

THE VAN DER WAAL'S INTERACTION OF PARTICLES

BY R. SANKAR

(Department of Applied Mathematics, Indian Institute of Science, Bangalore - 12)

Received on February 6, 1960

ABSTRACT

Recently Mrs. Vold [Proc. Ind. Acad. Sc., XLVI, Sec. A, No. 2, pp. 152-166, Aug. 1957] has evaluated an expression for the interaction energy of two ellipsoidal particles situated in any manner relative to each other. She has assumed the law of interaction as the inverse sixth power of the distance and has obtained the expression for the energy in terms of a series in ascending powers of $(1/R)$. She has given explicitly the co-efficients necessary to calculate the energy upto the first three terms of the series. In the present note the same problem has been reconsidered for the case in which each particle has three principal planes of symmetry. A series expression has been obtained as in Mrs. Vold's paper on the assumption that the law of interaction is the $(2k)$ th power of $(1/R)$, where k may be fractional. The result is expressed in terms of various order moments of the particles. These moments have been tabulated for the case of ellipsoids and elliptic cylinders. No applications have been attempted as the applications given in the paper under reference can easily be repeated for this also.

In a recent paper Vold¹ among other things has developed an expression for the interaction energy between two ellipsoidal particles with semiaxes a, b, c and α, β, γ situated in any manner relative to other, the distance between their centres being R . She has taken the inverse sixth power of distance as the law of interaction and has evaluated the interaction energy in terms of a series in ascending powers of $1/R$. She has recorded in an explicit form the coefficients which are necessary for calculating the energy upto the first three terms of this series. On account of the uncertainty about the law of interaction between the particles we have thought it fit to reconsider the problem discussed by Vold assuming the law of interaction as the $(2k)$ th power of the reciprocal of the distance, where k may have fractional values. We have expressed the main result (to the same degree of approximation as in the reference 1) in terms of the various order moments for the two particles and have recorded their explicit values for the cases when the particles are ellipsoids and elliptic cylinders in a table at the end. The values of the moments when the particles are spheroidal or spherical can easily be obtained from the first column (of the Table) as particular cases, while when the particles are circular cylinders the second column gives their values. We have not attempted any applications of the derived expression. In fact the whole of the discussion given in the reference 1 could easily be repeated for any specific law of force, any orientation and

any shape of the particles. We have assumed the particles to be symmetric about three mutually perpendicular planes passing through their centres.

Let the two particles be S and S' and their centres be at O and O' . The direction-cosines of the line OO' with respect to the axes of symmetry Ox_1, Ox_2, Ox_3 of S be $\lambda_1, \lambda_2, \lambda_3$ and the same with respect to the axes of symmetry $O'x'_1, O'x'_2, O'x'_3$ and of S' be $\lambda'_1, \lambda'_2, \lambda'_3$. Also let $(l_{11}, l_{12}, l_{13}), (l_{21}, l_{22}, l_{23}), (l_{31}, l_{32}, l_{33})$ be the direction-cosines of the axes of symmetry $O'x'_1, O'x'_2, O'x'_3$ of S' with respect to those of S . It follows that $(l_{11}, l_{12}, l_{13}), (l_{21}, l_{22}, l_{23}), (l_{31}, l_{32}, l_{33})$ are the direction-cosines of the axes of symmetry Ox_1, Ox_2, Ox_3 of S with respect to those of S' ,

$$\text{and} \quad \lambda'_j = \lambda_1 l_{1j} + \lambda_2 l_{2j} + \lambda_3 l_{3j}, \quad j = 1, 2, 3. \quad [1]$$

In the sequel we shall adopt the following convention with regard to the suffixes.

$$x_i = x_r, \quad i \equiv r \pmod{3} \quad \text{and} \quad 0 < r < 3, \quad [2.1]$$

$$x'_j = x'_s, \quad j \equiv s \pmod{3} \quad \text{and} \quad 0 < s < 3, \text{ etc.} \quad [2.2]$$

