

Analytic Potentials for Polyatomics

Nike Dattani and dattani.nike@fukui.kyoto.ac.jp

*Harvard Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge, Massachusetts, USA, and
McMaster University, Department of Chemistry and Chemical Biology, Hamilton, Ontario, Canada,*

Yu Zhai and yuzhai@mail.huiligroup.org

Institute of Theoretical Chemistry, Jilin University, Changchun, Jilin, China.

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A review of models for multi-dimensional potentials.

I. INTRODUCTION

The MLR (Morse/Long-range) function has been very successful for diatomic molecules (systems with one radial coordinate) [1–24]. Even for Van der Waals complexes, where the potential depends on one radial coordinate and one or many angular coordinates, it has been possible to build multi-dimensional MLR potential energy functions since for fixed values of all angular coordinates we can use the 1D-MLR to represent the energy dependence on the single radial coordinate [16, 25–29]. However the mathematics is much more complicated for systems with more than one radial coordinate and such systems are still commonly represented by splines (which are not analytic functions, do not extrapolate properly, and suffer from spurious oscillations between the points on which they are based). A very simple example of a system with two radial coordinates is CO_2 . We will focus our discussion on building a potential for CO_2 , and will generalize to systems with arbitrary numbers of radial and angular coordinates after.

II. REVIEW: MLR FOR DIATOMICS

$$V(r) = \mathfrak{D}_e \left(1 - \frac{u(r)}{u(r_e)} e^{-\beta(r)y_p(r)} \right)^2$$

$$y_p = \frac{r^p - r_e^p}{r^p + r_e^p}, \beta(r) = \beta_\infty y_p + (1 - y_p) \sum_{i=0}^{N_\beta} \beta_i (y_p)^i \quad (1)$$

Because of the fact that $\lim_{r \rightarrow \infty} y_p = 1$, we have:

$$\lim_{r \rightarrow \infty} \beta(r) = \beta_\infty, \lim_{r \rightarrow \infty} e^{-\beta(r)y_p(r)}. \quad (2)$$

Therefore we can define:

$$\beta_\infty = \ln \left(\frac{2\mathfrak{D}_e}{u(r_e)} \right), \quad (3)$$

which leads us to the famous long-range form for the MLR:

$$V_{\text{LR}}(r) = \mathfrak{D}_e \left(1 - \frac{u(r)}{2\mathfrak{D}_e} \right)^2 \quad (4)$$

$$= \mathfrak{D}_e - u(r) + \frac{u(r)^2}{4\mathfrak{D}_e}. \quad (5)$$

We can therefore decide by ourselves what we want the MLR potential to look like for large r , by defining $u(r_e)$ accordingly. For example theory tells us that an excited electronic state of Li_2 dissociating to $\text{Li}(S) + \text{Li}(P)$ should have a long-range potential of the form:

$$V_{\text{LR}}(r) = \mathfrak{D}_e - \frac{C_3}{r^3} - \frac{C_6}{r^6} - \dots, \quad (6)$$

so all we have to do is define:

$$u(r) = \frac{C_3}{r^3} + \frac{C_6 - \frac{C_3^2}{4\mathfrak{D}_e}}{r^6}, \quad (7)$$

and Eq. 5 becomes:

$$V_{\text{LR}}(r) = \mathfrak{D}_e - \frac{C_3}{r^3} + \frac{C_6}{r^6} + \frac{\frac{C_3^2}{4\mathfrak{D}_e}}{r^{12}} \quad (8)$$

$$= \mathfrak{D}_e - \frac{C_3}{r^3} + \frac{C_6}{r^6} \text{ (because } 1/r^{12} \text{ is much smaller than } 1/r^6 \text{ when } r \rightarrow \infty). \quad (9)$$

III. REVIEW: MLR FOR VAN DER WAALS COMPLEXES

A van der Waals complex consists of two systems very far away from each other. They are typically so far away from each other that the potential energy associated with their interaction doesn't depend on the internal structures of each system, and therefore only depends on the distance between them (r) and the angles formed with the various axes of the individual systems: $V = V(r, \theta_1, \theta_2, \theta_3, \dots)$. We can fix all angles and fit the resulting 1D potential using the above form.

