Potential energy function based on the narcissus constant, its square and its cube

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The narcissus constant, $N = 2.3983843828\ldots$, is defined as a number that fulfills the narcissistic infinite nested radical equation

$$\sqrt[N]{N + N \times \sqrt[N]{N + N \times \sqrt[N]{N + \cdots}}} = N = \sqrt[N]{N \times N + \sqrt[N]{N \times N + \sqrt[N]{N \times \cdots}}}.$$

Incorporation of this constant, its square and its cube into the generalized version of the Lennard-Jones potential function gives the narcissus constant potential function

$$\frac{U_{\mathrm{NLJ}}}{D} = \frac{1}{N-1}\left(\frac{R}{r}\right)^{N^3} - \frac{N}{N-1}\left(\frac{R}{r}\right)^{N^2},$$

which (a) is suitable for modeling van der Waals interaction due to its agreement with the Lennard-Jones (12-6) potential energy curve over long range, and (b) forms simple generalized hybrid interatomic–intermolecular potential energy function due to its correlation with the averaged form of Lennard-Jones, Morse, Buckingham and Linnett potential energy curve near the minimum well-depth.

KEY WORDS: mathematical constant, potential energy function

AMS subject classification: 03D80, 11Y60, 80A50, 81V55

1. Introduction

It has recently been shown that prominent mathematical constants such as $\pi = 3.141593$, $\phi = 1.618034$ and $e = 2.718282$ (correct up to six decimal points) can be incorporated into Lennard-Jones-type function [1]

$$U_C = D\left[\frac{1}{C-1}\left(\frac{R}{r}\right)^{nC} - \frac{C}{C-1}\left(\frac{R}{r}\right)^{n}\right], \quad C = \pi, \phi, e, \tag{1}$$

where D and R are the minimum well-depth and the equilibrium interatomic distance respectively, whilst r is the variable interatomic distance. The shape parameter n is obtainable through curve-fitting. Due to the definition of the golden ratio, ϕ, equation (1) reduces to

$$U_C = D \left[C \left(\frac{R}{r} \right)^{nC} - C^2 \left(\frac{R}{r} \right)^{n} \right] \quad \Leftrightarrow \quad C = \phi, \tag{2}$$

only for that specific case. The constants π and ϕ were later combined into two possible forms of potential functions

$$\frac{U}{D} = \frac{\phi}{\pi - \phi} \left(\frac{R}{r} \right)^{n\pi} - \frac{\pi}{\pi - \phi} \left(\frac{R}{r} \right)^{n\phi} \tag{3}$$

and

$$\frac{U}{D} = \frac{\phi}{\pi - \phi} e^{n\pi \left(1 - \frac{r}{R} \right)} - \frac{\pi}{\pi - \phi} e^{n\phi \left(1 - \frac{r}{R} \right)}, \tag{4}$$

which form the lower and upper estimates, respectively, for the van der Waals interaction in inert gases and the covalent bond interaction [2]. In this paper, a new mathematical constant is introduced and, together with its square and its cube, incorporated into the Lennard-Jones potential function.

2. Analysis

Expressions of the form

$$N_R = \lim_{k \to \infty} \left(x_0 + \sqrt{x_1 + \sqrt{x_2 + \sqrt{\cdots + \sqrt{x_k}}}} \right) \tag{5}$$

are called infinite nested radicals. Infinite nested radicals appear in the computation of pi [3–5]

$$\frac{2}{\pi} = \sqrt{\frac{1}{2}} \times \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{\frac{1}{2}}} \times \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{\frac{1}{2}}}} \times \cdots \tag{6}$$

and the golden ratio

$$\phi = \sqrt[n]{F_{n-1} + F_n \times \sqrt[n]{F_{n-1} + F_n \times \sqrt[n]{F_{n-1} + \cdots}}}, \tag{7}$$

where F_n is the Fibonacci number for the non-negative integer n. Equation (7) reduces to its simplest form by substituting $n = 2$ to give the well-known infinite nested radical equation for describing the golden ratio [6]

$$\phi = \sqrt{1 + \sqrt{1 + \sqrt{1 + \cdots}}}. \tag{8}$$

Infinite nested radicals can also be used for representing the Plastic constant [7, 8]

$$P = \sqrt[3]{1 + \sqrt[3]{1 + \sqrt[3]{1 + \cdots}}} \tag{9}$$

and the Silver constant [9, 10]

$$S = \sqrt[3]{7 + 7 \times \sqrt[3]{7 + 7 \times \sqrt[3]{7 + \cdots}}}. \tag{10}$$

