Extrapolation Procedure for the Low-Energy Deuteron-Deuteron Reaction Cross Section

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A semiempirical study is made of the deuteron-deuteron reaction cross section to determine its energy dependence at low energy and to permit more reliable extrapolation to energies below the experimental range. An energy-dependent correction to the simple WKB form is shown to be indicated by experimental data. The energy-independent normalization factor is then determined by comparison with the experimental data over the range of ten to one hundred kev bombarding energy. This provides a cross-section formula which is more suitable for extrapolation to the region around one kev.

INTRODUCTION

FOR many applications, such as stellar processes and proposed thermonuclear reactors, it is desirable to know the exact behavior of the reaction cross sections for deuterons impinging on deuterons with low collision energies. The reaction proceeds in the following two ways with about equal probabilities:

$$ {}_1H^2+{}_1H^2\rightarrow {}_2He^3+n, $$
$$ {}_1H^2+{}_1H^2\rightarrow {}_1H^3+p. $$

Unfortunately the cross sections for these processes are extremely small at low energy and are changing rapidly with energy in a manner characteristic of the behavior associated with penetration of a Coulomb barrier. Since the cross section is so low, it is very hard to measure it accurately. Several groups have measured the reaction cross section in the region from 10 kev to 100 kev. It is the purpose of this paper to investigate the validity of extrapolating these data to a bombarding energy of 1 kev or lower.

The three groups of deuteron reaction cross section data, which we shall refer to as those of APSST,[1] ERS,[2] and DJOPR,[3] cover slightly different energy ranges. The most extensive data are those of APSST, but McNeil[4] has pointed out that there is a calculational error in the reduction of their (d,n) branch. All of the groups have assumed a two-parameter equation for their data based on the simple WKB theory of barrier penetration. The empirical fits for each set of data are as follows:

APSST [total (d,n) and (d,p)], $13<E<113$ kev

$$ \sigma=(A/E)\exp[-B/E^{\frac{1}{2}}] $$
$$ =(2.88\times10^2/E)\exp[-45.8/E^{\frac{1}{2}}]\text{barns}; \quad (1\text{-a}) $$

ERS [either branch), $15.2<E<42.85$ kev

$$ \sigma=(1.32\times10^2/E)\exp[-44.758/E^{\frac{1}{2}}]; \quad (1\text{-b}) $$

DJOPR (either branch), $14.5<E<185.7$ kev

$$ \sigma=(1.48\times10^2/E)\exp[-45.29/E^{\frac{1}{2}}]. \quad (1\text{-c}) $$

These data are not inconsistent if one takes into consideration the experimental uncertainty.[5] The constant A depends upon, among other things, a specific nuclear process and probability whereas the constant B in the simple theory depends only upon the height of the Coulomb barrier. For the d-D reaction the theoretical expression for B is 44.4 in the same units as in the above equations. It is clear that each of the above experiments indicates a value of B which is higher than theory, and, in fact, a closer examination of the data indicates that B is increasing with energy.

In what follows we shall concentrate on the APSST data, try to see what assumptions of the simple WKB theory are no longer valid in the experimental energy range, and by assuming a more realistic model, show that the proper theoretical expression predicts a deviation of B from the value 44.4 indicated by the simple theory. The results of this analysis are not very sensitive to the details of the data so that the variations between the three sets of data do not significantly change the analysis.

One of the consequences of a more realistic theory will be the more accurate determination of the prefactor A from the experimental data. This will lead to a more accurate extrapolation of the cross section to the 1-kev region. Since the experimental data that have been obtained at low energies have an appreciable uncertainty, the following analysis can only be used to indicate qualitatively the size of the deviation from simple theory.

