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THE DIPOLE-DIPOLE DISPERSION FORCES FOR SMALL, INTERMEDIATE AND LARGE DISTANCES

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ABSTRACT

We obtain an improved expression for the dipole-dipole London dispersion force between closed shell atoms for small, intermediate and large distnaces compared with their linear dimensions.

RESUMO

Obtivemos uma expressão mais correta para a força de dispersão de London na interação dipolo-dipolo, para átomos neutros, a distâncias pequenas, intermediárias e grandes em relação as dimensões lineares dos mesmos.

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1. INTRODUCTION

The London(1) dispersion force theory for large distances has been treated, in details, by Longuet-Higgins(2) for intermediate and large distances. Since the usual multipole expansion fails for intermediate distances, he has written the interaction matrix elements without expanding the interatomic potential in multipoles. Lassettre(3) suggested to apply this method to calculate the interatomic electrostatic potential between neutral atoms. Following Lassettre's suggestion Csanak and Taylor(4) have applied this method to calculate the first terms of the transition matrix element of the charge denisty operator $X_{n,p}(q)$, also called polarization potential. They have also successfully obtained expressions for the polarization potential for the electron-atoms scattering.

Jacobi and Csanak(5) were the first to calculate(6) the dipole-dipole term of the London dispersion force for intermediate and large distances using an analytic representation of the Born amplitudes in momentum space and a general analysis of angular momentum.

According to Csanak and Taylor(4) the matrix element $X_{n1}(q)$ is given by:

$$X_{n1}(q) = D_n\left[\frac{q}{(\alpha^2+q^2)^3} - \frac{2q^3}{(\alpha^2+q^2)^4}\right]\alpha^6 + M_n\frac{16\,q^3\alpha^3}{\pi(\alpha^2+q^2)^4} \quad . \quad (1.1)$$

However, as will be shown in section 2, the matrix element $X_{n1}(q)$ defined in Eq. (1.1) is not correct and it must be replaced by:

$$x_{n1}(q) = \sqrt{\frac{2\pi}{3}}\, D_n\left[\frac{q}{(\alpha^2+q^2)^3} - \frac{2q^3}{(\alpha^2+q^2)^4}\right]\alpha^6 + M_n\,\frac{32\,q^3\alpha^3}{\pi(\alpha^2+q^2)^4} \quad . \tag{1.2}$$

In section 3, the dipole-dipole interaction energy between two neutral atoms in the ground state is calculated using only the term $\sqrt{2\pi/3}\, D_n\left[q/(\alpha^2+q^2)^3 - 2q^3/(\alpha^2+q^2)^4\right]\alpha^6$ of Eq. (1.2), since $D_n \gg M_n$, as one can easily verify. We see that for large distances our results agree with those of Dalgarno[7], as expected. On the other hand, for small distances we show that our results are different from those of Jacobi and Csanak[5].

2. THE MATRIX ELEMENT $X_{n1}(q)$

We use here the method adopted by Csanak and Taylor[4] to obtain $X_{n1}(q)$. According to them, the coefficients β and γ are determined by taking $X_{n1}(q)$ that is given by,

$$X_{n1}(q) = \beta\,\frac{q}{(\alpha^2+q^2)^3} + \gamma\,\frac{q^3}{(\alpha^2+q^2)^4} + \ldots , \tag{2.1}$$

in the limit $q\to 0$ and comparing it with the exact Taylor-series expansion of $X_{nL}(q)$ around $q\to 0$, defined by[4]:

$$X_{nL}(q) = \sum_{n=L}^{\infty} \frac{X_{nL}^{(x)}(q)}{x!}\, q^x \quad , \tag{2.2}$$

where

$$X_{nL}^{(x)}(q) = 4\pi\, i^L \sum_{i=1}^{N} \int \psi_0^*(\vec{r}_1\ldots\vec{r}_N)\, j_L(qr_i)\, Y_{LM}(\hat{r}_i)\, \psi_n(\vec{r}_1\ldots\vec{r}_N)\, d\vec{r}_1\ldots d\vec{r}_N \quad , \tag{2.3}$$

is the spectroscopic multipole oscillator strength.