Integers 2–4 can be expressed in terms of infinite nested radicals that consist of Fibonacci and Lucas number ratios, i.e.

$$2 = \sqrt{\left(\frac{F_2}{F_1}\right)^2 + \frac{F_2}{F_1}\sqrt{\left(\frac{F_3}{F_2}\right)^2 + \frac{F_3}{F_2}\sqrt{\left(\frac{F_4}{F_3}\right)^2 + \frac{F_4}{F_3}\sqrt{\left(\frac{F_5}{F_4}\right)^2 + \cdots}}}}, \tag{11}$$

$$3 = \sqrt{\left(\frac{F_3}{F_2}\right)^2 + \frac{F_3}{F_2}\sqrt{\left(\frac{F_4}{F_3}\right)^2 + \frac{F_4}{F_3}\sqrt{\left(\frac{F_5}{F_4}\right)^2 + \frac{F_5}{F_4}\sqrt{\left(\frac{F_6}{F_5}\right)^2 + \cdots}}}}, \tag{12}$$

$$4 = \sqrt{\left(\frac{L_2}{L_1}\right)^2 + \frac{L_2}{L_1}\sqrt{\left(\frac{L_3}{L_2}\right)^2 + \frac{L_3}{L_2}\sqrt{\left(\frac{L_4}{L_3}\right)^2 + \frac{L_4}{L_3}\sqrt{\left(\frac{L_5}{L_4}\right)^2 + \cdots}}}}. \tag{13}$$

A new mathematical constant N is herein conceptualized as one which fulfills the following infinite nested radical

$$\sqrt[N]{N + N \times \sqrt[N]{N + N \times \sqrt[N]{N + \cdots}}} = N = \sqrt[N]{N \times N + \sqrt[N]{N \times N + \sqrt[N]{N \times \cdots}}}. \tag{14}$$

The significance of equation (14) can be seen from three view points: (a) its narcissistic form whereby the terms N on the LHS and RHS are equal but with the addition and multiplication operations interchanged, (b) the root order N being equal to the terms, and that both the LHS and RHS are equal to N.

From

$$N = \sqrt[N]{N^N} \tag{15}$$

the LHS of equation (14) can be generated through the expansion

$$N = \sqrt[N]{N + N^N - N} = \sqrt[N]{N + (N^{N-1} - 1) \times N} = \sqrt[N]{N + (N^{N-1} - 1) \times \sqrt[N]{N^N}}. \tag{16}$$

Expanding the RHS of equation (16) recursively, we have

$$N = \sqrt[N]{N + (N^{N-1} - 1) \times \sqrt[N]{N + (N^{N-1} - 1) \times \sqrt[N]{N + \cdots}}}. \tag{17}$$

From equation (15) again, the RHS of equation (14) can be obtained by expanding

$$N = \sqrt[N]{N^N - N + N} = \sqrt[N]{N \times (N^{N-1} - 1) + N} = \sqrt[N]{N \times (N^{N-1} - 1) + \sqrt[N]{N^N}}. \tag{18}$$

Similar successive expansion on the RHS of equation (18) leads to

$$N = \sqrt[N]{N \times (N^{N-1} - 1) + \sqrt[N]{N \times (N^{N-1} - 1) + \sqrt[N]{N \times \cdots}}}. \tag{19}$$

Therefore, equation (14) is obtained upon substituting

$$(N^{N-1} - 1) = N \tag{20}$$

into both equations (17) and (19). Writing equation (20) as

$$f(N) = N^{N-1} - N - 1 \tag{21}$$

the solution to N is extracted when $f(N) = 0$. Solving equation (21) numerically gives a lower solution $N = 0.4758608124$ and an upper solution $N = 2.3983843828$ (both correct up to ten decimal places). The upper solution is selected herein since the definition of root loses its meaning when $0 < N < 1$. Hence we call the number $N = 2.3983843828$ as the Narcissus Constant.