LOW-ENERGY LIMIT

In the simplest theoretical approach to the reaction cross section, one divides the calculation into two parts, the probability that two deuterons impinging on each other will interpenetrate through the Coulomb and

[1] Arnold, Phillips, Sawyer, Stovall, and Tuck, Phys. Rev. **93**, 483 (1954).
[2] Eliot, Roaf, and Shaw, Proc. Roy. Soc. (London) **A216**, 57 (1953).
[3] Davenport, Jeffries, Owen, Price, and Roaf, Proc. Roy. Soc. (London) **A216**, 66 (1953).
[4] K. G. McNeil, Phil. Mag. **378**, 800 (1955).
[5] We shall assume that the branching ratio $(d,p)/(d,n)$ is unity, which is approximately true at these energies. Specific differences between the two modes of disintegration would depend upon a detailed nuclear model.

centrifugal barrier to within a distance R, called the interaction radius; and the probability that, the two having penetrated, a certain reaction will take place. This is basically the compound nucleus approach. It is not believed that the stripping reaction will contribute appreciably at such low energy. The first part, the probability of formation, is strongly energy-dependent for collision energies below the Coulomb barrier. For the collision of two deuterons this barrier height is about 200 kev. This probability of penetration is also dependent on the nuclear forces but to a much smaller extent because of the low energy and the short range of nuclear forces. The second factor, the inherent probability of disintegration in a certain decay mode, depends upon the interparticle forces which exist in the compound system. The complete analysis of this term would require a solution of the Schrödinger equation for the four bodies in interaction. This approach has been attempted by Flügge[6] and by Pruett *et al.*[7] but mathematical difficulties prevent a complete solution. For sufficiently low bombarding energy, this term should not be very sensitive to the kinetic energy and so in what follows it will be treated as a constant factor, independent of the bombarding energy.

Concentrating upon the first element of the cross section, the approach cross section can be calculated either by using the WKB approximation which is valid so long as the bombarding energy is low compared to the barrier height, or it can be calculated using exact Coulomb wave functions in the region external to the interaction radius R connected to wave functions obtained from some nuclear model inside the interaction radius.

Bethe[8] has evaluated the WKB expression for the penetration cross section, which is a quite complicated expression dependent upon the value of the interaction radius as well as upon the bombarding energy. It does not depend explicitly upon the depth of the nuclear potential well inside the range of forces. This complicated expression can be simplified in the low-energy limit.

The d-d approach cross section then takes the form

$$\sigma=(A/E)\exp[-2\pi\eta]=(A/E)\exp[-44.4/E^{\frac{1}{2}}], \quad (2)$$

where

$$\eta=e^2/\hbar v,$$

which was the form chosen by the experimentalists for empirical fit to their data. In this limit, it is assumed that the Coulomb barrier extends all the way to the origin and the nuclear and centrifugal potentials are ignored. Equation (2) represents a quite accurate approximation to the decay of a heavy nucleus by alpha-particle emission since the barrier is very high. But for the interaction of light nuclei where the Coulomb barrier is quite low, this approximation is valid only at extremely low energy.

A comparison of the exponential constant obtained in the limiting theoretical expression above with the empirical constants obtained by the various groups indicates that the drastic simplifications required to obtain Eq. (2) are not entirely justified in the energy range above 13-kev bombarding energy.

If, then, one wishes to describe the correct analytical behavior of the approach cross section in the range of experimental data, one can either choose the more complicated and more exact WKB formula,[8] or one can proceed directly to the Coulomb wave function solutions. We shall follow the second approach, obtaining low-energy approximations to the exact Coulomb solutions.

COULOMB WAVE APPROXIMATION

The procedure in brief is to assume a Coulomb field between the deuterons down to some radius R, and beyond that an attractive nuclear one-body potential. Ostrofsky, Breit, and Johnson[9] have derived the reaction cross section for such a one-body model, assuming small attenuation of the incoming wave which corresponds to small absorption, in terms of the regular and irregular Coulomb functions (unbound solutions of the Schrödinger equation) and the internal wave functions which are solutions of the assumed nuclear potential. A phase shift is needed to match smoothly the wave functions at the boundary R. The cross section has the form

$$\sigma_L=\frac{4\pi PR^3(2L+1)(F_L^2/\rho^2)\langle u_L^2\rangle}{v(1-F_LG_L\delta_L)^2+F_L^4\delta_L^2}, \quad (3)$$

where

$$\langle u_L^2\rangle=\int_0^R w_Lu_L^2dr;\quad \int_0^R w_L(r)dr=1.$$

The F_L and G_L are the regular and irregular Coulomb functions for angular momentum L normalized to be asymptotic to the sine and cosine of the same phase for large r. The u_L are the internal wave functions, solutions of the assumed nuclear potential. δ_L is the phase shift caused by the presence of the nuclear potential and ρ is the dimensionless length, kr. v is the relative velocity of collision and w_L is the relative intrinsic probability of inducing the disintegration in a distance dr around r. This will be taken to be constant, $1/R$. P is a parameter representing the probability of the reaction occurring if the bombarding particle is inside the nuclear boundary. This will, in general, vary with energy and angular momentum, but in what follows it will be assumed to be constant.

