Title
THE SCATTERING OF HIGH VELOCITY NEUTRAL PARTICLES BY ORIENTATION DEPENDENT POTENTIAL

Permalink
https://escholarship.org/uc/item/1np5q12r

Author
Sinanoglu, Oktay.

Publication Date
1958-08-01
UNIVERSITY OF CALIFORNIA

Radiation Laboratory

TWO-WEEK LOAN COPY
This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 5545

BERKELEY, CALIFORNIA
DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.
THE SCATTERING OF HIGH VELOCITY NEUTRAL PARTICLES BY AN ORIENTATION DEPENDENT POTENTIAL

Oktay Sinanoğlu

August 1958

Printed for the U. S. Atomic Energy Commission
The scattering of high velocity neutral particles by an orientation dependent potential

Oktay Sinanoglu
Department of Chemistry and Radiation Laboratory, University of California, Berkeley, California

This note was written under the support of the U.S. Atomic Energy Commission.

In a recent article, 1 Amour, Mason, and Jordan have determined the high velocity scattering cross sections of He and A in thermal N2, and deduced from these data effective interatomic potentials for He-N and A-N2. These potentials are in turn used to obtain an average intermolecular potential for the N2-N2 interaction.

The interaction between He or A and N2 is orientation dependent and can be represented as the sum of effective interatomic potentials. To interpret the scattering cross section data, the authors first average the interaction between say an He and an N2 over all orientations of N2 and use the resulting potential (after fitting it into an inverse power form) in the usual small angle scattering formula 2 to obtain the cross section.


The use of a "pre-averaged" potential for the interpretation of cross sections obtained in such experiments implies that the rotational period of the scattering molecule is small compared to the "time of collision." However, in many experiments where a high velocity particle is scattered by thermal gas molecules, this condition is not satisfied, and it is desirable to have a procedure to interpret cross sections taking into account the effect of orientation. In the following we shall give a method for obtaining approximate orientation dependent cross sections and discuss it primarily with reference to the work of Anand, Mason, and Jordan.

In their experiments, the scattering of an He or A atom takes place under conditions such that, during the "time of collision" an N₂ remains practically in the same orientation; N₂ rotates only by about 0.1°. Moreover, a rough estimate based on the equations of motion treating rotations classically shows that starting from an initial orientation, the angular momentum imparted to N₂ during collision with He, by the angle dependent part of the potential, can change this orientation only by about 0.1°. Therefore, it will be interesting to see, for instance, in this case, to what extent the cross section obtained as the average of cross sections corresponding to equally probable fixed orientations of N₂ might differ from the "pre-averaged" value. Orientation dependent cross sections can be obtained quite readily, if in addition to the fixed orientation of N₂, we assume that during the "time of collision" the relative orientation of N₂ with respect to He remains fixed. This assumption is quite justified since in
high velocity scattering with steep repulsive potentials, the
main part of the interaction takes place over a small range near
the distance of closest approach. Once this assumption is made,
it is necessary to consider only one angle \( \beta \), determining the
approximately fixed relative orientation of \( N_a \) with respect to
He in one plane and at the range of maximum interaction, and
non-planar effects can be ignored.

The orientation dependent potential is conveniently expres-
sed in terms of "Gegenbauer" polynomials (see for example
Frigoriev\textsuperscript{3}). Using the inverse power form of interatomic

\textsuperscript{3}I. Frigoriev, et al., "Molecular Theory of Solutions."

potential with \( \frac{K'}{r} \) and \( \nu \) as parameters we get for the homo-
nuclear diatomic molecule - atom interaction:

\[
\mathbf{V}(r) = \frac{2K'}{r^\nu} \left[ 1 + C_4(\nu)(\frac{\alpha}{r})^4 + C_6(\nu)(\frac{\alpha}{r})^6 + \ldots \right]
\]

\( \alpha \) is half the N-N distance. \( \nu \) has to be a full or half integer;
however, this restriction on \( \nu \) does not sacrifice any accuracy
of fit if the range of \( r \), to which \( \mathbf{V}(r) \) is fitted is small.

For Ne-\( N_a \), once \( K' \) and \( \nu \) are chosen the use of terms through
\( C_6 \) is sufficient for a few tenths of a percent accuracy (even
\( C_8 \) term is about 1%). The use of Eq. (1) in the usual small
angle scattering formula,\textsuperscript{2} along with the stated assumptions,
gives an approximate orientation dependent cross section

\[
S_\theta(v) = \pi r_0^2(v), \text{ where } r_0^2(v) \text{ has to be solved from:}
\]

\[
r_0^2(v) = 1 + \frac{4K'}{\nu \sqrt{\alpha}} \left[ 1 + C_4 \frac{\nu(v+1)}{\nu(v)} \left( \frac{\alpha}{r_0} \right)^4 + C_6 \frac{\nu(v+4)}{\nu(v)} \left( \frac{\alpha}{r_0} \right)^6 + \ldots \right]^{\frac{1}{2}}
\]
\[ \theta_a \] is the effective aperture and \( \Psi(2\nu) = \frac{1}{\nu} \left( \frac{2\nu+1}{2\nu} \right) \]

The "pre-averaging" procedure adopted by Armer, Kuson and Jordan corresponds to using Eq. (1) with the averaged coefficients

\[ C_n^N = \frac{1}{\pi^2} \int_0^{\pi/2} C_n^N(\omega) \cos \omega d\omega \]

and then solving Eq. (2) for \( E^N \). Representing their equation for the He-N potential by \( V_{He-N} = 1.86 \times 10^{-7} / r^6 \) within ca. 2%, \( V(\xi) \) from Eq. (1) agrees with their average \( V(r)_{He-N} \) to ca. 2%.

Now, to obtain orientation dependent cross sections we solve for \( E^N(\gamma) \) from Eq. (2) for several values of \( \gamma \) chosen between 0 and \( \pi/\beta \) by a rapid iterative procedure. Taking \( \beta^2 = 1000 \) a. u. and \( \theta_a = 10^{-3} \) radians for illustration, we find that \( E^N(\gamma) \) varies from 5.77 A to 3.73 A (computed to 0.2% accuracy) as \( \gamma \) goes from 0 to \( \pi/3 \). This gives (taking every orientation of \( \hat{r}_2 \) in an approximately every relative orientation, equally probable) \( E^N(\gamma) = \int_{\gamma}(\gamma) \cos \gamma d\gamma = 5.49 A \) as compared to the "pre-averaged" value \( E^N = 5.38 A \), i.e., pre-averaging more leads to cross sections that are ca. 5% high. (Conversely, this treatment would deduce slightly weaker interatomic potentials).

The assumption of fixed relative orientation somewhat overestimates the effect of orientation, so that this difference of pre-averaged procedures is nearly within experimental uncertainty; and "pre-averaging" is quite justified at least for He-N.

However, e.g., for A-N, i.e., with steeper potentials, and greater experimental accuracy (apparently ca. 2% for A-N) the difference would become more significant.

In any case, the method given here provides a means of estimating the effect of orientation on the cross sections.
and where the difference from the "pre-averaged" cross sections proves large, can be used to interpret these data and obtain interatomic potentials. The results are extendable to heteronuclear diatomic (where odd powers of \( \frac{a}{R_0} \) also enter Eqs. (1) and (2)) and to certain polystylic molecules so long as the assumptions of fixed relative orientation and additivity of interatomic potentials is justified.

ACKNOWLEDGEMENT

The author is indebted to Professor Ambar for correspondence on this subject and his valuable criticism.