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# *CALCULATION OF THE INTERACTION POTENTIAL OF ATOMS*

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The sum of the Coulomb interaction between atomic nuclei and the change in electron energy connected with the mutual approach of the nuclei is taken as the interaction potential. The electron energy is computed on the basis of the statistical model.

**I.** It was shown in a previous article[1] that the energy $H_0$ of electrons, in the approximation of the Thomas-Fermi statistical model and for the presence of two nuclei, lies between the two values $H$ and $H_1$, which differ by not more than 5 per cent:

$$\frac{1}{e^2}H = \int\left\{\lambda\left[\frac{3}{5}(\rho_{01}+\rho_{02})^{5/3} - \frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02})\right] - \frac{1}{2}\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)(\rho_{01}+\rho_{02})\right\}dv,$$

$$\frac{1}{e^2}H_1 = \int\left\{\lambda\left[\frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02}) - \frac{2}{5}(\rho_{01}^{2/3}+\rho_{02}^{2/3})^{5/2}\right] - \frac{1}{2}\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)(\rho_{01}+\rho_{02})\right\}dv, \quad (1)$$

where $\lambda = \frac{1}{2}(3\pi^2)^{2/3}\hbar^2/me^2 = 2.52\times10^{-8}$ cm, $Z_1e$ and $Z_2e$ are the nuclear charges, $\rho_{01}(r_1)$ and $\rho_{02}(r_2)$ are the Thomas-Fermi electron densities in the atoms without consideration of the mutual interaction, $r_1$ is the distance to the nucleus of the first atom, $r_2$, to the nucleus of the second atom.

The relative difference between H and $H_1$ decreases montonically to zero upon increase in the distance between the nuclei from zero to infinity.

Under the condition that the electrons are always in the ground states, we have for the interaction potential between the atoms, in accord with (1), $U_1(R) < U_0(R) < U(R)$, where

$$U(R) = e^2Z_1Z_2/R + H - H(\infty),\ U_1(R) = e^2Z_1Z_2/R + H_1 - H_1(\infty). \tag{2}$$

It is evident that as $R \rightarrow 0$, $\rho_{01} \rightarrow 0$, where $\rho_{02}$ differs from zero; conversely, for $r_1 \rightarrow \infty$, $\rho_{01}(r_1) \sim 1/r_1^6$. Therefore,

$$\begin{aligned}\frac{1}{e^2}U(R) &= \frac{Z_1Z_2}{R} + \int\left\{\lambda\left[\frac{3}{5}(\rho_{01}+\rho_{02})^{5/3} - \frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02}) - \frac{1}{10}(\rho_{01}^{5/3}+\rho_{02}^{5/3})\right] - \frac{1}{2}\left(\frac{Z_1}{r_1}\rho_{02}+\frac{Z_2}{r_1}\rho_{01}\right)\right\}dv,\\ \frac{1}{e^2}U_1(R) &= \frac{Z_1Z_2}{R} + \int\left\{\lambda\left[\frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02}) - \frac{2}{5}(\rho_{01}^{2/3}+\rho_{02}^{2/3})^{5/2} - \frac{1}{10}(\rho_{01}^{5/3}+\rho_{02}^{5/3})\right] - \frac{1}{2}\left(\frac{Z_1}{r_1}\rho_{02}+\frac{Z_2}{r_2}\rho_{01}\right)\right\}dv,\end{aligned} \tag{3}$$