Now, following the approach of Johnson and Jones,[10]

[6] S. Flügge, Z. Physik **108**, 545 (1938).
[7] Pruett, Beiduk, and Konopinski, Phys. Rev. **77**, 628 (1950).
[8] H. A. Bethe, Revs. Modern Phys. **9**, 178 (1937).
[9] Ostrofsky, Breit, and Johnson, Phys. Rev. **49**, 22 (1936).
[10] J. L. Johnson and H. M. Jones, Phys. Rev. **93**, 1286 (1954).

this cross section can be expanded about zero bombarding energy if there are no low-lying resonances in the compound system, which seems to be the case for the (d,d) system.[11] In their notation[12] the first two terms of this expansion are as follows:

$$\sigma=\frac{8\pi PH\beta}{9(\mathcal{R}+S\alpha)^2}\left(\frac{2\pi\eta}{e^{2\pi\eta}-1}\right)\times\left\{1+\left(\frac{1}{\eta^2}\right)\left[\frac{M+N\alpha+O\beta}{\mathcal{R}+S\alpha}+\left(\frac{x}{2}\right)^4\frac{\gamma}{\beta}\right]+\cdots\right\}, \quad (4)$$

where $x=(8\rho\eta)^{\frac{1}{2}}$ and H, $\mathcal{R}$, S, M, N, and O are algebraic expressions involving Bessel functions of imaginary argument, defined in reference 10. They are completely determined by the value of R which is chosen. η is the Sommerfeld parameter, $e^2/\hbar v$, and α, β, and γ are parameters defined through an expansion of the logarithmic derivative of the wave function inside the nuclear potential evaluated at R. Their exact definitions are contained in Appendix I.

The first term in the expansion is practically identical with Eq. (2), the extreme low-energy limiting expression. The next term in the expansion includes the effects of the finite values of the nuclear well parameters. This procedure is analogous to the effective-range expansion of the neutron-proton scattering cross section[13] except that the presence of charged particle interactions is complicating. But in analogy to effective-range theory it will be shown that the first two terms of the cross section are not sensitive to the details of the nuclear potential but only to the average range and depth parameters.

Since the expansion is valid at low energy only, the shape of the nuclear potential should not be significant.[14] Therefore a nuclear potential is assumed which has a constant depth, $-U$, out to a radius R and is zero beyond. This potential is certainly not directly related to the basic internucleon potential but is an auxiliary potential which one deuteron experiences when it penetrates to within R of the other deuteron. In other words, it has the same average effect on the penetration process at low energy as does the more nearly correct and much more complicated interaction between all four particles.

Since the parameter P is undetermined in this procedure, it is useful to eliminate it and this can be done by considering the slope of the cross section as a function of energy, specifically $d\ln(\sigma E)/d(E^{-\frac{1}{2}})$. To the same order of approximation as the cross section, this slope has the form

$$\frac{d\ln(\sigma E)}{d(E^{-\frac{1}{2}})}=-2\pi\eta E^{\frac{1}{2}}\times\left\{1+\left(\frac{1}{\pi\eta^3}\right)\left[\frac{M+N\alpha+O\beta}{\mathcal{R}+S\alpha}+\left(\frac{x}{2}\right)^4\frac{\gamma}{\beta}\right]+\cdots\right\}. \quad (5)$$

Note that the first term in this slope, $2\pi\eta E^{\frac{1}{2}}=44.4$, is identical to the constant B which is the slope of the low-energy WKB formula, Eq. (2). Thus, the second term in the expression above is a correction term which will depend on the nuclear force parameters. Our problem is now to decide whether the analytic form of the cross section, Eq. (4), and of the slope, Eq. (5), can be made to account for the behavior of the experimental data.