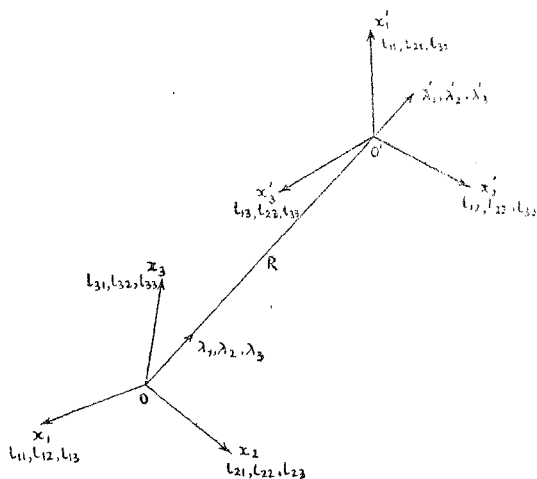


FIG. I

The axes of symmetry of the two particles and their relative Orientation

The various order moments used in the result are defined below :

$$M = \text{mass of } S \qquad M' = \text{mass of } S' \qquad [3.1]$$

$$A_i = \int_S x_i^2 \rho \, dv \qquad A'_j = \int_{S'} x_j'^2 \rho' \, dv' \qquad [3.2]$$

$$B_i = \int_S x_i^2 \rho \, dv \qquad B'_j = \int_{S'} x_j'^4 \rho' \, dv' \qquad [3.3]$$

$$C_i = \int_S x_{i+1}^2 x_{i+2}^2 \rho \, dv \qquad C'_j = \int_{S'} x_{j+1}'^2 x_{j+2}'^2 \rho' \, dv' \qquad [3.4]$$

$$D_i = \int_S x_i^6 \rho \, dv \qquad D'_j = \int_{S'} x_j'^6 \rho' \, dv' \qquad [3.5]$$

$$E_i = \int_S x_{i+1}^4 x_{i+2}^2 \rho \, dv \qquad E'_j = \int_{S'} x_{j+1}'^4 x_{j+2}'^2 \rho' \, dv' \qquad [3.6]$$

$$F_i = \int_S x_{i+1}^3 x_{i+2}^4 \rho \, dv \qquad F'_j = \int_{S'} x_{j+1}'^3 x_{j+2}'^4 \rho' \, dv' \qquad [3.7]$$

$$H = \int_S x_1^2 x_2^2 x_3^2 \rho \, dv \qquad H' = \int_{S'} x_1'^2 x_2'^2 x_3'^2 \rho' \, dv' \qquad [3.8]$$

Assuming the law of interaction to be

$$\frac{Gmm'}{r^{2k}} \qquad [4]$$

between two particles of masses m and m' at a distance r apart the interaction energy V between the two bodies S and S' is given by

$$V = G \int \dots \int \frac{\rho \, dx_1 \, dx_2 \, dx_3 \, \rho' \, dx_1' \, dx_2' \, dx_3'}{[(x_1 - x_1')^2 + (x_2 - x_2')^2 + (x_3 - x_3')^2]^k}, \qquad [5]$$

where the integration extends over the entire masses of the two interacting bodies. Following the usual methods of expansion and retaining terms upto $(2k + 6)$ th power of $1/R$, we find