$Z_2/R - \int r_1^{-1}\rho_{02}(r_2)\,dv$ is the Thomas-Fermi potential of the second atom at the distance R. Therefore, we can write (3) in the form

$$\begin{aligned}\frac{1}{e^2}U(R) &= \frac{Z_1Z_2}{2R}\left[\chi\left(Z_1^{1/3}\frac{R}{a}\right)+\chi\left(Z_2^{1/3}\frac{R}{a}\right)\right] + \lambda\int\left[\frac{3}{5}(\rho_{01}+\rho_{02})^{5/3} - \frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02}) - \frac{1}{10}(\rho_{01}^{5/3}+\rho_{02}^{5/3})\right]dv,\\ \frac{1}{e^2}U_1(R) &= \frac{Z_1Z_2}{2R}\left[\chi\left(Z_1^{1/3}\frac{R}{a}\right)+\chi\left(Z_2^{1/3}\frac{R}{a}\right)\right] + \lambda\int\left[\frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})(\rho_{01}+\rho_{02}) - \frac{1}{2}(\rho_{01}^{2/3}+\rho_{02}^{2/3})^{5/2} - \frac{1}{10}(\rho_{01}^{5/3}+\rho_{02}^{5/3})\right]dv,\end{aligned} \tag{4}$$

$$a = (9\pi^2/128)^{1/3}\hbar^2/me^2 = 4.68\cdot 10^{-9}\ \text{cm},$$

where $\chi(x)$ is the Thomas-Fermi function, the tabulation of which was taken from the book of Gombas.[2] The densities $\rho_{01}(r_1)$ and $\rho_{02}(r_2)$ are expressed in terms of the Thomas-Fermi function

$$\rho_{01}(r_1) = \left(\frac{Z_1}{r_1\lambda}\cdot\chi\left(Z_1^{1/3}\frac{r_1}{a}\right)\right)^{3/2},$$

and similarly for $\rho_{02}(r_2)$.

**2.** If we write the potential $U_0(R)$ in the form

$$U_0(R) = Z_1Z_2e^2f_0(R)/R,$$

then for small R,

$$f_0 \approx 1 - 1.59x + \ldots,\ x = \frac{3}{7}\frac{(Z_1+Z_2)^{7/3} - Z_1^{7/3} - Z_2^{7/3}}{Z_1Z_2}\frac{R}{a}. \tag{5}$$

This follows from the fact that for $R \rightarrow 0$, $U(R)$ differs from the Coulomb interaction by the difference of the electron energy at $R \rightarrow \infty$ and $R = 0$, which, in accord with the Thomas-Fermi model, are respectively equal to

$$-1.59\,\frac{3}{7}(Z_1+Z_2)^{7/3}\frac{e^2}{a}\ \text{and}\ -1.59\cdot\frac{3}{7}\left(Z_1^{7/3}+Z_2^{7/3}\right)\frac{e^2}{a}.$$

The first two terms in (5) coincide with the expansion of the Thomas-Fermi function of argument x.

With the aid of perturbation theory, we can obtain,[3] for $Z_2/Z_1 \rightarrow 0$ or $Z_1/Z_2 \rightarrow 0$:

$$f_0(R) \rightarrow \chi\left(Z_1^{1/3}\frac{R}{a}\right) \quad \text{or} \quad f_0(R) \rightarrow \chi\left(Z_2^{1/3}\frac{R}{a}\right), \tag{6}$$

which coincides with (5) for $R \rightarrow 0$ under these limiting conditions. Obviously, $f_0(R)$ ought to be a symmetric function relative to a substitution of $Z_2$ for $Z_1$.

We now consider the more general expression for the electron energy

$$\frac{1}{e^2}H(R = \frac{3}{5}\int\lambda\rho^{5/3}dv - \int\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)\rho\,dv + \frac{1}{2}\iint\frac{\rho(\bar{r})\rho(\bar{r}')\,dv\,dv'}{|\bar{r}-\bar{r}'|}$$

The density ought to be such that H is minimal. Therefore,

$$\frac{3}{5}\lambda\int\rho_0^{5/3}dv = \frac{\lambda}{e^2}\frac{\partial H_0}{\partial\lambda};\ -\int\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)\rho_0\,dv = \frac{Z_1}{e^2}\frac{\partial H}{\partial Z_1} + \frac{Z_2}{e^2}\frac{\partial H}{\partial Z_2}. \tag{7}$$