COMPARISON OF LOS ALAMOS DATA WITH THEORY

If, instead of assuming, as did the Los Alamos group, APSST, that the data can be fit by an empirical equation like Eq. (1), one assumes an empirical equation with the form of Eq. (4), what parameters in the assumed nuclear model could account for the data? Let us assume then that the slope of the cross section can be represented by

$$d\ln(\sigma E)/d(E^{-\frac{1}{2}})=-44.4(1+CE^{\frac{3}{2}}), \quad (6)$$

rather than the constant slope, B, assumed by the experimentalists. The dependence of the correction term to the slope upon energy is suggested by the form of Eq. (5), but it is interesting to note that if the more exact form of the WKB expression[8] were used, the energy dependence would be the same as assumed in Eq. (6). If a least-squares analysis of the (d,p) branch of the APSST data is performed subject to the constraint that the first term in the slope should be the constant $B=44.4$, one obtains the result

$$\ln(\sigma E)=11.586-44.4E^{-\frac{1}{2}}+0.00188E, \quad (7)$$

or, for the slope by differentiation,

$$d\ln(\sigma E)/d(E^{-\frac{1}{2}})=-44.4-0.00376E^{\frac{3}{2}}.$$

These numbers are to be considered as order-of-magnitude estimates only, since the data are not precise enough to validate the number of significant figures used.

Our procedure is to determine what values of the parameters of the theoretical slope, Eq. (5), are needed to reproduce the empirical equation, Eq. (7). From this, since the parameters are functions of the assumed nuclear potential, one can find what range and depth a nuclear potential must have to give the observed reaction cross section.

Writing, for the energy-dependent correction to the theoretical slope,

$$t=\frac{M+N\alpha+O\beta}{\mathcal{R}+S\alpha}+\left(\frac{x}{2}\right)^4\frac{\gamma}{\beta},$$

[11] D. D. Phillips (private communication).

[12] $\mathcal{R}$ is used to distinguish the expression from radius R.

[13] R. G. Sachs, *Introduction to Nuclear Theory* (Addison Wesley Press, Cambridge, 1955), Chap. 4.

[14] The effect of rounded edges is not so important for the light nuclei. See D. C. Peaslee, *Annual Review of Nuclear Science* (Annual Reviews Inc., Stanford, 1955), Vol. 5, p. 127.

one has, rewriting Eq. (5),

$$\frac{d\ln(\sigma E)}{d(E^{-\frac{1}{2}})}=-2\pi\eta E^{\frac{1}{2}}\left\{1+\frac{t}{\eta^3\pi}\right\}$$
$$=-44.4\{1+9\times10^{-4}tE^{\frac{3}{2}}\}. \quad (8)$$

Now t can be expressed as a transcendental function of the phase of the wave function evaluated at the radius R in the limit of zero energy. In Appendix I the analytic forms of the parameters are obtained in terms of the nuclear potential parameters. If the correct nuclear potential were known, the phase z of the wave function would be specified uniquely and therefore t would be determined uniquely. However, if one proceeds in the reverse order as one must, a knowledge of t gained from experiment does not specify the range and depth uniquely. Even the range-depth relationship is contained in a multiple-root solution of the transcendental equation. However, it is possible to select the correct root from physical arguments so that a range-depth relationship can be obtained.

A comparison of the empirical relation, Eq. (7), and the theoretical relation, Eq. (8), shows that the potential must be chosen such that $t\cong0.094$. In Fig. 1 a plot is made of t *versus* the phase z of the nuclear wave function at R. In order to simplify the numerical work, a value for $R=7\times10^{-3}$ cm has been chosen. This is customary for the d-D reaction work and is based on some theoretical justification.[7] Now it is seen from the diagram that a root exists in the first quadrant, in the third quadrant, in the fifth, etc. Since the ground state of the system is some 20 Mev below the energy of the compound nucleus, and since the first known excited state is several Mev above the excitation energy, one selects the third-quadrant root as the physically meaningful result. For the chosen value of R, quoted above, this means that the depth of the potential must be about 9 Mev. If a different value of R were chosen, this would change the diagram, Fig. 1, only slightly

