Upper Bounds on Scattering Lengths for Compound Systems: n-D Quartet Scattering*†

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In the zero-energy scattering of a particle by a compound system under the conditions that (1) only one exit channel is open (elastic scattering) and (2) no composite bound state exists for the particle and the scattering system in the state of given total angular momentum, the Kohn variational principle gives an upper bound on the scattering length. This is one of several results given previously for the case of scattering by a center of force which may be taken over directly, provided conditions (1) and (2) are satisfied. As a particular application of these results, several previous calculations of the n-D quartet scattering length, A_Q, based on the Kohn principle (the method of Verde and the static approximation of Buckingham and Massey are included) are reanalyzed using the rigorous criterion that the best result is the one giving the lowest value. Further, some calculations of A_Q based on the Rubinow formulation, which do not necessarily provide a bound, are converted to the Kohn form, thereby obtaining, in addition to a bound, an improved approximation to the scattering length. Some limitations and possible extensions of the method are discussed.

I. INTRODUCTION

IN a previous paper,[1] to be referred to in the following as I, it was shown that for the zero energy, zero orbital angular momentum scattering of a particle by a center of force, the Kohn variational principle gives an upper bound on the scattering length provided no bound state of zero orbital angular momentum exists. We now wish to present the appropriate generalization of this result to the case in which the scatterer is a compound system. The knowledge that a variational calculation gives a bound is considerably more useful in the many-body problem where it is more difficult to choose a good trial function. In fact, results obtained from different trial functions may vary over so wide a range that practically no information is gained from the calculations unless one has a reliable criterion to enable one to choose the "best" among a set of results. This point is illustrated by an example given previously for the e^+H problem[2] in which two trial functions, each containing dependence on all the relevant coordinates, and each containing three linear variational parameters gave qualitatively different results, one showing an effective attraction between the positron and hydrogen atom and the other an effective repulsion.

The proof that the Kohn principle gives an upper bound on the scattering length is presented in Sec. II. In its essential points the argument follows rather closely the one given in I for the one-body problem. The proof is valid under the following conditions:

(1) Elastic scattering, including Pauli exchange, is the only process which is allowed on the basis of conservation of energy, angular momentum, parity, and any other conservation law which can be taken to be valid. Since, as will be seen, at zero energy only one exit channel is then open, the zero energy scattering is completely characterized by a single real parameter, the scattering length. (For the present we restrict ourselves to the case for which the scattered particle and the scattering system do not both carry a net charge.)

(2) No composite bound state exists for the particle and scattering system in the state of given total angular momentum, parity, and any other quantum number that can be assumed to be conserved. For example, in the scattering of a spin $\frac{1}{2}$ particle from a system of angular momentum I, where the total angular momentum can take the values $J=J\pm\frac{1}{2}$ ($J=\frac{1}{2}$ for $I=0$), if a composite bound state exists for one of these values of J then the scattering state with that value of J is excluded from our present considerations. The condition that no composite bound state should exist is listed separately even though the existence of a bound state, which in turn implies the possibility of the radiative capture process, is excluded by condition (1). However, both conditions are required if the proof is to be applied in a problem in which the interaction with the radiation field is ignored. This approximation is often made, for example, for the problem of low-energy n-D scattering so that a real scattering length may be defined for each J value. Thus, according to condition (2), the Kohn principle provides a bound on the quartet scattering length; when applied to the doublet case it need not give a bound.

The proof, in Sec. II, is presented in terms of neutron scattering by a nucleus. It is clear, however, that applications can be made in problems of electron or positron scattering by neutral atoms as well. (While Coulomb forces are present in this type of problem the effective interaction between the scattered particle and

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[1] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1033 (1959) (to be referred to as I).

[2] L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1959).

the scattering system falls off sufficiently rapidly so that a phase shift can be defined.) The e^+H calculation referred to earlier is in fact one such application. The fact that the Kohn variational principle gave a bound was justified there[2] on the basis of the Kato method. The desirability of giving a proof which is independent of the Kato method is discussed in I.[3]

In Sec. III the particular case of quartet scattering of neutrons by deuterons is considered. Here we reanalyze some previous variational calculations with the aid of the rigorous criterion that the best result is the one which gives the lowest value for the scattering length. Since the method of Verde[4] as well as that of Buckingham and Massey,[5] who derive an equivalent one-body formulation, can be obtained from the Kohn principle (see Appendix), calculations based on these methods are included in the analysis. Further, we find that results obtained using the Rubinow formulation[6,7] are improved when converted to the Kohn form. This is generally to be expected when, in addition to the conditions under which the Kohn principle gives a bound, the scattering length is positive and the trial function is sufficiently accurate such that third order terms can be neglected[8] (see I).

In Sec. IV some limitations and possible extensions of the method are discussed.