Recalling the generalized Lennard-Jones potential function

$$\frac{U_{\text{LJ}}}{D} = \frac{n}{m-n}\left(\frac{R}{r}\right)^m - \frac{m}{m-n}\left(\frac{R}{r}\right)^n \tag{22}$$

where $0 < n < m$, the commonly used Lennard-Jones (12–6) is recovered when $m = 2n = 6$. Substituting

$$n = N^2 \tag{23}$$

and

$$m = N^3 \tag{24}$$

into equation (22) converts it into a molecular potential function that consists of N^i ($i = 1, 2, 3$), i.e.

$$\frac{U_{\mathrm{NLJ}}}{D} = \frac{1}{N-1}\left(\frac{R}{r}\right)^{N^3} - \frac{N}{N-1}\left(\frac{R}{r}\right)^{N^2}. \tag{25}$$

Although this paper's objective is to express the van der Waals interaction, the Morse-version to equation (25)

$$\frac{U_{N-\mathrm{Morse}}}{D} = \frac{1}{N-1}e^{N^3\left(1-\frac{r}{R}\right)} - \frac{N}{N-1}e^{N^2\left(1-\frac{r}{R}\right)} \tag{26}$$

is also considered for illustration purposes in the next section.

3.   Results and Discussion

To examine the validity of equation (25), we compare it with a recently established flexible potential function

$$\frac{U}{D} = \frac{n^x \xi_2^{1-x}}{m^y \xi_1^{1-y} - n^x \xi_2^{1-x}}\left(\frac{R}{r}\right)^{my} e^{\xi_1\left(1-\frac{r}{R}\right)(1-y)}$$

$$- \frac{m^y \xi_1^{1-y}}{m^y \xi_1^{1-y} - n^x \xi_2^{1-x}}\left(\frac{R}{r}\right)^{nx} e^{\xi_2\left(1-\frac{r}{R}\right)(1-x)}, \tag{27}$$

which can be reduced into the generalized versions of Lennard-Jones [11, 12], Morse [13], Buckingham [14, 15] and Linnett [16, 17] potential functions through the substitution of (x, y)=(1,1), (0,0), (1,0) and (0,1), respectively, into equation (27). The scaling factors and ξ_2 are functions of m and n, and are useful in relating the generalized potential functions for either short range or long range. In the case of short range relationship between Lennard-Jones and Morse potential functions, the relations are

$$\xi_1 \xi_2 = mn \tag{28}$$

and

$$\xi_1 + \xi_2 = m + n + 3, \tag{29}$$

while that between Buckingham and Linnett potential functions is

$$\frac{\xi_1 n \left[\xi_1 - (n+1)\right]}{\xi_1 - n} = \frac{\xi_2 m \left[\xi_2 - (m+1)\right]}{\xi_2 - m}. \tag{30}$$

Due to the proposed application of equation (25) for van der Waals interaction, we are concerned with the long range relationship. For such a case, the scaling factors are simply

$$\begin{Bmatrix} \xi_1 \\ \xi_2 \end{Bmatrix} = \begin{Bmatrix} m \\ n \end{Bmatrix}. \tag{31}$$

Substituting $m = \xi_1 = 2n = 2\xi_2 = 12$ into equation (27) with $(x, y)=(1,1)$, $(0,0)$, $(1,0)$ and $(0,1)$ gives

$$U_{\text{LJ}(12-6)} = D \left[\left(\frac{R}{r} \right)^{12} - 2 \left(\frac{R}{r} \right)^{6} \right], \tag{32}$$

$$U_{\text{Morse}} = D \left[e^{12(1-\frac{r}{R})} - 2e^{6(1-\frac{r}{R})} \right], \tag{33}$$

$$U_{\text{Buck}} = D \left[e^{12(1-\frac{r}{R})} - 2 \left(\frac{R}{r} \right)^{6} \right], \tag{34}$$

$$U_{\text{Linn}} = D \left[\left(\frac{R}{r} \right)^{12} - 2e^{6(1-\frac{r}{R})} \right], \tag{35}$$

respectively.

Figure 1 compares the Narcissus Constant potential function, equation (25), with the Lennard-Jones, Morse, Buckingham and Linnett potential functions whereby $m = \xi_1 = 2n = 2\xi_2 = 12$, as described in equations (32)–(35). It can be seen that for $r > R$ the Narcissus Constant potential energy, denoted by circles, lies close to the Lennard-Jones (12-6) and Buckingham potential energy curves. This is attributed to the similarity of the functional form (R/r), in the attractive parts. By similar reasoning, plot of equation (26), denoted by triangles, lies close to the Morse and Linnett potential energy curves for $r > R$ due to the similar exponential form in the attractive parts.