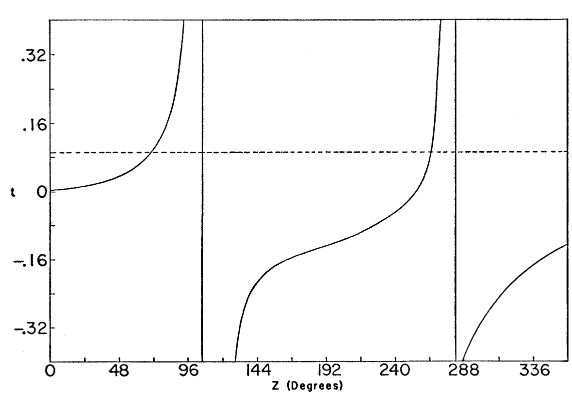

FIG. 1. The slope correction parameter t plotted against the phase z of the wave function at the boundary of the nucleus.

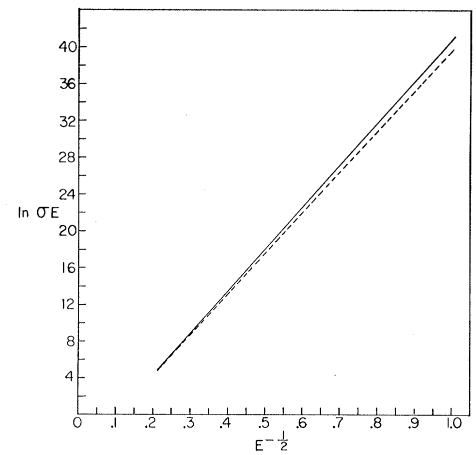

FIG. 2. A comparison of the d-D cross section extrapolated to 1 kev is shown. The solid line represents the direct extrapolation of the Los Alamos empirical equation. The dashed line represents the extrapolation with the theoretically modified equation of this paper. For graphical clarity, the logarithm of σE is plotted *versus* $E^{-\frac{1}{2}}$.

and so the diagram essentially determines a range-depth relationship for the assumed square well shape. This can be written

$$U_0R^2\cong4.4\times10^{-24}\text{ Mev-cm}^2,$$

and can then be used to determine corresponding depths if other values of the range are chosen. Note that small changes in z lead to large changes in the value of t in certain regions, especially near crossing points. This being true, it follows that experimental uncertainties which lead to uncertainties in the value of t will not change significantly the range-depth relationship quoted above. As a matter of fact, if one analyzes the ERS and DJOPR data in the same way as has been done with the APSST data, the value of t is different but this does not require a large change in the nuclear force parameters.

It is well to reiterate that this potential which we have obtained is an auxiliary potential whose average effect on the penetration cross section at low energies is equivalent to the actual interparticle potential. One would certainly not be justified in using this auxiliary potential for a determination of the factor P, the intrinsic probability of decay of the compound nucleus, as this will depend intimately upon the interparticle potential within the radius R.

EXTRAPOLATION TO VERY LOW ENERGY

For certain applications, such as some stellar problems, it is of interest to know the reaction cross section for bombarding energies even lower than the present experimental range. But to do this, using the low-energy limiting cross section, Eq. (2), it is necessary to know the normalization factor A. If our theory leading to Eq. (4) is adequate to describe the energy behavior in the experimental energy range, then the factor P

should turn out to be a constant as we postulated. A comparison of Eq. (4) with the APSST data for all energy values between 13 and 113 kev shows that P is essentially constant for this range with a value of

$$P=6.6\times10^{18}\ \text{sec}^{-1}.$$

If we wish to extrapolate to a lower bombarding energy of about 1 kev, the second term in the expansion of the cross section, Eq. (4), is negligible and the first term is now of the same form as the low-energy limiting equation. Therefore, by inserting the value of P obtained above, it is possible to evaluate the normalization constant A. Therefore, the extrapolated cross section, (d,p) branch, becomes

$$\sigma=(107/E)\exp[-44.4E^{-\frac{1}{2}}].$$

This expression gives a value for the cross section about three times larger than the APSST empirical equation (1−a) for a bombarding energy of 1 kev. (See Fig. 2.)