II. GENERAL FORMULATION

We consider the scattering of a neutron from a nucleus of angular momentum I, consisting of Z protons and N neutrons. The total system is assumed to satisfy the properties outlined in Sec. I. To prove that the Kohn variational principle provides an upper bound on the scattering length we begin by deriving the generalization of the Kato identity[9] for this system; this will be done for arbitrary scattering energy. The wave function, Ψ, satisfies the equation

$$-(2\mu/\hbar^2)(T+V-E)\Psi\equiv\Lambda\Psi=0,$$

where T and V are the total kinetic and potential energy operators, respectively. E is the total energy of the system and μ is the reduced mass of one neutron with respect to the rest of the system. The wave function may be represented as

$$\Psi=\sum_i(-1)^i\psi_i, \tag{2.1}$$

where

$$\psi_{Z+N+1}=\psi_{Z+N+1}(1,\cdots,Z;Z+1,\cdots,Z+N,Z+N+1)$$

is taken to be antisymmetric in the coordinates (space and spin) of the Z protons, and in the coordinates of the neutrons labelled by $Z+1$ through $Z+N$. (Here and in the following $\sum_i$ will be understood to represent a summation over the indices $Z+1$ through $Z+N+1$.) The set of functions ψ_i, $Z+1\leq i\leq Z+N$, is defined in terms of ψ_{Z+N+1} by the rule that ψ_i may be obtained from ψ_{i+1} by interchanging the coordinates of neutrons i and $i+1$. While ψ_{Z+N+1} is not uniquely defined by a knowledge of Ψ and by Eq. (2.1) (a function, $\Delta\psi_{Z+N+1}$, may be added to ψ_{Z+N+1} without changing Ψ provided $\sum_i(-1)^i\Delta\psi_i=0$), its asymptotic form is, and that is all that will be relevant for our purposes. Now let

$$F_i=F_i(1,\cdots,Z;Z+1,\cdots,i-1,i+1,\cdots,Z+N+1)$$

be the wave function of the unperturbed nucleus (consisting of all the $N+Z+1$ particles except neutron i) in its ground state, with energy E_g; F_i is normalized to unity. The total energy, E, may be expressed as

$$E=E_g+(\hbar^2/2\mu)k^2,$$

where $\hbar k$ is the relative momentum of the incoming neutron with respect to the nucleus. The asymptotic form of ψ_i will be different for different values of the total angular momentum, J, and its z projection, J_z. For simplicity it will be assumed in the following that $J=J_z=I+\frac{1}{2}$, but the formal results of this section may be readily obtained for the other possible values of J and J_z as well. Thus, with q_i defined as the distance of neutron i from the center of mass of the other $Z+N$ particles, r_{mn} defined as the distance between particles m and n, and $\chi_{ss_z}(i)$ the spin function of neutron i, the asymptotic form of ψ_i, for $Z+1\leq i\leq Z+N+1$, may be written as

$$\psi_i\to D\chi_{\frac{1}{2}\frac{1}{2}}(i)F_i\sin(kq_i+\eta)/[q_i\sin(\eta-\theta)], \quad \text{for} \quad q_i\to\infty,$$

$$\psi_i\to 0, \quad \text{for} \quad r_{mn}\to\infty, \quad m,n\neq i. \tag{2.2}$$

Here η is the phase shift, θ is an arbitrary normalization parameter, and D is an arbitrary parameter to be chosen later for convenience. A trial function, Ψ_t, is now defined, satisfying the same type of boundary conditions as Ψ, with η_t replacing the true phase shift, η. The expression,

$$K=\int\Psi_t^*\Lambda\Psi d\tau-\int\Psi^*\Lambda\Psi_t d\tau,$$

with $\int d\tau$ understood to represent an integration over configuration space as well as a summation over spin indices, may be evaluated in two ways. On the one

[3] The point is that in the present method of proof no connection between the zero energy phase shift and the number of bound states (a generalization of Levinson's theorem) need be assumed. Further, the effects of the Pauli principle are taken into account in a simple way.

[4] M. Verde, Helv. Phys. Acta **22**, 339 (1949).

[5] R. A. Buckingham and H. S. W. Massey, Proc. Roy. Soc. (London) **A179**, 123 (1941).

[6] S. I. Rubinow, Phys. Rev. **98**, 183 (1955).

[7] L. Sartori and S. I. Rubinow, Phys. Rev. **112**, 214 (1958).

[8] More precisely, in order that conversion from the Rubinow to the Kohn form give an improved result it is sufficient that (in the notation of I) A_t be positive and $|(A_t\int u_t\mathfrak{L}u_t d\mathbf{r})|$ be small compared to unity. We note that these conditions may be satisfied even for an inaccurate trial function.