IV. POLY-MLR: AN MLR FOR TRIATOMICS

Things get complicated when we care not just about inter-molecular forces (as in van der Waals complexes) but also on the intra-molecular forces, which depend on more than on radial coordinate when the number of atoms is larger than two. For example the CO_2 potential has the form: $V = V(r_1, r_2, \theta)$. The θ -dependence is of no theoretical concern since we can treat it the way we did for the van der Waals complexes. So let's start by thinking about a CO_2 molecule with θ fixed at $180^\circ = \pi$ (ie. fixed to stay linear). The poly-MLR for the two radial coordinates can look like this:

$$V(r_1, r_2) = y_{p,+} (V_{\text{CO}(1)}(r_1) + V_{\text{CO}(2)}(r_2) + V_{\text{OO}}(r_{\text{OO}})) + V_{\text{Triatomic}}(r_1, r_2) \quad (10)$$

$$V_{\text{LR}}(r_1, r_2) = V_{\text{LR,CO}(1)}(r_1) + V_{\text{LR,CO}(2)}(r_2) + V_{\text{LR,OO}}(r_{\text{OO}}) + V_{\text{LR,Triatomic}}(r_1, r_2) \quad (11)$$

$$\lim_{r_1 \rightarrow \infty} V(r_1, r_2) = \quad (12)$$

$$V_{\text{Triatomic}}(r_1, r_2) = \mathfrak{D}_e \left(1 - \frac{u(r_1, r_2)}{u(r_{e,1}, r_{e,2})} e^{-\beta(r_1, r_2) y_p(r_1, r_2)} \right)^2 \quad (13)$$

$$y_p = \frac{y_{p,1} + y_{p,2}}{2}, \quad (14)$$

$$\beta = \beta_\infty y_p + (1 - y_p) \sum_{i,j=0}^{N_\beta} \beta_{i,j} (y_{p,1})^i (y_{p,2})^j \quad (15)$$

Because of the fact that $\lim_{r_1, r_2 \rightarrow \infty} y_p = 1$, we have:

$$\lim_{r_1, r_2 \rightarrow \infty} \beta(r) = \beta_\infty, \quad \lim_{r_1, r_2 \rightarrow \infty} e^{-\beta(r) y_p(r)} = 1/e^{\beta_\infty}. \quad (16)$$

Therefore we can define:

$$\beta_\infty = \ln \left(\frac{2\mathfrak{D}_e}{u(r_{e,1}, r_{e,2})} \right), \quad (17)$$

and we get:

$$V_{\text{LR}}(r_1, r_2) = \mathfrak{D}_e \left(1 - \frac{u(r_1, r_2)}{2\mathfrak{D}_e} \right)^2 \quad (18)$$

$$= \mathfrak{D}_e - u(r_1, r_2) + \frac{u(r_1, r_2)^2}{4\mathfrak{D}_e}. \quad (19)$$

This looks exactly like it did for the 1D case. Let's try to see if it works though:

$$u(r_1, r_2) = \frac{C_{6,\text{CO}}}{r_1^6} + \frac{C_{6,\text{CO}}}{r_2^6} + \frac{C_{6,\text{OO}}}{r_{\text{OO}}^6}, \quad (20)$$

$$V_{\text{LR}}(r_1, r_2) = \mathfrak{D}_e - \frac{C_{6,\text{CO}}}{r_1^6} - \frac{C_{6,\text{CO}}}{r_2^6} - \frac{C_{6,\text{OO}}}{r_{\text{OO}}^6} \quad (21)$$

$$+ \frac{C_{6,\text{CO}}^2}{r_1^{12}} + \frac{C_{6,\text{CO}}^2}{r_2^{12}} + \frac{C_{6,\text{OO}}^2}{r_{\text{OO}}^{12}} + \frac{2C_{6,\text{CO}}^2}{r_1^6 r_2^6} + \frac{2C_{6,\text{CO}}C_{6,\text{OO}}}{r_1^6 r_{\text{OO}}^6} + \frac{2C_{6,\text{CO}}C_{6,\text{OO}}}{r_2^6 r_{\text{OO}}^6}. \quad (22)$$