For $L=x=1$, Eq.(2.3) follows as

$$X_{n1}^{(1)} = \sqrt{\frac{2\pi}{3}}\, D_n \quad , \tag{2.4}$$

where

$$D_n = \sqrt{\frac{8\pi}{3}}\, i \sum_{i=1}^{N} \int \psi_0^*(\vec{r}_1\ldots\vec{r}_N)\, r_i\, Y_{10}(\hat{r}_i)\, \psi_n(\vec{r}_1\ldots\vec{r}_N)\, d\vec{r}_1\ldots d\vec{r}_N \quad , \tag{2.5}$$

is the dipole oscillator strength.

For $x=L+2$, $L=1$, Eq. (2.3) becomes

$$x_{n1}^{(3)}(q) = 4\pi\, i \sum_{i=1}^{N} \int \psi_0(\vec{r}_1\ldots\vec{r}_N)\, j_1(qr_i)\, Y_{10}(\hat{r}_i)\, \psi_n(\vec{r}_1\ldots\vec{r}_N)\, d\vec{r}_1\ldots d\vec{r}_N \quad , \tag{2.6}$$

where

$$j_1(qr) = \frac{1}{3}(qr) - \frac{1}{5!}(qr)^3 + \ldots \quad , \qquad (2.7)$$

is a spherical Bessel function of the first kind[10].

Substituting Eq. (2.5) in Eq. (2.6), for $x=3$, $L=1$, the following result is obtained

$$X_{n1}^{(3)}(q) = \sqrt{\frac{2\pi}{3}}\, D_n q + \ldots \quad , \qquad (2.8)$$

neglecting higher order terms in q.

From Eqs. (2.1) and (2.8) we see that the coefficient β is given by

$$\beta = \sqrt{\frac{2\pi}{3}}\, D_n \alpha^6 \quad . \qquad (2.9)$$

In the next step γ will be determined by using the exact first moment M_n that is defined by[4]:

$$M_n = \int_0^\infty q\, X_{n1}(q)\, dq \quad . \qquad (2.10)$$

Then, substituting Eqs. (2.1) and (2.9) into Eq. (2.10) we found

$$M_n = \sqrt{\frac{2\pi}{3}}\, D_n \int_0^\infty \frac{q}{(1+q^2/\alpha^2)^3}\, dq + \frac{\gamma}{\alpha^8}\int_0^\infty \frac{q^4}{(1+q^2/\alpha^2)^4}\, dq \quad . \qquad (2.11)$$

that permit us to find

$$\gamma = -\sqrt{\frac{2\pi}{3}}\, D_n (2\alpha^6) + \frac{32\, M_n\, \alpha^3}{\pi} \qquad (2.12)$$

taking into account the integrals[9]

$$\int_0^\infty \frac{dn}{(x^2+a^2)^n} = \frac{(2n-3)!!}{2(2n-2)!!} \cdot \frac{\pi}{a^{2n-1}} \quad , \qquad (2.13)$$

where $n = 1,2,3$ and 4.

Now, substituting Eqs. (2.9) and (2.12) in Eq. (2.1) we get,

$$X_{n1}(q) = \sqrt{\frac{2\pi}{3}}\, D_n \left[\frac{q}{(\alpha^2+q^2)^3} - \frac{2q^3}{(\alpha^2+q^2)^4}\right]\alpha^6 + \frac{32\, M_n q^3 \alpha^3}{\pi(\alpha^2+q^2)^4} \quad . \qquad (2.14)$$

Comparing Csanak and Taylor[4] result, given by Eq. (1.1), with our Eq. (2.14), we see that they are different by a factor $\sqrt{2\pi/3}$ in the first term and by a factor 2 in the second one.

In the next section we use the matrix element $X_{n1}(q)$ given by Eq. (2.14) to calculate the interaction energy $W^{(1,1)}(R)$ for two neutral atoms in the ground state.