[9] T. Kato, Progr. Theoret. Phys. (Kyoto) **6**, 394 (1951).

hand, since $\Lambda\Psi=0$, we have

$$K=-\int \Psi^*\Lambda\Psi_t d\tau.$$

On the other hand we have

$$K=-(2\mu/\hbar^2)\int (\Psi_t{}^*T\Psi-\Psi^*T\Psi_t)d\tau.$$

This may be simplified by introducing the representation, Eq. (2.1), for Ψ (and the analogous one for Ψ_t) and recognizing that because of the boundary conditions, Eq. (2.2), T is Hermitian when between functions ψ_i and ψ_{jt}, with $i\neq j$ (since then there exists no surface at infinity on which both ψ_i and ψ_{jt} are nonvanishing). We therefore obtain

$$K=-(2\mu/\hbar^2)\sum_i \int (\psi_{it}{}^*T\psi_i-\psi_i{}^*T\psi_{it})d\tau$$

$$=-(2\mu/\hbar^2)(N+1)\int (\psi_{jt}{}^*T\psi_j-\psi_j{}^*T\psi_{jt})d\tau,$$

where j is any one of the $N+1$ indices which label the neutrons. Now T may be written

$$T=-(\hbar^2/2\mu)\nabla_j{}^2+t \qquad (2.3)$$

where t contains no derivatives with respect to q_j ($\nabla_j{}^2$ is the operator with respect to $\mathbf{q}_j$). Therefore, with this form for T, and with the aid of the boundary conditions on ψ_j and ψ_{jt}, we obtain

$$K=(N+1)\int (\psi_{jt}{}^*\nabla_j{}^2\psi_j-\psi_j{}^*\nabla_j{}^2\psi_{jt})d\tau$$

$$=D^2(N+1)[k\cot(\eta-\theta)-k\cot(\eta_t-\theta)].$$

Here use has been made of the fact that F_j is normalized to unity. We choose $D^2=(N+1)^{-1}$, and equate the two forms for K to obtain the identity

$$k\cot(\eta-\theta)=k\cot(\eta_t-\theta)-\int \Psi_t{}^*\Lambda\Psi_t d\tau+\int \Omega^*\Lambda\Omega d\tau, \qquad (2.4)$$

where Ω is defined as

$$\Omega=\Psi_t-\Psi.$$

It now remains to show that for $k=0$, and $\theta>0$, the second order term, $\int\Omega^*\Lambda\Omega d\tau$, is nonpositive. (The specification of $\theta\neq 0$ corresponds to choosing the appropriate generalization of the boundary conditions, Eqs. (2.5), of I.) In analogy with the presentation given in I for the static problem we define

$$\Omega(\lambda)=\Omega\exp(-\lambda\textstyle\sum_i q_i).$$

For $\lambda>0$, $\Omega(\lambda)$ is quadratically integrable. From the fact that no composite bound state exists we conclude that

$$M(\lambda)\equiv\int \Omega^*(\lambda)\Lambda\Omega(\lambda)d\tau<0, \quad \lambda>0.$$

To establish the continuity of $M(\lambda)$ at $\lambda=0$ we examine

$$M(\lambda)-M(0)=\int [\exp(-2\lambda\textstyle\sum_i q_i)-1]\Omega^*\Lambda\Omega d\tau$$

$$+(N+1)\lambda^2\int |\Omega|^2\exp(-2\lambda\textstyle\sum_i q_i)d\tau$$

$$-(N+1)2\lambda\int (q_j\Omega^*)\left[\frac{\partial}{\partial q_j}(q_j\Omega)\right]$$

$$\times\exp\{-2\lambda\textstyle\sum_i q_i\}d\tau/q_j{}^2, \qquad (2.5)$$

where again the index j labels any one of the neutrons. In evaluating the commutator of Λ with each of the factors $\exp(-\lambda q_j)$, to arrive at Eq. (2.5), the representation for T given in Eq. (2.3) has been used. The right-hand side of Eq. (2.5) may be shown to be vanishingly small, in absolute magnitude, in the limit as $\lambda\to 0$. It is useful, in checking this, to recognize that with $\Omega_i=\psi_{it}-\psi_i$, and $\Omega=\sum_i(-1)^i\Omega_i$, we have

$$\int |\Omega|^2\exp(-2\lambda\textstyle\sum_i q_i)d\tau$$

$$=\textstyle\sum_i\int |\Omega_i|^2\exp(-2\lambda\sum_{i'} q_{i'})d\tau+R$$

$$=(N+1)\int |\Omega_j|^2\exp(-2\lambda\textstyle\sum_{i'} q_{i'})d\tau+R,$$

where R is an integral which results from the cross terms and therefore remains finite as $\lambda\to 0$. A similar decomposition may be made for the third integral in Eq. (2.5). The proof then proceeds just as it did in the treatment of the static problem. Here Ω_j satisfies the boundary conditions

$$q_j\Omega_j\to \text{const}\chi_{\frac{1}{2}\frac{1}{2}}(j)F_j, \quad \text{for} \quad q_j\to\infty$$
$$\Omega_j\to 0, \quad \text{for} \quad r_{mn}\to\infty, \quad m,n\neq j.$$