Where $r_{\text{OO}} = \sqrt{r_1^2 + r_2^2 - 2r_1r_2 \cos \theta}$. While it looks like the cross-terms (such as the one with $C_{6,\text{CO}}C_{6,\text{CO}}$) might be problematic because it has the same r_i -dependence as the r_i^6 terms, we must keep in mind that Eq. 21 was only valid for the case where r_1 **and** r_2 were very large, so indeed the last three terms of Eq. 21 are much smaller than the rest of the terms when and we have:

$$V_{\text{LR}}(r_1, r_2) = \mathfrak{D}_e - \frac{C_{6,1}}{r_1^6} - \frac{C_{6,2}}{r_2^6} - \frac{C_{6,\text{OO}}}{r_{\text{OO}}^6}. \quad (23)$$

Let's see what happens if $r_1 \rightarrow \infty$ but r_2 does not:

$$\lim_{r_1 \rightarrow \infty} \beta(r_1, r_2) = \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} e^{-\bar{\beta}_{ij}(r_2)y_{p,2}(r_2)} \right)^2 \quad (24)$$

which turns out to be exactly the 1D-MLR for the diatomic CO in terms of r_2 , except without a β_∞ . We could define a β_{∞, r_2} , however this does not yet seem to be necessary because if $r_2 \rightarrow \infty$, we have already shown that this equation collapses to the global long-range function.

V. SYMMETRIC TRIATOMICS

A. Jensen

Power series in Morse transformed bond lengths. But even when one bond length goes to infinity, the potential depends on the angle. P. Jensen, J. Mol. Spectrosc. 128, 478 (1988).

B. Partridge-Schwenke (modified from something in Varandas's book "Molecular Potential Energy Functions (1984)")

$$V(r_1, r_2, \theta) = V^a(r_1) + V^a(r_2) + V^b(r_{12}) + V^c(r_1, r_2, \theta) \quad (25)$$

$$V^a(r) = D \left(1 - e^{-a(r-r_{\text{ref}})} \right)^2 \quad (26)$$

$$V^b(r) = Ae^{-br} \quad (27)$$

$$V^c(r) = e^{-\beta((r_1-r_e)^2 + (r_2-r_e)^2)} \sum_{ijk} c_{ijk} \left(\frac{r_1-r_e}{r_e} \right)^i \left(\frac{r_2-r_e}{r_e} \right)^j (\cos \theta - \cos \theta_e)^k \quad (28)$$

Let's evaluate the limits:

$$\lim_{r_1 \rightarrow \infty} V(r_1, r_2, \theta) = V^a(r_2) \quad (29)$$

$$\lim_{r_2 \rightarrow \infty} V(r_1, r_2, \theta) = V^a(r_1) \quad (30)$$

$$\lim_{\theta \rightarrow 180^\circ} V(r_1, r_2, \theta) = \text{nothing special} \quad (31)$$

$$\lim_{r_1, r_2 \rightarrow \infty} V(r_1, r_2, \theta) = 0 \quad (32)$$

C. Huang-Schwenke-Tashkun-Lee

$$V = V_{\text{short}} + V_{\text{long}} \quad (33)$$

$$V_{\text{short}} = f_{\text{damp}} \sum_n C_{ijk}^n P \left[\left(1 - e^{-\beta(r_1 - r_{\text{ref}})} \right)^i \left(1 - e^{-\beta(r_2 - r_{\text{ref}})} \right)^j \right] \cos^k(\pi - \theta) \quad (34)$$

$$f_{\text{damp}} = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m} - \bar{d}_m(1 + \cos \theta)^{2m})} \quad (35)$$