It was found in Ref. 1 [Eq. (7)] that

$$\frac{1}{e^2} H_0 = \frac{\lambda}{10}\int \rho_0^{5/3} dv - \frac{1}{2}\int\left(\frac{Z_1}{r_1}+\frac{Z_2}{r_2}\right)\rho_0\, dv.$$

Hence, by virtue of (7), we have

$$H_0 = \frac{1}{6}\lambda\, \partial H_0/\partial\lambda - \frac{1}{2}(Z_1\, \partial H_0/\partial Z_1 + Z_2\, \partial H_0/\partial Z_2). \tag{8}$$

From (8), $H_0$ can be written in the form

$$(Z_1 Z_2 e^2/R)\,\Theta\,(Z_1^{1/3}R/a,\ Z_2^{1/3}R/a). \tag{9}$$

Consequently, $U_0(R)$ also reduces to the same form.

**3.** In the table below, the screening functions $f(R)$ and $f_1(R)$ have been computed as functions of the argument $x$ [Eq. (5)] for the ratio $\alpha = Z_2/Z_1 = 1/4,\ 2/3,\ 1$.

| $\alpha$ | $x$ | 0,2 | 0,3 | 0,5 | 0,7 | 1 | 1,5 | 2 | 3 | 5 | 7 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | $\chi(x)$ | 0,79 | 0,72 | 0.61 | 0,52 | 0,425 | 0,315 | 0,242 | 0,158 | 0,079 | 0,046 | 0,0244 |
| $1/4$ | $f(x)$ | 0,80 | 0.73 | 0,61 | 0.52 | 0,42 | 0,31 | 0,23 | 0.14 | 0,063 | 0,026 | 0,013 |
| $1/4$ | $f_1(x)$ | 0,79 | 0,71 | 0,59 | 0,50 | 0,40 | 0,28 | 0,21 | 0,12 | 0,052 | 0,024 | 0,010 |
| $2/3$ | $f(x)$ | 0.80 | 0,73 | 0,61 | 0,52 | 0,42 | 0,31 | 0,23 | 0,14 | 0,056 | 0,026 | 0,011 |
| $2/3$ | $f_1(x)$ | 0,79 | 0,71 | 0,5 | 0,49 | 0,39 | 0,28 | 0,20 | 0,12 | 0,046 | 0,021 | 0,008 |
| 1 | $f(x)$ | 0,80 | 0.73 | 0,61 | 0,47 | 0,42 | 0,30 | 0,22 | 0,13 | 0,055 | 0,028 | 0,015 |
| 1 | $f_1(x)$ | 0,79 | 0,70 | 0,58 | 0,44 | 0,39 | 0,28 | 0,20 | 0,11 | 0,046 | 0,024 | 0,012 |

The integrals in Eq. (4) were computed with an accuracy ~ 2 per cent. These integrals are negative and for large values of R are close in value to the first term in Eqs. (4). Therefore, the error in computing $f$ and $f_1$ amounts to about 10 per cent at $x \sim 10$. Moreover, at some points there are evidently small random errors, because the computation was carried out "by hand" by a single person. Since the statistical model is generally valid only with accuracy ~ 20 per cent, these errors have no significant importance here.

It follows from the table that the screening function $f_0(x)$, whose values lie between $f(x)$ and $f_1(x)$ for large values of $x$, differs appreciably from $\chi(x)$ even at $\alpha = 1/4$. This corresponds to $f_0(x)$ for $\alpha \to 0$. For $x = 10$, the ratio $f_0(x)/\chi(x)$ is $\sim 1/2$. Further change of $\alpha$ up to 1 does not lead to a significant change in $f_0(x)$.