For completeness it is noted that the Rubinow formulation, as applied to quartet n-D scattering,[7] may be derived from the Kato variational principle, which in turn follows from Eq. (2.4) upon dropping the second order term, $\int\Omega^*\Lambda\Omega d\tau$. With $\theta=0$, an inside wave function is introduced and the variationally determined value of the parameter $k\cot\eta_t$ is inserted. Identification with the form given in reference 7 may then be made. This is straightforward and the details are omitted here. We note that the analogous identification has

previously been made by Kato[10] for the case of scattering by a static potential.

III. THE *n-D* QUARTET SCATTERING LENGTH

The experiments on low-energy *n-D* scattering are consistent with the assumption of either of two sets of scattering lengths, for the quartet (A_Q) and doublet (A_D) states, respectively. They are[11]

$$A_Q=6.4\text{f}, \quad A_D=0.7\text{f}; \quad \text{Set I}$$
$$A_Q=2.6\text{f}, \quad A_D=8.3\text{f}; \quad \text{Set II}.$$

Thus a determination of one of the scattering lengths leads to a determination of the other. However, since almost all *n-D* calculations to date have ignored the presence of the tensor force and the repulsive core, such calculations provide more information about the ability of the assumed potentials to represent the true potentials than about the true scattering lengths. (We note that a calculation has been performed recently, by Delves and Brown,[12] in which the tensor force, though not the repulsive core, was taken into account. The authors come to the conclusion that Set II is correct. However, as the authors themselves point out, the theory has been rather severely simplified and it appears to the present authors that their conclusions must remain tentative.) Therefore our main concern here is with the reliability of the calculations for an assumed set of potentials rather than with a determination of which set of scattering lengths is the correct one. Our viewpoint in this regard is the same as that expressed by Sartori and Rubinow.[7] Of course the effects of the tensor force and repulsive core are included to some extent since the strengths of the assumed central potentials are adjusted to match the experimental two-body data. We shall in fact assume in the following that these effective central potentials are sufficiently realistic so that they introduce no spurious composite bound states for H^3 with $J=\frac{3}{2}$. This is almost surely true in all cases of interest. It may well be that the effective central potentials do give reliable results, but from the point of view of the present investigation the point is that one cannot now rigorously prove this. (Though it will not be our present concern, it might be noted that if the correct potential were known, and used in a calculation which provided an upper bound on A_Q, a bound lying below 6.4f would prove that Set II is correct. One could not, in this way, prove that Set I is correct.)

According to the conditions outlined in Sec. I, and the proof given in Sec. II, it follows that a calculation of the quartet scattering length, A_Q, using the Kohn variational principle, will provide an upper bound on A_Q. (We are here ignoring the radiative capture process. As mentioned in Sec. I, the Kohn principle need not lead to a bound on A_D since the *n-D* system can be bound in the doublet state.) Now a sizable number of calculations of A_Q have appeared in the literature. It is then of interest to determine how the methods used are related to the Kohn principle, and to reanalyze the calculations accordingly.

To begin with, we consider some calculations which do not take into account specific polarization. This means that apart from the effect of the Pauli principle the deuteron is assumed to be unperturbed in the scattering process. With χ_Q representing one of the quartet spin functions (all four of which are of course totally symmetric in the spin coordinates) the wave function may be written, in this approximation,

$$\Psi=\chi_Q[\phi(12;3)-\phi(13;2)], \tag{3.1}$$

where

$$\phi(12;3)=2^{-\frac{1}{2}}R(r_{12})f(q_3)/q_3. \tag{3.2}$$

Here $R(r_{12})$ is the exact deuteron wave function and $f(q_3)$ is a function, satisfying the proper boundary conditions, of the position of the scattered neutron with respect to the center of mass of the deuteron. From the assumed form of the wave function, Eqs. (3.1), and (3.2), Buckingham and Massey have defined an effective one-body problem, described by an integro-differential equation[13] which we write symbolically as

$$\mathcal{L}_s f(q_3)=0. \tag{3.3}$$

(The subscript s is used to denote the static approximation.) At zero energy the exact solution of Eq. (3.3) is characterized by a scattering length, A_{Qs}. On the other hand, a function of the form given by Eqs. (3.1) and (3.2) may be used as a trial function in a variational calculation. If the Kohn principle is employed it may be shown (see Appendix) that the approximate scattering length thus determined must be greater than or equal to A_{Qs}, the equality obtaining only if the trial function is constructed using the exact solution of Eq. (3.3). Therefore A_{Qs} represents an upper bound on the true scattering length, A_Q.

