 > \right] dx.
\]

Using these integrals, Eq. (A1.4) can be solved:

\[
\begin{align*}
I_0 &= A_0 < 2 >' \\
I_1 &= A_1 (3 >' - 2 >') \\
I_2 &= A_2 (4 >' - 2 < 3 >' + 2 >') \\
I_3 &= A_3 (5 >' - 3 < 4 >' + 3 < 3 >' - 2 >') \\
I_4 &= A_4 (6 >' - 4 < 5 >' + 6 < 4 >' - 4 < 3 >' + 2 >') \\
I_5 &= A_5 (7 >' - 5 < 6 >' + 10 < 5 >' - 10 < 4 >' + 5 < 3 >' - 2 >')
\end{align*}
\]

Consider now the rest of the terms in Eq. (A1.3):

\[
\int \sum_{j=0}^{2} \frac{C_{2j+6}}{\delta + x^{2j+6}} x^2 dx = - \int \frac{C_6}{\delta + x^6} x^2 dx - \int \frac{C_8}{\delta + x^8} x^2 dx - \int \frac{C_{10}}{\delta + x^{10}} x^2 dx
\]

\[
= \{ J_6 + J_8 + J_{10} \}
\]

where:

\[
J_6 = C_6 \int_{\delta + x^6}^\infty dx = C_6 \left[ \frac{1}{3\sqrt{\delta}} \arctg \left( \frac{x^3}{\sqrt{\delta}} \right) \right]_{\delta + x^6}^\infty = C_6 \left[ \frac{\pi}{3\sqrt{\delta}} - \frac{1}{3\sqrt{\delta}} \arctg \left( \frac{r_c^3}{r_m^3} \right) \right].
\]

(A1.30)
for \( J_8 \) and \( J_{10} \) an approximation has to be used. Since \( \delta = 0.01 \) and \( x = \frac{r}{r_m} > 0.9 \) (practically always), we can infer that \( x^8 \gg \delta \) and \( x^{10} \gg \delta \) so it is possible to write:

\[
J_8 = C_8 \int_{r_e/r_m}^{\infty} \frac{x^2}{\delta + x^8} \, dx \approx C_8 \int_{r_e/r_m}^{\infty} \frac{1}{x^6} \, dx = C_8 \left\{ -\frac{1}{5} \frac{1}{x^5} \right\} \bigg|_{r_e/r_m}^{\infty} = C_8 \left\{ -\frac{1}{5} \left( \frac{r_c}{r_m} \right)^5 \right\} \quad (A1.31)
\]

\[
J_{10} = C_{10} \int_{r_e/r_m}^{\infty} \frac{x^2}{\delta + x^{10}} \, dx \approx C_{10} \int_{r_e/r_m}^{\infty} \frac{1}{x^8} \, dx = C_{10} \left\{ -\frac{1}{7} \frac{1}{x^7} \right\} \bigg|_{r_e/r_m}^{\infty} = C_{10} \left\{ -\frac{1}{7} \left( \frac{r_c}{r_m} \right)^7 \right\} \quad . \quad (A1.32)
\]

Using the integrals calculated, we can finally write:

\[
E_{lrc}^{2b} = 2\pi N \rho r_m^3 \left[ \sum_{i=0}^{5} I_i - \sum_{j=0}^{2} J_{2j+6} \right] \]

For the pressure we have the expression (see Eq. (2.101)):

\[
P_{lrc}^{2b} = -\frac{2\pi \rho^2}{3} \int_{r_e}^{\infty} \frac{du_{2b}}{r^3} \, dr = -\frac{2\pi \rho^2}{3} r_m^3 \int_{r_e/r_m}^{\infty} \frac{du_{2b}(x)}{dx} \, dx \quad . \quad (A1.33)
\]

Considering the formula for integration by part:

\[
\int_{a}^{b} f(x)g'(x) \, dx = f(x)g(x) \bigg|_{a}^{b} - \int_{a}^{b} f'(x)g(x) \, dx \quad (A1.34)
\]

we can write:
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\[ I = \int_{r_c}^{r_m} \left( \frac{du^{2b}(x)}{dx} \right) dx = x^3 u^{2b}(x) \bigg|_{r_c}^{r_m} - 3 \int_{r_c}^{r_m} x^2 u^{2b}(x) dx = \]

\[ -\left( \frac{r_c}{r_m} \right)^3 \varepsilon \sum_{i=0}^{5} A_i \left( \frac{r_c}{r_m} - 1 \right) \exp \left[ \alpha (1 - \frac{r_c}{r_m}) \right] - \sum_{j=0}^{2} \frac{C_{2j+6}}{\delta + \left( \frac{r_c}{r_m} \right)^{2j+6}} \]  

(A1.35)

\[ -3\varepsilon \left[ \sum_{i=0}^{5} I_i - \sum_{j=0}^{2} J_{2j+6} \right] \]

thus,

\[ p_{lrc}^{2b} = -\frac{2\pi \rho^2}{3} r_m^3 I \]  

(A1.36)