3. THE DIPOLE-DIPOLE TERM

Following Jacobi and Csanak[5] the second order dipole-dipole interaction energy between two neutral atoms in the ground state is given by

$$W^{(1,1)}(R) = -\frac{2}{\pi^4}\int_0^\infty du \int_0^\infty dq \int_0^\infty dq' \sum_{LL'\ell} \begin{pmatrix} L & L' & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 \cdot$$

$$\cdot\, j_L(qR)\, j_{L'}(q'R) \cdot \left[\frac{(2L+1)(2L'+1)(2\ell+1)}{4\pi}\right] \cdot$$

$$\cdot \sum_{n\neq 0} \frac{\left(E_{nL}^{(1)} - E_0^{(1)}\right) X_{nL}(q)\, X^*_{nL'}(q')}{\left(E_{nL}^{(1)} - E_0^{(1)}\right)^2 + u^2} \cdot$$

$$\cdot \sum_{m\neq 0} \frac{\left(E_{mL}^{(2)} - E_0^{(2)}\right) X_{mL}(q)\, X^*_{mL'}(q')}{\left(E_{mL}^{(2)} - E_0^{(2)}\right)^2 + u^2} \quad , \qquad (3.1)$$

where R is the distance between the centre of mass of the two systems, E_{nL} refers to the unperturbed excited state energy of the atom with energy in the gorund state E_0, $X_n(q)$ is the spatial Fourier transform of the transition density matrix between the ground and the n^{th} excited state and $j_L(qR)$ is the Bessel spherical function.

In Ref. (5) only the first term of $X_{nL}(q)$ for $L = L' = 1$ was used to calculate the dipole-dipole interaction energy and claimed without any justification to be the leading term. Indeed, as it will become apparent from our calculations, the first and the second terms have the same order of magnitude for all R values.

Substituting Eq. (1.2) in Eq. (3.1), for $L = L' = 1$, the following result is obtained, taking into account the q-integrals shown explicitely in appendix A:

$$W^{(1,1)}(R) = \frac{-2\alpha^{24} A}{3\pi^3} \left\{ \left[I_1^2(\alpha R) + 2 I_2^2(\alpha R)\right] + \right.$$

$$+ 8\left[2J_1^2(\alpha R) - I_1(\alpha R)J_1(\alpha R) + 2K_1^2(\alpha R) - 4J_1(\alpha R)K_1(\alpha R) + I_1(\alpha R)K_1(\alpha R)\right] +$$

$$\left. + 16\left[2J_2^2(\alpha R) - I_2(\alpha R)J_2(\alpha R) + 2K_2^2(\alpha R) - 4J_2(\alpha R)K_2(\alpha R) + I_2(\alpha R)K_2(\alpha R)\right]\right\}, \qquad (3.2)$$

where the functions $I_i(\alpha R)$, $J_i(\alpha R)$ and $K_i(\alpha R)$ are seen in Appendix A,

$$A = \int_0^\infty d\omega\, \alpha_1(i\omega)\alpha_2(i\omega) \quad , \qquad (3.3)$$

with $\alpha_j(i\omega)$, denoting the frequency-dependent dipole polarizability, defined by

$$\alpha_j(i\omega) = \sum_n \frac{\left(E_{nL}^{(j)} - E_0^{(j)}\right) D_n D_n^*}{\left(E_{nL}^{(j)} - E_0^{(j)}\right)^2 + u^2} \quad . \qquad (3.4)$$

Taking into account $I_i(\alpha R)$, $J_i(\alpha R)$ and $K_i(\alpha R)$, shown in Appendix A, Eq. (3.2) becomes:

$$W^{(1,1)}(R) = V^{(1,1)}_{disp}(R) + U^{(1,1)}_{disp}(R) \quad , \tag{3.5}$$

where

$$V^{(1,1)}_{disp}(R) = \frac{-3A}{\pi R^6}\left\{\left[1 - e^{-\alpha R} P_7(\alpha R)\right]^2 + \frac{2}{9}(\alpha R)^6\left[e^{-\alpha R} P_A(\alpha R)\right]^2\right\} \quad , \tag{3.6}$$

$$U^{(1,1)}_{disp}(R) = \frac{-3A}{\pi R^6}\left\{\frac{(\alpha R)^6\, e^{-2\alpha R}}{2^7.3^2}\left[\frac{1}{2^{10}}\left(Q_7(\alpha R) - Q_6(\alpha R)\right)^2 + P_4(\alpha R)\left(Q_7(\alpha R) - Q_6(\alpha R)\right)\right] + \right.$$

$$+ \frac{e^{-2\alpha R}}{2^{14}.3^2}\left(A_9(\alpha R) - A_8(\alpha R)\right)^2 +$$

$$\left. + \frac{e^{-\alpha R}}{2^6.3}\left(A_9(\alpha R) - A_8(\alpha R)\right).\left[1 - e^{-\alpha R} P_7(\alpha R)\right]\right\} \quad , \tag{3.7}$$