While Eq. (3.3) is arrived at by making an approximation in the formalism (i.e., the no polarization approximation) it may now be solved numerically, leading to an exact determination of A_{Qs}. Values of A_{Qs} for the ordinary, Serber, and symmetric force mixtures, and a variety of potential ranges, have been calculated by Burke and Robertson.[14] To check the relative merits

[10] T. Kato, Phys. Rev. **80**, 475 (1950).

[11] D. G. Hurst and J. Alcock, Can. J. Phys. **29**, 36 (1951); Wollan, Shull, and Koehler, Phys. Rev. **83**, 700 (1951).

[12] L. M. Delves and D. Brown, Nuclear Phys. **11**, 432 (1959). We note that an investigation of high energy *n-D* scattering, using the Born approximation, has been performed in which tensor forces were included [B. H. Bransden, Proc. Roy. Soc. (London) **A209**, 380 (1951)].

[13] See Eq. (36) of footnote 5.

[14] P. G. Burke and H. H. Robertson, Proc. Phys. Soc. (London) **70**, 777 (1957). The work here was carried out with potentials of Gaussian radial dependence. For a recent extension to the Yukawa interaction see F. A. Haas and H. H. Robertson, Proc. Phys. Soc. (London) **73**, 160 (1959). See also P. G. Burke and F. A. Haas, Proc. Roy. Soc. (London) **A252**, 177 (1959), where polarization effects are included.

of the Kohn and Hulthén methods, Burke and Robertson performed no polarization variational calculations, using different sets of exponential variational parameters, for several small (but nonzero) values of the scattering energy. (The symmetric force mixture was used.) In all those calculations for which the plot of $k\cot\eta$ *vs* k^2 is very nearly a straight line the extrapolation back to zero energy of the quartet results leads to approximations to the scattering length which we find to lie above A_{Qs}, as they must by the arguments given above. For the one trial function (corresponding, in their notation, to $\nu\approx 0.07\times 10^{26}$ cm^{-2}) which leads to values of $k\cot\eta$ showing the proper energy dependence for both the Hulthén and Kohn methods, the latter provides a better extrapolated result. This is also consistent with our previous statements (see I). The results of the Hulthén, Kohn, and exact calculations are 5.6f, 5.4f, and 5.24f, in that order.

As a further check it is noted that Christian and Gammel[15] have also determined A_{Qs} exactly, for the Serber force, basing their calculation on the variational principle given by Verde.[4] The value[16] differs from the corresponding value obtained by Burke and Robertson by a fraction of a percent (see Table I). Of course exact agreement should not be expected since different deuteron wave functions were used in the two calculations, and since the "exact" solutions of the approximate one-body equations involve the replacement of differential equations by difference equations.

An earlier application of the Verde principle was made by Troesch and Verde,[17] who ignored specific polarization. Their variational results are in agreement with the second set of scattering lengths quoted above. Even if the assumed central potentials do provide accurate compensation for the effects of the tensor force and repulsive core this should still not be taken as evidence that Set II is the correct one. The reason for this is that their variational result for the quartet scattering length lies considerably below the corresponding value of A_{Qs} determined exactly by Burke and Robertson, and we have shown that it cannot lie below. The value obtained by Kohn[18] in a no polarization variational calculation also lies below the exact value. The explanation for these results, the only ones that we have found for which a bound is violated, is very likely the fact that a relatively crude deuteron function, namely a single Gaussian, is used in both the Kohn calculation and that of Troesch and Verde. (Burke and Robertson, and Christian and Gammel use two and three Gaussians, respectively, to represent the deuteron wave function.) That Kohn obtains a reasonably accurate result, in spite of the crudity of his deuteron function, is presumably accidental, as he himself points out. The considerable sensitivity of variational results to the assumed form of the deuteron wave function, even for one consisting of three Gaussians, has been discussed and illustrated by Sartori and Rubinow. On the other hand, as we have already noted, the values of A_{Qs} calculated by Burke and Robertson, and by Christian and Gammel, who used different deuteron functions, are practically identical. It seems possible that the error introduced in using an inaccurate deuteron function is significantly magnified by the inaccuracies in the scattering trial function. (It should be stated that since none of the calculations involve the use of the correct deuteron function, *complete* rigor cannot be claimed for any of the bounds quoted here.)

