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ON SCALING FACTOR OF LENNARD-JONES AND EXPONENTIAL-6 POTENTIAL FUNCTIONS

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Abstract: Lennard-Jones and Buckingham have proposed potential function for famous Van der Waal equation in 1924 and 1934 respectively. A modified simple representation with appropriate scaling factor has been proposed in the literature. Approach for writing equations and obtaining scaling factor is irrespective but the scaling is the unique.

Key words: Van der waal equation, Linnard Jones potential, Buckinghams potential, exponential function etc.

Introduction

Typical Van-der-Waal (Vdw) potential energy functions are attributed to LENNARD-JONES (LJ)(1924):

$$U_{LJ} = \frac{A_{LJ}}{r^m} - \frac{B_{LJ}}{r^n} = D\left[\frac{n}{m-n}\left(\frac{R}{r}\right)^m - \frac{m}{m-n}\left(\frac{R}{r}\right)^n\right] \qquad 1$$

And BUCKINGHAM (1938)

$$U_B = Ae^{-Br} - \frac{C}{r^n} \qquad 2$$

In most of the practices, these potentials are utilized as 12-6 function(RIGBY & ROE (1987, 1988, 1989):

$$U_{12-6} = D\left[\left(\frac{R}{r}\right)^{12} - \left(\frac{R}{r}\right)^6\right] \qquad 3$$

And exponential-6 function (RIGBY & ROE, 1990); KARASAWA et al., (1991)

$$U_{X6} = Ae^{-Br} - \frac{C}{r^6} \qquad 4$$

respectively. The choice of 12-6 depends on the circumstances and simplicity to compute.

$$U_{X6} = D\left[\frac{6}{\xi-6}e^{\xi\left(1-\frac{r}{R}\right)} - \frac{\xi}{\xi-6}\left(\frac{R}{r}\right)^6\right] \qquad 5$$

LIM (2001) has proposed following equation in which scaling factor $\xi = 12.0$ gives same long range attraction as LJ (12-6) form, and $\xi = 13.772$ gives equal curvatures at the minimum well depth ($r=R$). The scaling factor $\xi=13.772$ sacrifices the accuracy beyond the minimum well depth (r=R). This has been attributed to the vdW interactions occurring beyond the vicinity of the minimum well-depth. He has proposed alternate scaling that attain overall good agreement between two vdW potential energy functions.

Analysis

LIM (2007) developed following approach in which, inter-atomic potential functions have relied on imposition of equal curvatures at minimum well-depth as;

$$\left(\frac{\partial^p U_1}{\partial r^p}\right)_{r=R}=\left(\frac{\partial^p U_2}{\partial r^p}\right)_{r=R};(p=-1,0,1,2) \qquad 6$$

-1, 0, 1, 2 corresponds to integration (anti-derivative), ($U_1=U_2$), differentiation of 1st and 2nd order respectively. That yields a set of equations;

$$\int_R^\infty U_{X6}dr=\frac{A}{B}e^{-BR}-\frac{C}{5R^5},\int_R^\infty U_{12-6}dr=-\frac{17}{55}DR \qquad 7a$$

$$U_{X6}|_{r=R}=\frac{A}{B}e^{-BR}-\frac{C}{R^6},U_{12-6}|_{r=R}=-D \qquad 7b$$

$$\left.\frac{\partial U_{X6}}{\partial r}\right|_{r=R}=-ABe^{-BR}-\frac{6C}{R^7},\left.\frac{\partial U_{12-6}}{\partial r}\right|_{r=R}=0 \qquad 7c$$

$$\left.\frac{\partial^2 U_{X6}}{\partial r^2}\right|_{r=R}=-AB^2e^{-BR}+\frac{42C}{R^8},\left.\frac{\partial^2 U_{12-6}}{\partial r^2}\right|_{r=R}=-\frac{72D}{R^2} \qquad 7d$$

Lim used first three equations from above set, however, in present approach last three equations are used to obtain constants. Manual computations and computations using Maple 14 agree to yield same results as; A = 0.722 $De^{-13.722}$, B = 13.772/R , C = 0.722 DR^6. The factor 13.772 re-ocurs as in the calculation of LIM(2007) hence the scaling proposed by LIM may be confirmed.

Conclusion

The scaling factor of 13.772 for exponential-6 mimic LJ (12-6) function for short range. Consideration of integral form or double differentiation hardly matters the scaling provided it exists.

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