and the $P_n(\alpha R)$, $Q_n(\alpha R)$, and $A_n(\alpha R)$ are given by:

$$P_4(x) = \frac{1}{2^9}\left(7 + \frac{7}{2}x + 3x^2 + \frac{2}{3}x^3 + \frac{1}{15}x^4\right) \quad , \tag{3.8}$$

$$P_7(x) = \left(1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{57}{1536}x^4 + \frac{31}{3840}x^5 + \right.$$

$$\left. + \frac{33}{17280}x^6 + \frac{1}{11520}x^7\right) \quad , \tag{3.9}$$

$$Q_6(x) = \left(49 + \frac{7}{3}x + \frac{23}{6}x^2 + \frac{1}{3}x^3 - \frac{1}{15}x^4 - \frac{1}{45}x^5\right) \quad , \tag{3.10}$$

$$Q_7(x) = \left(\frac{35}{2} - \frac{5}{2}x + \frac{7}{4}x^2 - \frac{1}{12}x^3 - \frac{1}{15}x^4 - \frac{1}{90}x^5 + \frac{1}{630}x^6\right) \quad , \tag{3.11}$$

$$A_8(x) = \left(\frac{7}{3}x^4 - \frac{5}{12}x^5 - \frac{13}{30}x^6 + \frac{1}{6}x^7 + \frac{1}{90}x^8\right) \quad , \tag{3.12}$$

$$A_9(x) = \left(x^4 - \frac{3}{8}x^5 - \frac{61}{280}x^6 + \frac{29}{210}x^7 - \frac{1}{252}x^8 - \frac{1}{1269}x^9\right) \quad . \tag{3.13}$$

Comparing our $P_4(x)$ and $P_7(x)$ with those calculated by Jacobi and Csanak[5] we verify that some of their coefficients are not correct. We must note also that the polarizability integral W, defined by them in page 370, is not correct. Indeed, comparing W with the polarizability, that is indicated by A, in Eq. (3.3), we verify that, in the $R \to 0$ limit, W must be multiplied by a factor 1/9.

Considering Eqs. (3.6) and (3.7) we have the following limits for $R \to 0$ and $R \to \infty$:

$$V^{(1,1)}_{disp}(R \to 0) = U^{(1,1)}_{disp}(R \to \infty) = 0 \quad , \tag{3.14}$$

and

$$V^{(1,1)}_{disp}(R \to 0) = -\frac{A\alpha^6}{6\pi}\left(\frac{7}{256}\right)^2 \quad . \tag{3.15}$$

$$V^{(1,1)}_{disp}(R \to \infty) = -\frac{3A}{\pi R^6} \quad . \tag{3.16}$$

From Eq. (3.16), we see that for large-R distances our prediction for $V_{disp}^{(1,1)}(R\to\infty) = -3A/\pi R^6$ coincides with that obtained by Dalgarno[7], as expected. For small-R distances $V_{disp}^{(1,1)}(R\to 0) = -(A\alpha^6/6\pi)(7/256)^2$ is different from that shown by Jacobi and Csanak[5].

In figures 1 and 2 are seen our results for $W^{(1,1)}(R)/A$, given by Eq. (3.5), for two values of α^2, compared with those of Jacobi and Csanak[5]. We verify that our and Jacobi and Csanak[5] results agree for intermediate and large-R distances; for small-R distances they are different. According to our predictions the interaction potential is very much more attractive than that obtained by Jacobi and Csanak[5].

In future works we intend to introduce higher order dispersion forces terms, such as the dipole-quadrupole, dipole-octupole, quadrupole-quadrupole, and to compare our predictions with experimental results in scattering problems, in virial coefficients[5] and for compressed solid hydrogen[11].