$$\begin{aligned} \frac{V}{G} = & \frac{MM'}{R^{2k}} + \frac{1}{R^{2k+2}} \left[M' \sum \alpha_i A_i + M \sum' \alpha'_j A'_j \right] \\ & + \frac{1}{R^{2k+4}} \left[M' \sum (\beta_i B_i + \gamma_i C_i) + \sum \sum' (\delta_i + \epsilon_i \lambda_i^2 + \zeta_i l_{ij}^2 + \eta_i l_{ij} \lambda'_j) A_i A'_j + \right. \\ & \quad \left. + M \sum' (\beta'_j B'_j + \gamma'_j C'_j) + \sum \sum' (\delta'_j + \epsilon'_j \lambda_j'^2 + \zeta'_j l_{ij}'^2 + \eta'_j l_{ij} \lambda_i) A_i A'_j \right] + \\ & + \frac{1}{R^{2k+6}} \left[M' \sum (\theta_i D_i + \kappa_i E_i + \mu_i F_i + \nu_i H) \right. \\ & \quad + \sum \sum' (\xi_i + \alpha_i \lambda_i^2 + \omega_i l_{ij}^2 + \rho_i l_{ij} \lambda'_j) B_i A'_j + \\ & \quad + \sum \sum' (\sigma_i + \tau_i \lambda_i^2 + \phi_i l_{ij}^2 + x_i l_{i+1,j} l_{i+2,j} + \\ & \quad \quad + \psi_i l_{i+1,j} \lambda'_j + \omega_i l_{i+2,j} \lambda'_j) C_i A'_j + \\ & \quad + M \sum (\theta'_j D'_j + \kappa'_j E'_j + \mu'_j F'_j + \nu'_j H') \\ & \quad + \sum \sum' (\xi'_j + \alpha'_j \lambda_j'^2 + \omega'_j l_{ij}'^2 + \rho'_j l_{ij} \lambda_i) B'_j A_i \\ & \quad + \sum \sum' (\sigma'_j + \tau'_j \lambda_j'^2 + \phi'_j l_{ij}'^2 + x'_j l_{i+1,j} l_{i+2,j} \\ & \quad \quad + \psi'_j l_{i+1,j} \lambda_i + \omega'_j l_{i+2,j} \lambda_i) C'_j A_i \left. \right] \qquad [6] \end{aligned}$$

The suffixes i and j run over 1, 2, 3 and the dimensionless coefficients

$\alpha_i, \beta_i, \dots, \omega_i$ and $\alpha'_j, \beta'_j, \dots, \omega'_j$ are given by

$$\alpha_i = c_1 + 4 c_2 \lambda_i^2 \quad [7.1]$$

$$\beta_i = c_2 + 12 c_3 \lambda_i^2 + 16 c_4 \lambda_i^4 \quad [7.2]$$

$$\gamma_i = 2 c_2 + 12 c_3 - 12 c_3 \lambda_i^2 + 96 c_4 \lambda_{i+1}^2 \lambda_{i+2}^2 \quad [7.3]$$

$$\delta_i = c_2 + 12 c_3 \lambda_i^2 \quad [7.4]$$

$$\epsilon_i = 48 c_4 \lambda_i^3 \quad [7.5]$$

$$\zeta_i = 2 c_2 \quad [7.6]$$

$$\eta_i = 24 c_3 \lambda_i \quad [7.7]$$

$$\theta_i = c_3 + 24 c_4 \lambda_i^3 + 80 c_5 \lambda_i^4 + 64 c_6 \lambda_i^5 \quad [7.8]$$

$$\kappa_i = 3c_3 + 24c_4(2\lambda_{i+1}^2 + \lambda_{i+2}) + 80c_5(\lambda_{i+1}^4 + 6\lambda_{i+1}^2 \lambda_{i+2}^2) + 960c_6 \lambda_{i+1}^4 \lambda_{i+2}^2 \quad [7.9]$$

$$\mu_i = 3c_3 + 24c_4(\lambda_{i+1}^2 + 2\lambda_{i+2}^2) + 80c_5(\lambda_{i+1}^4 + 6\lambda_{i+1}^2 \lambda_{i+2}^2) + 960c_6 \lambda_{i+1}^2 \lambda_{i+2}^4 \quad [7.10]$$

$$\nu_i = 2 c_3 + 16 c_4 + 480 c_5 \lambda_{i+1}^3 \lambda_{i+2}^3 + 1920 c_6 \lambda_{i+1}^3 \lambda_{i+2}^3 \quad [7.11]$$

$$\xi_i = 3 c_3 + 48 c_4 \lambda_i^3 + 80 c_5 \lambda_i^4 \quad [7.12]$$

$$\sigma_i = 24 c_4 + 480 c_5 \lambda_i^3 + 960 c_6 \lambda_i^4 \quad [7.13]$$

$$\tilde{\omega}_i = 12 c_3 + 96 c_4 \lambda_i^2 \quad [7.14]$$

$$\rho_i = 192 c_4 \lambda_i + 640 c_5 \lambda_i^3 \quad [7.15]$$

$$\sigma_i = 18 c_3 + 144 c_4 - 144 c_4 \lambda_i^2 + 480 c_5 \lambda_{i+1}^2 \lambda_{i+2}^2 \quad [7.16]$$