To examine the characteristics of the Narcissus Constant potential function near the ground state, reference is made to figure 2. The Narcissus Constant potential function is bounded above by the Morse and Linnett potential functions and bounded below by the Lennard-Jones and the Buckingham potential functions for the region $r > R$. For the region $0 < r < R$, the Narcissus Constant potential energy hovers very close to the Lennard-Jones (12-6) and the Linnett potential functions due to the similarity of the repulsive parts, as expressed by (R/r).

To compare the Narcissus Constant potential function with the averaged form of the Lennard-Jones, Morse, Buckingham and Linnett potential functions,
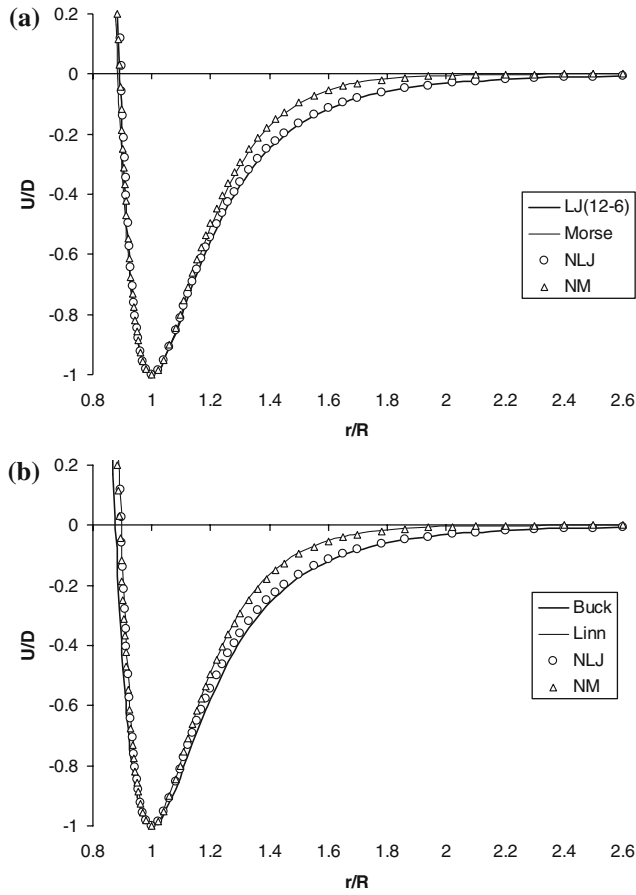
Figure 1. Plots of the Narcissus Constant potential function (NLJ) based on the Lennard-Jones form in comparison with (a) Lennard-Jones ($m = 2n = 12$) and Morse ($\xi_1 = 2\xi_2 = 12$), and (b) Buckingham ($\xi_1 = 2n = 12$) and Linnett ($m = 2\xi_2 = 12$) potential functions. The Narcissus Constant in Morse form (NM) is included for comparison.

we substitute $\xi_1 = m = 12$, $\xi_2 = n = 6$ and $x = y = 0.5$ into equation (27) to yield

$$\frac{U}{D} = \left(\frac{R}{r}\right)^6 e^{6(1-\frac{r}{R})} - 2\left(\frac{R}{r}\right)^3 e^{3(1-\frac{r}{R})}. \tag{36}$$