$$= e^{-d_1((r_1 - r_{\text{ref}})^2 + (r_2 - r_{\text{ref}})^2) - d_2((r_1 - r_{\text{ref}})^4 + (r_2 - r_{\text{ref}})^4) - d_3(\pi - \theta)^2 - d_4(\pi - \theta)^4} \quad (36)$$

$$V_{\text{long}} = \sum_m \left(D_{e,m} \sum_i \left(1 - e^{-\beta(r_i - r_{\text{ref}})} \right)^{2m} + e^{-\bar{d} \sum_i (r_i - r_{\text{ref}})^2} A_{e,m} (1 + \cos \theta)^{2m} \right) \quad (37)$$

Here $P[]$ is a permutation operator used to ensure that:

$$P \left[(r_1 - r_{\text{ref}})^i (r_2 - r_{\text{ref}})^j \right]$$

is totally invariant with respect to the interchange of two O atoms.

$$\lim_{r_1 \rightarrow \infty} V(r_1, r_2, \theta) = \sum_m \left(D_{e,m} \left(1 - e^{-\beta(r_2 - r_{\text{ref}})} \right)^{2m} \right) \quad (38)$$

$$\lim_{r_2 \rightarrow \infty} V(r_1, r_2, \theta) = \sum_m \left(D_{e,m} \left(1 - e^{-\beta(r_1 - r_{\text{ref}})} \right)^{2m} \right) \quad (39)$$

$$\lim_{\theta \rightarrow 180^\circ} V(r_1, r_2, \theta) = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m})} \sum_n C_{ijk}^n P \left[\left(1 - e^{-\beta(r_1 - r_{\text{ref}})} \right)^i \left(1 - e^{-\beta(r_2 - r_{\text{ref}})} \right)^j \right] \quad (40)$$

$$+ \sum_m \left(D_{e,m} \sum_i \left(1 - e^{-\beta(r_i - r_{\text{ref}})} \right)^{2m} \right) \quad (41)$$

$$= V^a(r_1) + V^a(r_2) + V^c(r_1, r_2) \quad (42)$$

$$\lim_{r_1, r_2 \rightarrow \infty} V(r_1, r_2, \theta) = 0 \quad (43)$$

D. New Model

$$V(r_1, r_2, \theta) = V_{\text{long,CO}}(r_1) + V_{\text{long,CO}}(r_2) + V_{\text{long,OO}}(r_{\text{HH}}) + V_{\text{long,nonadditive,LR}}(r_1, r_2, \theta) + V_{\text{short}}(r_1, r_2, \theta) \quad (44)$$

$$V_{\text{longCO}}(r) = \text{MLR}_{\text{CO}} \quad (45)$$

$$V_{\text{longOO}}(r) = \text{MLR}_{\text{OO}} \quad (46)$$

$$V_{\text{short}}(r_1, r_2, \theta) = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m})} \left(1 - e^{-\beta_{p,q}^{r_{\text{ref}}}(r_1) y_p^{r_e(\theta)}(r_1)} e^{-\beta_{p,q}^{r_{\text{ref}}}(r_2) y_p^{r_e(\theta)}(r_2)} \right) \quad (47)$$

$$\times e^{-\sum_m \bar{d}_m (1 + \cos \theta)^{2m} \cos^k(\pi - \theta) - e^{-(r_1 + r_2 - 2r_e)} \mathfrak{D}_e} \quad (48)$$

$$\lim_{r_1 \rightarrow \infty} V_{\text{short}}(r_1, r_2, \theta) = 0 \quad (49)$$

$$\lim_{r_2 \rightarrow \infty} V_{\text{short}}(r_1, r_2, \theta) = 0 \quad (50)$$

$$\lim_{r_1, r_2 \rightarrow \infty} V_{\text{short}}(r_1, r_2, \theta) = 0 \quad (51)$$