APPENDIX A

THE q-INTEGRALS RESULTS

The q-integrals that appear in section 3 are the following[9,10]:

$$\int_0^\infty \frac{x^{\nu+1}J_\nu(ax)}{(x^2+K^2)^{\mu+1}}\,dx = \frac{a^\mu K^{\nu-\mu}}{2^\mu\Gamma(\mu+1)}\,K_{\nu-\mu}(ak) \quad , \tag{1A}$$

$$K(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} e^{-z}\sum_{r=0}^{N}\frac{(n+r)!}{(n-r)!(2z)^r} \quad , \tag{2A}$$

$$\int_0^\infty \frac{\operatorname{sen}(ax)}{x(\beta^2+x^2)^{n+1}}\,dx = \frac{\pi}{2\beta^{2n+2}}\left[1-\frac{e^{-\alpha\beta}}{2^n.n!}F_n(\alpha\beta)\right] \quad , \tag{3A}$$

$$F_0(z) = 1\,,\ F_1(z) = z+2\,,\ \ldots\,,\ F_n(z) = (z+2n)F_{n-1}(z) - zF'_{n-1}(z)\ . \tag{4A}$$

For $\ell = 0,2$ we get:

$$I_1(\alpha R) = \int_0^\infty dq\,\frac{q^2.j_0(qR)}{(\alpha^2+q^2)^6} = \frac{\pi\,e^{-\alpha R}}{\alpha^9}\,P_4(\alpha R) \quad , \tag{5A}$$

$$J_1(\alpha R) = \int_0^\infty dq\,\frac{q^4.j_0(qR)}{(\alpha^2+q^2)^7} = \frac{\pi\,e^{-\alpha R}}{2^{11}\alpha^9}\,Q_6(\alpha R) \quad , \tag{6A}$$

$$K_1(\alpha R) = \int_0^\infty dq\, \frac{q^6 \cdot j_0(qR)}{(\alpha^2+q^2)^8} = \frac{\pi\, e^{-\alpha R}}{2^{11}\,\alpha^9}\, Q_7(\alpha R) \quad , \tag{7A}$$

$$I_2(\alpha R) = \int_0^\infty dq\, \frac{q^2 \cdot j_2(qR)}{(\alpha^2+q^2)^6} = \frac{3\pi}{2\,\alpha^{12} R^3} \left[1 - e^{-\alpha R}\, P_7(\alpha R)\right] \quad , \tag{8A}$$

$$J_2(\alpha R) = \int_0^\infty dq\, \frac{q^4 \cdot j_2(qR)}{(\alpha^2+q^2)^7} = \frac{\pi\, e^{-\alpha R}}{2^{10} \cdot \alpha^{12} R^3}\, A_8(\alpha R) \quad , \tag{9A}$$

$$K_2(\alpha R) = \int_0^\infty dq\, \frac{q^6 \cdot j_2(qR)}{(\alpha^2+q^2)^8} = \frac{\pi\, e^{-\alpha R}}{2^{10} \cdot \alpha^{12} R^3}\, A_9(\alpha R) \quad , \tag{10A}$$

where the polynomials $P_4(x)$, $P_7(x)$, $Q_6(x)$, $Q_7(x)$, $A_8(x)$, and $A_9(x)$ are indicated by Eqs. [(3.7)-(3.12)].

For $i = 1,2$ we have,

$$J_i(\alpha R) = I_i(\alpha R) + \frac{\alpha}{12} \left[\frac{d\, I_i(\alpha R)}{d\alpha}\right] \quad , \tag{11A}$$

$$K_i(\alpha R) = J_i(\alpha R) + \frac{\alpha}{14} \left[\frac{d\, J_i(\alpha R)}{d\alpha}\right] \quad . \tag{12A}$$

Substituting Eq. (2.13) in Eqs. (5A) and (8A) results:

$$I_1(\alpha R) = \frac{\pi}{2} \left(\frac{7}{256}\right) \frac{1}{\alpha^9} \quad , \tag{13A}$$

$$I_2(\alpha R) = \frac{3\pi}{2R^3} \cdot \frac{1}{\alpha^{12}} \tag{14A}$$

Now, we will derive the $W^{(1,1)}(R)$ limits for small-R and large-R values.