APPENDIX I

In order to evaluate the correction term to the cross section, Eq. (4), it is necessary to assume some shape dependence for the nuclear potential. We assume a square well of range R and depth U_0. Beyond R the potential is that of a repulsive Coulomb force. The wave function inside R is given by

$$u(r)=\frac{\sin\kappa r}{\sin\kappa R},\quad \frac{\hbar^2\kappa^2}{2\mu}=E+U_0,$$

where we have chosen the normalization so that

$$u(R)=1.$$

The parameters α, β, and γ are defined through the expansion of

$$\rho(u^{-1}du/d\rho)_{r=R}=\alpha+(1/\eta^2)[-\beta/8(x/2)^4]_{E=0}+\cdots,$$
$$2\langle u^2\rangle=\beta+(1/\eta^2)[\gamma(x/2)^4]_{E=0}+\cdots,$$

where $\rho=kr$, $\eta=e^2/\hbar v$, $\hbar^2k^2/2\mu=E$, and $x=(8\rho\eta)^{\frac{1}{2}}$. Now if we let $z=\kappa R$, then as E approaches zero, we have

$$z\rightarrow(2\mu/\hbar^2)^{\frac{1}{2}}(U_0R^2)^{\frac{1}{2}},$$

so as E approaches zero. z, the phase of the wave function, depends on the range-depth relationship of the nuclear potential. Now, by expanding the logarithmic derivative in power of the energy, we obtain the definitions for the three parameters as

$$\alpha=z\cot z|_{E=0},$$
$$\beta=(\csc^2 z-\cot z/z)_{E=0},$$
$$\gamma=(1/8z^2)[\csc^2 z+\cot z/z-2z\cot z\csc^2 z]_{E=0}.$$

Thus the limiting value of z specifies α, β, and γ and in turn the limiting value of z is specified by the product U_0R^2, the range-depth relationship.

Now as shown in the text, a comparison of the theoretical slope, Eq. (8), and the least-squares analysis of the experimental data, Eq. (7), shows that the value of z that we are seeking is such that

$$t\cong9.4\times10^{-2}.$$

From Eq. (8), we can express t as follows:

$$t=\tfrac{1}{6}(x/2)^4\left\{\frac{(\alpha+3\beta-3)+K_3(x)/K_1(x)(1-\alpha)}{(2\alpha-2)+[K_3(x)/K_1(x)-1](x/2)^2}+\frac{6\gamma}{\beta}\right\}.$$

This is a complicated transcendental equation. It is convenient to specify R, solve for z such that t will assume the right value, and then determine the proper value of the depth U_0 for the choice of R. We take the usual choice for R, namely

$$R=7\times10^{-13}\ \text{cm}.$$

Thus we seek a solution to the equation

$$t(z)=0.03933\times\left\{\frac{(\alpha(z)+3\beta(z)-3)+7.2939(1-\alpha(z))}{2\alpha(z)+1.05769}+6\frac{\gamma(z)}{\beta(z)}\right\},$$

In Fig. 1, $t(z)$ is plotted against z. It is clear that there are multiple solutions of z which give the proper value for t. If we consider that z is the phase of the nuclear wave function at the boundary, and that the incident scattering energy is below the first known virtual state of He^4, we are led to select the root in the third quadrant as that which corresponds to the physical situation. This solution, $z=264°$, yields a value for

$$U_0\cong9\ \text{Mev}.$$

This, as we expected, is quite shallow, consistent with the broad range. The product U_0R^2 is the important quantity so that changes in the range would lead to corresponding changes in the depth but would leave the parameters α, β, and γ practically unchanged.

Having determined α, β, and γ by the procedure outlined above, one can then evaluate the theoretical expression for the cross section, Eq. (4), except for the (assumed) constant P, the intrinsic disintegration probability. Comparing the theoretical expression with the experimental cross section, one gets the value for P, 6.6×10^{18} sec^{-1}. It would be of interest to try to evaluate this parameter P in terms of a more realistic nuclear model involving the interactions of nucleons.