It was shown in I, for the one-body case, how one could convert results obtained using the Rubinow principle to the Kohn form. No new calculations need be performed provided one knows the values of the integrals A_B, B, and C defined in I. Sartori and Rubinow have generalized the Rubinow formulation from the static case to the three-body problem and applied it to zero energy neutron-deuteron scattering.[7] (This was also done, independently, by Efimov.[19]) They have (by private communication) kindly made available to us the numerical values of the integrals corresponding, in this generalized form, to the expressions A_B, B, and C for some of their calculations using the ordinary (WB) force mixture. The results obtained for the Rubinow form,[20] and Kohn results derived from them, appear in Table I. The rather large difference between the results of the two variational principles, with no specific polarization, indicates that the trial function can be improved, without introducing polarization. This is verified by observing the corresponding value of A_{Qs} (for the ordinary force mixture) obtained by Burke and Robertson.

Sartori and Rubinow also performed calculations using a trial function which allowed for specific polarization. This function, a generalization of the trial function used in the no polarization calculation, contained two free exponential parameters which were chosen to give an extremum. Again, conversion to the Kohn form leads to an improved approximation, as well as a bound on A_Q. While it is true that the Kohn polarization result (column V in Table I) represents an improvement over the Kohn no polarization value for the same potential (column II) this is not a *necessary* consequence of the fact that the Kohn principle is here

[15] R. S. Christian and J. L. Gammel, Phys. Rev. **91**, 100 (1953).
[16] We refer to the result corresponding to Eq. (44′) in reference 15. Actually, two other results are presented for the Serber force; the three values would be identical if the correct deuteron wave function were used. The other two results are not considered here for reasons discussed by Sartori and Rubinow (see footnote 7).
[17] A. Troesch and M. Verde, Helv. Phys. Acta **24**, 39 (1951).
[18] W. Kohn, Phys. Rev. **74**, 1763 (1948).
[19] Y. N. Efimov, J. Exptl. Theoret. Phys. (U.S.S.R.) **35**, 137 (1958) [translation: Soviet Phys. JETP **35**(8), 98 (1959)].
[20] Two variational principles are given in reference 7, which would yield the same results if the correct deuteron wave function were used. Only the results obtained using one of them (referred to in reference 7 as variational principle B) are considered here.

TABLE I. A summary (by no means exhaustive) and an analysis thereof of calculations of the n-D quartet scattering length. In all cases the interparticle potentials were of the form $V_{ij}(r_{ij}) = V_0 \exp(-r_{ij}^2/b^2)[w+mP_{ij}+bQ_{ij}+hP_{ij}Q_{ij}]$, where Q_{ij} and P_{ij} represent spin and space exchange operators, respectively. The symbols WB, S, and SYM stand for ordinary, Serber, and symmetric force mixtures, respectively. The potential range, b, and the scattering lengths are expressed in units of 10^{-13} cm. According to the analysis given in the text the results for a given potential should satisfy the relations II>III>A_Q and V>A_Q. For a sufficiently accurate trial function (see footnote 8) one should also find I>II, and III>IV>V. Here I, II, etc., represent the values which appear in those columns for a particular row. There are values in the literature which do not agree with the first mentioned set of inequalities. We give one example, placed in parentheses. It is assumed that the explanation for this disagreement lies in the fact that deuteron wave functions were used which were not sufficiently accurate.

Potential		No polarization approximation variational principle			Polarization considered variational principle	
		Rubinow	Kohn	"Exact"	Rubinow	Kohn
Type	Range	I	II	III	IV	V
SYM	1.29		5.4[a]	5.24[a]		
S	1.33	7.5[b]	···	5.33,[c] 5.32[a]	6.3[b]	···
WB	1.33	6.9[d]	5.8[e]	5.26[a]	6.5[d]	5.7[e]
WB	1.9		(2.8)[f]	5.9[a]		

[a] Footnote 14. Each of these values represents the result of an extrapolation to zero energy.
[b] Footnote 19. A rearrangement of the data used in obtaining this value would enable one to fill in the dashed portion in the column to the right.
[c] Footnote 15.
[d] Footnote 7.
[e] Calculated by present authors from the data which was used by Sartori and Rubinow in obtaining the number in the column to the left.
[f] Footnote 17.

a minimum principle since a variational determination of the parameters in the trial function, using the Rubinow form, will not generally yield the optimum set (i.e., that which gives a minimum) in the Kohn form. (However, as pointed out in I, conversion from the Rubinow to the Kohn form does give a result which corresponds to the optimum choice of one of the variational parameters, namely the trial scattering length.)