For small-R values we found

$$W^{(1,1)}(R \to 0) = \frac{-2\,\alpha^{24} A}{3\pi^3} \left[I_1^2 + 8(2J_1^2 - I_1 J_1 + 2K_1^2 - 4J_1 K_1 + I_1 K_1)\right] \quad , \tag{15A}$$

that we will give

$$\left|V_{disp}^{(1,1)}(R \to 0)\right| = \left|U_{disp}^{(1,1)}(R \to 0)\right| = \frac{\alpha^6 A}{6\pi} \left(\frac{7}{256}\right)^2 \quad ; \tag{16A}$$

taking into account Eqs. (11A-13A) and the following integrals[9,10]

$$\int_0^\infty \frac{x\, \mathrm{sen}\, ax}{(\beta^2+x^2)}\, dx = \frac{\pi}{2}\, e^{-a\beta} \quad , \tag{17A}$$

$$\int_0^\infty \frac{\mathrm{sen}\, ax}{n(\beta^2+x^2)}\, dx = \frac{\pi}{2\beta^2} \left(1 - e^{-a\beta}\right) \quad . \tag{18A}$$

$$\int_0^\infty \frac{\cos ax}{(\beta^2+x^2)}\, dx = \frac{\pi}{2\beta}\, e^{-a\beta} \quad . \tag{19A}$$

For large-R values we found

$$W^{(1,1)}(R\to\infty) = V^{(1,1)}_{disp}(R\to\infty) = -\frac{4\alpha^{24}A}{3\pi^3} I_2^2 , \qquad (20A)$$

that we will give

$$W^{(1,1)}(R\to\infty) = -\frac{3A}{\pi R^6} , \qquad (21A)$$

taking into account Eqs. (11A-14A) and (17A-19A).

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FIGURE CAPTIONS

Fig. 1 - The Van der Waals potential. Our predictions $W^{(1,1)}(R)/A$ (●) are compared with those of Jacobi and Csanak $V^{(1,1)}_{disp}(R)/A$ (○) at large-R distances, for $\alpha^2 = 3.391$ and $\alpha^2 = 2.896$.

Fig. 2 - The Van der Waals potential. Our predictions $W^{(1,1)}(R)/A$ (●) are compared with those of Jacobi and Csanak $V^{(1,1)}_{disp}(R)/A$ (○) at small-R distances, for $\alpha^2 = 3.391$ and $\alpha^2 = 2.896$.