$$V_{\text{short}}(r_1, r_2, \pi) = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m})} \left(1 - e^{-\beta_{p,q}^{r_{\text{ref}}}(r_1) y_p^{r_e(\theta)}(r_1)} e^{-\beta_{p,q}^{r_{\text{ref}}}(r_2) y_p^{r_e(\theta)}(r_2)} \right) - e^{-(r_1 + r_2 - 2r_e)} \mathfrak{D}_e \quad (52)$$

$$V_{\text{short}}(r_e, r_2, \pi) = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m})} \left(1 - e^{-\beta_{p,q}^{r_{\text{ref}}}(r_2) y_p^{r_e(\theta)}(r_2)} \right) - e^{-(r_2 - r_e)} \mathfrak{D}_e \quad (53)$$

$$V_{\text{short}}(r_1, r_e, \pi) = e^{-\sum_{i,m} (d_m(r_i - r_{\text{ref}})^{2m})} \left(1 - e^{-\beta_{p,q}^{r_{\text{ref}}}(r_1) y_p^{r_e(\theta)}(r_1)} \right) - e^{-(r_1 - r_e)} \mathfrak{D}_e \quad (54)$$

$$V_{\text{short}}(r_e, r_e, \pi) = -\mathfrak{D}_e \quad (55)$$

APPENDIX: POLY-MLR WHEN $r_1 \rightarrow \infty$ BUT r_2 DOES NOT

Let's see what happens if $r_1 \rightarrow \infty$ but r_2 does not:

$$\lim_{r_1 \rightarrow \infty} \beta(r_1, r_2) = \beta_{\infty} \left(\frac{1 + y_{p,2}}{2} \right) + \left(\frac{1 - y_{p,2}}{2} \right) \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j \quad (56)$$

$$\lim_{r_1 \rightarrow \infty} e^{-\beta(r_1, r_2) y_p(r_1, r_2)} = e^{-\beta_{\infty} \left(\frac{1 + y_{p,2}}{2} \right)^2 - \frac{1 - y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \quad (57)$$

$$= e^{-\beta_{\infty} \left(\frac{1 + y_{p,2}}{2} \right)^2} e^{-\frac{1 - y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \quad (58)$$

$$= \left(\frac{u(r_{e,1}, r_{e,2})}{2\mathfrak{D}_e} \right)^{\left(\frac{1 + y_{p,2}}{2} \right)^2} e^{-\frac{1 - y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \quad (59)$$

$$\lim_{r_1 \rightarrow \infty} V_{\text{LR}}(r_1, r_2) = \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} \left(\frac{u(r_{e,1}, r_{e,2})}{2\mathfrak{D}_e} \right)^{\left(\frac{1 + y_{p,2}}{2} \right)^2} e^{-\frac{1 - y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \right)^2 \quad (60)$$

$$= \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} \left(\frac{u(r_{e,1}, r_{e,2})}{2\mathfrak{D}_e} \right)^x e^{-\frac{1}{4} + \frac{y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \right)^2, \quad 0 < x < 1 \quad (61)$$

$$= \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} \bar{x} e^{\frac{y_{p,2}^2}{4} \sum_{i,j}^{N_{\beta}} \beta_{i,j}(y_{p,2})^j} \right)^2, \quad e^{-1/4} < \bar{x} < \frac{u(r_{e,1}, r_{e,2}) e^{-1/4}}{2\mathfrak{D}_e} \quad (62)$$

$$= \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} e^{-\sum_{i,j}^{N_{\beta}} \bar{\beta}_{ij}(y_{p,2})^{j+2}} \right)^2 \quad (63)$$

$$= \mathfrak{D}_e \left(1 - \frac{u(r_2)}{u(r_{e,1}, r_{e,2})} e^{-\bar{\beta}_{ij}(r_2) y_{p,2}(r_2)} \right)^2, \quad (64)$$

VI. 2D HARMONIC OSCILLATOR

$$V(r_1, r_2) = \frac{1}{2} \left(k_1 (r_1 - r_{1,e})^2 + k_2 (r_2 - r_{2,e})^2 \right) \quad (65)$$

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