$$\tau_i = 144 c_4 + 480 c_5 - 480 c_5 \lambda_i^2 + 5760 c_6 \lambda_{i+1}^2 \lambda_{i+2}^2 \quad [7.17]$$

$$\phi_i = -12 c_3 - 96 c_4 \quad [7.18]$$

$$\chi_i = 576 c_4 \lambda_{i+1} \lambda_{i+2} \quad [7.19]$$

$$\psi_i = 1920 c_5 \lambda_{i+1} \lambda_{i+2}^2 \quad [7.20]$$

$$\omega_i = 1920 c_5 \lambda_{i+1}^2 \lambda_{i+2} \quad [7.21]$$

c_1, c_2, \dots, c_6 being the binomial coefficients, viz.

$$c_r = (-1)^r \frac{k(k+1) \dots (k+r-1)}{r!} \quad [8]$$

We get $\alpha'_j, \beta'_j, \dots, \omega'_j$ from $\alpha_i, \beta_i, \dots, \omega_i$ by changing λ_i to λ'_i .

In the following table we give the expressions for the various order moments required in the above approximate expression for V , in the two cases, viz. :

- (i) when the particle is an ellipsoid, and
 (ii) when it is an elliptic cylinder.

TABLE I

	Ellipsoid with semi axes a, b, c along Ox_1, Ox_2, Ox_3 respectively	Cylinder with elliptic section having semi-axes a, b parallel to Ox_1, Ox_2 respectively and height $2h$ parallel to Ox_3
M	$(4/5) \pi abc$	$2 \pi abh$
A_1	$(4/15) \pi a^2bc$	$(1/2) \pi a^2bh$
A_2	$(4/15) \pi ab^2c$	$(1/2) \pi ab^2h$
A_3	$(4/15) \pi abc^3$	$(2/3) \pi abh^3$
B_1	$(4/35) \pi a^5bc$	$(1/4) \pi a^5bh$
B_2	$(4/35) \pi ab^5c$	$(1/4) \pi ab^5h$
B_3	$(4/35) \pi abc^5$	$(2/5) \pi abh^5$
C_1	$(4/105) \pi ab^3c^3$	$(1/6) \pi ab^3h^3$
C_2	$(4/105) \pi a^3bc^3$	$(1/6) \pi a^3bh^3$
C_3	$(4/105) \pi a^3b^3c$	$(1/12) \pi a^3b^3h$
D_1	$(4/63) \pi a^7bc$	$(5/32) \pi a^7bh$
D_2	$(4/63) \pi ab^7c$	$(5/32) \pi ab^7h$
D_3	$(4/63) \pi abc^7$	$(2/7) \pi abh^7$
E_1	$(4/315) \pi ab^5c^3$	$(1/12) \pi ab^5h^3$
E_2	$(4/315) \pi a^3bc^5$	$(1/10) \pi a^3bh^5$
E_3	$(4/315) \pi a^5b^3c$	$(1/32) \pi a^5b^3h$
F_1	$(4/315) \pi ab^3c^5$	$(1/10) \pi ab^3h^5$
F_2	$(4/315) \pi a^5bc^3$	$(1/12) \pi a^5bh^3$
F_3	$(4/315) \pi a^3b^5c$	$(1/32) \pi a^3b^5h$
H	$(4/945) \pi a^3b^3c^3$	$(1/36) \pi a^3b^3h^3$

We may mention here that the above expression for V is valid only when L/R , where L is a characteristic length defining the size of a particle, is so small that

the terms of order $(L/R)^8$ and higher powers of (L/R) are negligibly small in comparison with 1.

ACKNOWLEDGMENT

I am grateful to Prof. P. L. Bhatnagar for the suggestion of the problem and guidance throughout the preparation of the paper.

REFERENCE

1. Vold, M. J. . . *Proc. Ind. Acad.* 1957, 46, Sec. A, 152-166.