We can, however, introduce another scale factor in the definition of $x$. This factor would coincide with Eq. (5) when $Z_2/Z_1$ or $Z_1/Z_2$ tended to zero and would reduce for this same value of R to smaller values of $x$ in the old definition. Then $f(x')$, for the new definition of $x$, will differ less from $\chi(x')$ at larger $x'$. For example, the Bohr scale factor $(Z_1^{2/3} + Z_2^{2/3})$ gives the following changes in $x$ for various values of $\alpha$:

$$\alpha = 0,\quad 1/4,\quad 2/3,\quad 1$$
$$x'/x = 1,\quad 0.93,\quad 0.92,\quad 0.92,$$

i.e., if we introduce

$$x' = \sqrt{Z_1^{2/3} + Z_2^{2/3}}\, R/a,$$

in place of the value of $x$ defined by Eq. (5), then at $\alpha = 0$, $x' = x$, while at $\alpha = 1$, $x' = 0.92\, x$. Then the values of $f(x')$ in the table above remain practically unchanged for $x' < 0.2$, in the interval $0.5 < x' < 3$, they increase by ~ 8 per cent, and for $x' \sim 7 - 10$, they increase by ~ 20 per cent. The difference between $f(x')$ and $\chi(x')$ will be much less. It would be even better to introduce a scale factor by the relation

$$x' = (Z_1^{1/2} + Z_2^{1/2})^{2/3} R/a.$$

Then the ratio $x'/x$ will be

$$\alpha = 0,\quad 1/4,\quad 2/3,\quad 1,$$
$$x'/x = 1,\quad 0.84,\quad 0.82,\quad 0.82.$$

In this case, $f(x')$ differ from $\chi(x')$ by not more than 20 per cent throughout the entire range of variation of $x'$ from 0 to 10. Since

$$R \approx 4.7\cdot 10^{-9}\ \text{cm}\cdot x'/(\sqrt{Z_1} + \sqrt{Z_2})^{2/3},$$

then, for $x' = 10$, even for $Z_1 = Z_2 = 100$, $R = 0,64 \times 10^{-8}$ cm. However, at distances $R > 10^{-8}$ cm, the calculation of the interaction potential of atoms on the basis of a statistical model loses its meaning.

Thus, in the limits of accuracy of the Thomas-Fermi statistical model of the atom, the interaction between atoms at distances between atoms less than $10^{-8}$ cm can be described by the potential

$$U(R) = \frac{Z_1 Z_2 e^2}{R} \cdot \chi\left([\sqrt{Z_1} + \sqrt{Z_2}]^{2/3} \frac{R}{a}\right), \tag{10}$$

where $\chi(x)$ is the Thomas-Fermi screening function.

This fact, that the screening function can be expressed approximately as a function a single argument, allows us to compute (within a suitable interval of energy of relative motion and for suitable scattering angles) the effective differential scattering cross section at once for an arbitrary pair of colliding atoms.

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# *CYLINDRICAL SELF-SIMILAR ACOUSTICAL WAVES*

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A one-parameter family of self-similar solutions for cylindrical motion is constructed in the acoustical approximation. This construction is accomplished by superposition of plane waves and is expressed in elementary form by quadratures. For motion with a finite pressure discontinuity on the wave front of a converging cylindrical wave, the results agree with those obtained previously.[1] It is found again that the pressure in the reflected wave is infinite. The maximum pressure is estimated and allowances are made for the deviations from the acoustical approximation for large amplitudes.

ZABABAKHIN and Nechaev[1] have treated the propagation of a weak cylindrical shock wave and its reflection from the axis in the acoustical approximation.* Their solution for the reflected wave has an unexpected property: the pressure on the front diverges logarithmically, and is the same before and behind the front, that is

$$p \sim \frac{a}{\sqrt{r_f}} \ln\left|\frac{b r_f}{r - r_f}\right| \quad \text{for} \quad |r - r_f| \ll r_f$$

(where $p$ is the pressure change, and the solution is valid only for $p \ll p_0$).

No such singularity occurs when a spherical acoustical wave converges onto a center and is reflected, or for strong cylindrical and spherical shock waves.[2] It is therefore desirable to obtain the result of Zababakhin and Nechaev differently, by a method in which the necessity for their solution would become clearer.

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