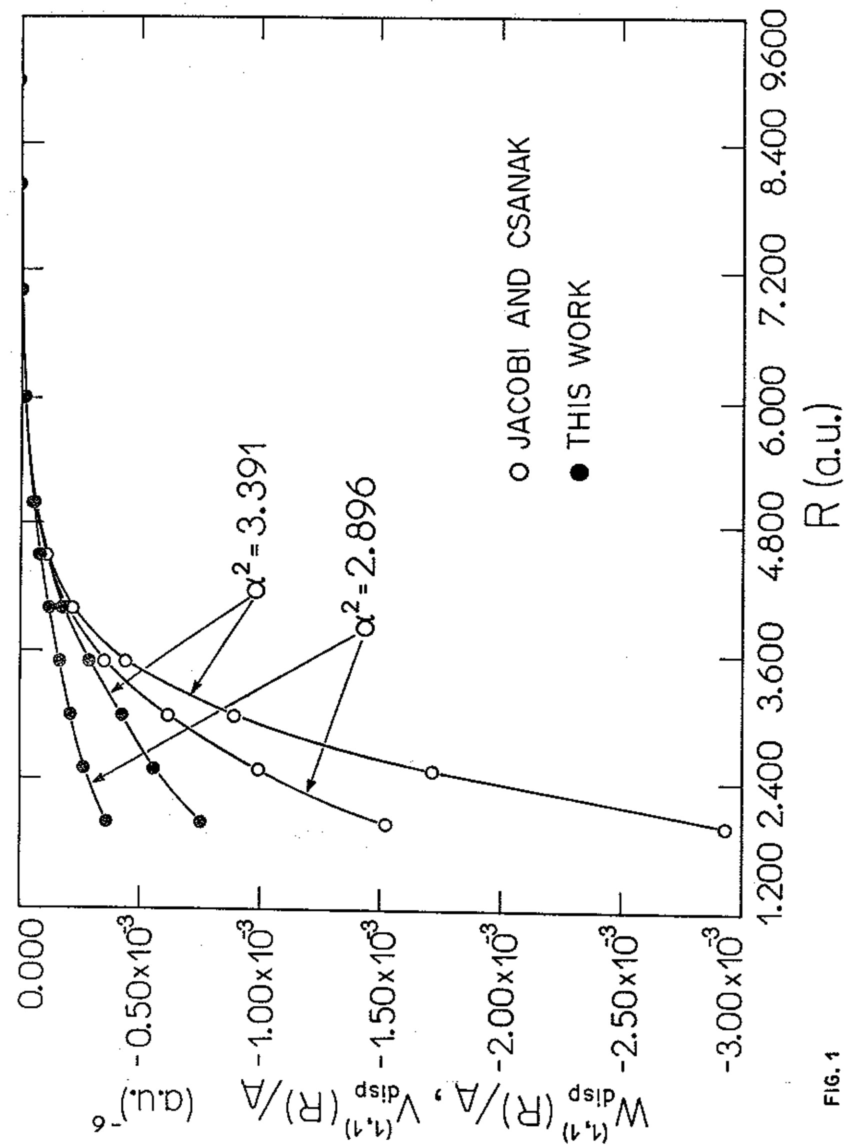

FIG. 1

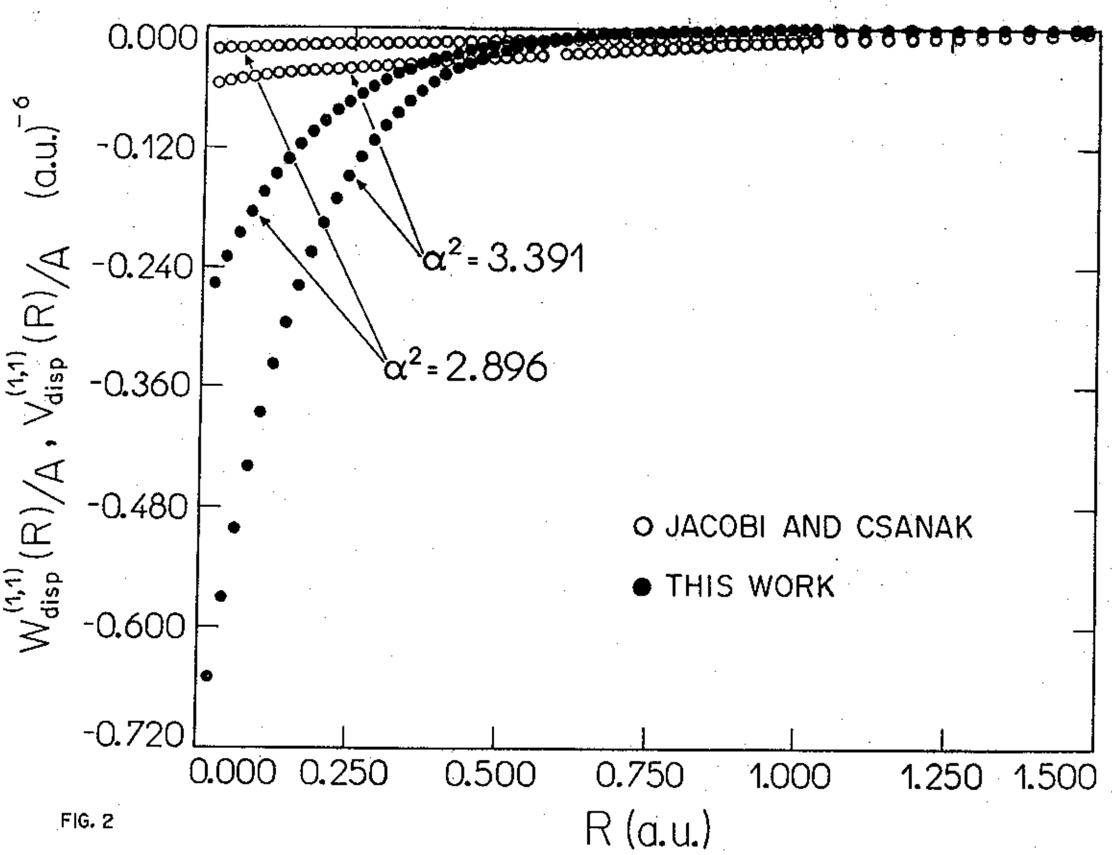
0.000
-0.120
-0.240
-0.360
-0.480
-0.600
-0.720
$W_{disp}^{(1,1)}(R)/A$, $V_{disp}^{(1,1)}(R)/A$ $(a.u.)^{-6}$
$\alpha^2 = 3.391$
$\alpha^2 = 2.896$
O JACOBI AND CSANAK
● THIS WORK
0.000 0.250 0.500 0.750 1.000 1.250 1.500
R (a.u.)

FIG. 2