Additional numerical results, based on the present work, have been recorded by Rubinow and Sartori.[21]

IV. DISCUSSION

It is found that the results which are summarized in Section IV of I, presented there in terms of the problem of scattering by a center of force, are valid in the wider class of problems in which the scatterer may be a compound system, provided the conditions which are outlined in Sec. I of the present paper are satisfied. In addition to the n-D quartet system discussed in Sec. III, the results may be applied, for example, to zero energy n-H^3 scattering for both the singlet and triplet states, as well as to n-α scattering. On the other hand, the n-He^3 problem cannot be treated by the present methods. A bound state with $J=0$ (He^4) exists which is sufficient to exclude the singlet scattering state from the present type of treatment. Even if a bound state did not exist, however, the fact that in addition to elastic scattering the reaction $n+He^3 \rightarrow p+H^3$ can take place means that the zero energy scattering *cannot* be completely characterized by a real scattering length, for either the $J=0$ or $J=1$ states.

The method can be extended to take into account the effect of a Coulomb field[22] so that the case of proton scattering from nuclei, as well as electron or positron scattering from atomic ions, or from nuclei, may be included. For example, one could, in this way, study zero energy p-p, p-α, p-He^3 (both spin states), as well as quartet p-D and triplet p-H^3 scattering (provided the radiative capture process is ignored). The doublet p-D and the singlet p-H^3 states would be excluded from the present type of analysis due to the existence of the bound systems, He^3 and He^4, respectively. Note that in the $J=2$ scattering of protons by Li^7, while the reaction $p+Li^7 \rightarrow \alpha+\alpha$ is not excluded on the basis of conservation of energy and angular momentum, it is forbidden by the assumed conservation of parity for strong interactions, leaving only one exit channel open, if we ignore the possibility of gamma emission. (For $J=1$ the reaction $p+Li^7 \rightarrow \alpha+\alpha$ is forbidden by angular momentum conservation.)

In the preceding discussion it has been assumed that the orbital angular momentum, L, of the scattered particle relative to the scattering system is zero before the reaction and that it is zero after the reaction has taken place, i.e., no additional states with higher L values are introduced asymptotically. This is in fact necessary in order that the scattering process may be completely characterized by a single real parameter. It is of course true that if the scattering energy is not zero the above assumption will not be valid in general. The point is that at zero energy, for scattering in which the region of interaction is in effect finite, the long range centrifugal barrier prevents the scattered particle from escaping to infinity in states for which L is not zero. One has a somewhat analogous situation in a low-energy scattering problem, e^- on H, say. In the region of interaction there exist an infinite number of compound states which, however, decay asymptotically; for these states the hydrogen atom is excited so that the scattered electron lacks sufficient energy to escape. Thus the present method is applicable for a system in which tensor forces exist. An explicit proof that at zero energy there is no mixing of states of higher L values (even asymptotically) has been given for the n-p triplet system[23] and, recently, for the more general case of the scattering of one compound system by another.[24]

Other possible extensions of the method would be to the case where the relative orbital angular momentum has some nonzero value in the initial and final states, and to the problem of the scattering of two compound

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systems. However, one of the simplest types of compound-compound scattering problems, *D-D* scattering, may be excluded from consideration immediately, due to the possibility of the reactions $D+D\rightarrow n+\mathrm{He}^3$ and $D+D\rightarrow p+\mathrm{H}^3$. (Further, for $J=0$, the bound system, the alpha particle, exists.) Note that for $J=2$ conservation of angular momentum does not forbid the above reactions; nonzero values of the relative orbital angular momentum are possible in the final states, due to the kinetic energy which is gained in the reaction.

Finally, we wish to point out that in the case where the particle and the scattering system can form a composite bound state, but where no exothermic reactions are possible (again, we ignore the radiative capture process) the present method can be modified so that upper bounds on the scattering length may be obtained. This will be discussed in a future communication.[25]

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APPENDIX

It will now be established that the integro-differential equation used by Massey and his collaborators to describe *n-D* scattering may be derived from the Kohn variational principle. (The discussion is restricted to the quartet state.) The trial function may be written, in the notation of Sec. II,

$$\Psi_t=\psi_{3t}-\psi_{2t},$$

where ψ_{3t} and ψ_{2t} differ by an interchange of the coordinates of neutrons 2 and 3. In the no polarization approximation, ψ_{3t} takes the form

$$\psi_{3t}=(2^{-\frac{1}{2}})\chi_Q R(r_{12})f_t(q_3)/q_3. \tag{A.1}$$

(In the following the subscripts on r and q will be dropped.) Here $f_t(q)$ is a function which satisfies the boundary conditions

$$f_t(0)=0$$

$$f_t(q)\rightarrow \sin kq+\tan\eta_t\cos kq, \quad \text{for} \quad q\rightarrow\infty;$$