Figure 3 compares the Narcissus Constant potential function, equation (25), with the averaged form of the four classical potential functions, equation (36). The Narcissus Constant potential function compares well with the averaged potential function for all r except for the region $1.3R < r < 2.2R$ whereby the former underestimates the former by less than 3.6% of D. For region near the
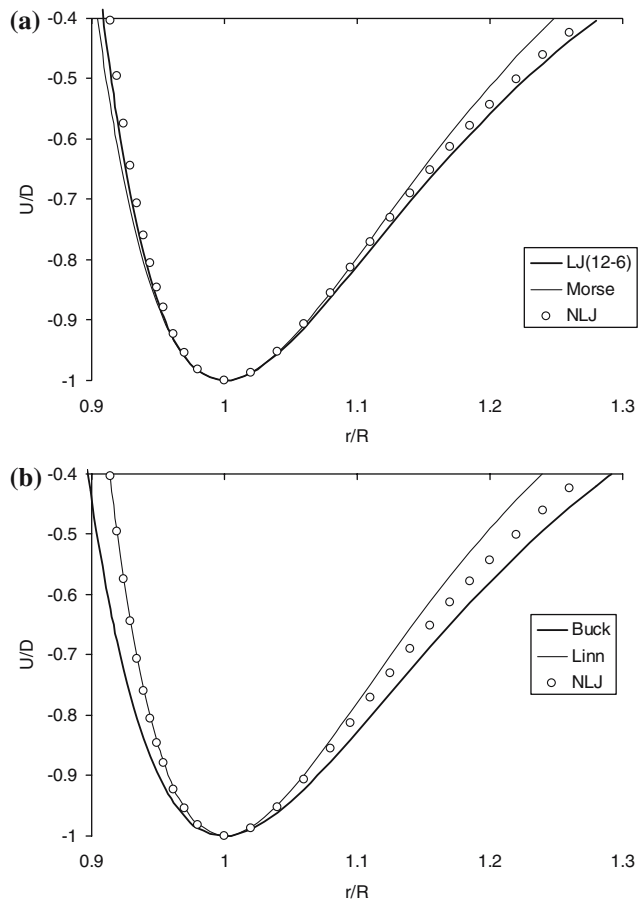
Figure 2. The Narcissus Constant potential function is shown to be bounded by Morse and Linnett potential functions as upper estimates, and by Lennard-Jones and Buckingham potential functions as lower estimates for $r > R$.

equilibrium point the Narcissus Constant potential function agrees well with the averaged potential functions, as evident from Fig. 3(b).

4. Conclusions and recommendation

Apart from fulfilling the interesting narcissistic nested radical equation described in equation (14), the Narcissus Constant, its square and its cube can be incorporated into a Lennard-Jones-type potential function to give a potential energy curve that is bounded by the classical potential functions of Lennard-Jones, Morse, Buckingham and Linnett. Further investigation reveals that the Narcissus Constant potential function correlates with the averaged form of the four classical potential functions. This observation suggests the uniqueness of the Narcissus
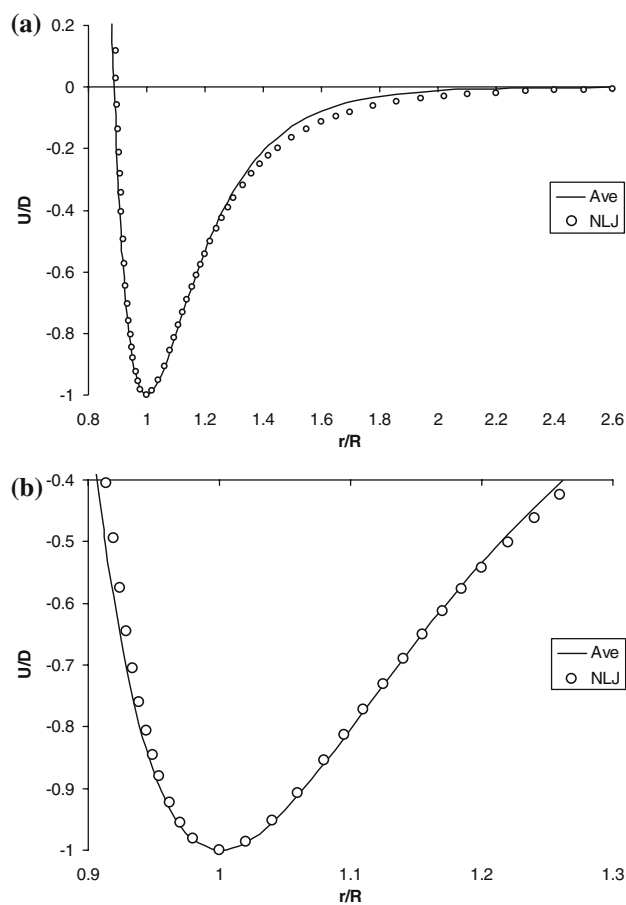
Figure 3. Comparison between the averaged form of the four classical potential function curve with the Narcissus potential energy: (a) long range view, and (b) short range view.

Constant in enabling its potential function to easily represent the central form of the four classical potential functions. It is worth mentioning that in a recent development a constant 2.398, which is the Narcissus Constant correct up to three decimal points, was applied in an algorithm for one-warehouse multi-retailer computational problem [20]. Investigation on the significance of the Narcissus Constant in geometry and other chemical systems is suggested for future work.

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