$R(r)$ is the spatial part of the deuteron wave function (normalized to unity) and χ_Q is the spin function defined in Sec. III. The Kohn variational principle may be written

$$k\tan\eta\approx k\tan\eta_t+I,$$

where

$$I\equiv\int\Psi_t\Lambda\Psi_t d\tau=2\int\psi_{3t}\Lambda\Psi_t d\tau.$$

With ψ_{3t} of the form given by Eq. (A.1), I becomes

$$\begin{aligned} I&=\sqrt{2}\int[f_t(q)/q]\chi_Q R(r)\Lambda\Psi_t d\tau \\ &=\int_0^\infty f_t(q)\mathfrak{L}_s f_t(q)dq, \end{aligned} \tag{A.2}$$

which defines the operator $\mathfrak{L}_s$.[26] This definition agrees in form with the Massey integro-differential operator.[13] The Kohn principle, in the no polarization approximation, may be written in the equivalent one-body form

$$k\tan\eta\approx k\tan\eta_t+\int_0^\infty f_t(q)\mathfrak{L}_s f_t(q)dq. \tag{A.3}$$

Since the right-hand side of Eq. (A.3) provides, at zero energy, an upper bound on the true scattering length, A_Q, it follows that, in particular, the scattering length, A_{Qs}, obtained from an exact solution of Eq. (3.3), lies above A_Q, as stated in Sec. III. Further it is seen that A_{Qs} represents the best (i.e., lowest) value obtainable from Eq. (A.3). This follows from an application of the theorem proved in Sec. II to the one body problem defined by the operator $\mathfrak{L}_s$. (The fact that the potential is now an integral operator does not affect the validity of the result.) We verify the applicability of the theorem by noting that $\mathfrak{L}_s$ admits no bound state solutions since it is defined on a sub-space of those functions for which the operator, Λ, is defined, and no bound state exists for the latter. It is to be noted that the static approximation is applicable to a wide range of problems, not only the *n-D* case considered here.

We now turn to the relationship between the Verde variational principle (which was developed in terms of the isotopic spin formalism) and the Kohn form, for *n-D* quartet scattering. The equivalence may be established by identifying the wave function Ψ with a linear combination of the functions ψ' and ψ'' defined by Verde.[27] We find that

$$\Psi=c(3^{-\frac{1}{2}}\psi'-\psi'')\chi_Q, \tag{A.4}$$

[25] *Note added in proof.*—The technique for handling the case where bound states exist was developed in conjunction with T. F. O'Malley [Phys. Rev. (to be published)]. The method has been used by the present two authors in an analysis of zero-energy *n-D* doublet scattering [Nuclear Phys. (to be published)]. Efimov[19] obtained a variational estimate of $1.1f$ for the doublet scattering length A_D. It is shown that a conversion of Efimov's data (not all of which appeared in the published article) to the appropriate normalization will provide an upper bound on A_D. To the extent that his assumed potentials are realistic, and to the extent that the inappropriate normalization used will not significantly alter the result, both of which assumptions are not unreasonable, it follows that a value close to $1.1f$ serves as an upper bound on A_D, from which it may be concluded that Set I is the correct set.

[26] $\mathfrak{L}_s$ is not *uniquely* defined by Eq. (A.2) but this is irrelevant for our purposes.

[27] For a comprehensive discussion of the nuclear three-body problem which, in particular, includes an analysis of the symmetry properties of the wave function in the isotopic spin formalism, see M. Verde, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 144.

where c is a constant. As Sartori and Rubinow have already observed, the two coupled differential equations satisfied by ψ' and ψ'' [Eqs. (14) and (15) of reference 4] may be combined to yield the Schrödinger equation for the system, in which the spin and isotopic spin variables have been removed [see Eq. (10) of reference 7]. Verde defines an integral J, involving ψ' and ψ'', which vanishes if the correct functions are used and whose first variation is zero. With the aid of Eq. (A.4) and the symmetry properties of ψ' and ψ'' it may be shown that

$$J=\text{const}\int \Psi\Lambda\Psi d\tau.$$

The normalization used by Troesch and Verde in their application of the Verde principle is equivalent to the choice $\theta=\pi/2$ [see Eq. (2.2)], i.e., it corresponds to that proper to the Kohn principle. The variational parameters were evaluated according to the prescription of Hulthén, i.e.,

$$J=0,$$
$$\partial J/\partial a_i=0, \quad i=1, 2, \cdots, N,$$

where the a_i are the N variational parameters in the trial function, excluding the trial scattering length. As discussed in I, the Kohn method for evaluating the parameters, in a problem in which it provides a bound, is superior to that of Hulthén but the results in the latter case still give an upper bound on the true scattering length.

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Electron Capture Decay of Tm^{168} and Tm^{166}

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The electron capture of Tm^{168} (87 day) to levels in Er^{168} was investigated with permanent magnet spectrographs and coincidence scintillation spectrometers. The following levels in Er^{168} have been established: 79.8(2+), 264.3(4+), 548.9(6+), 822.4(2+), 897.0(3+), 996.2(4+), 1095.1(3− and $T_{\frac{1}{2}}=1.2\times10^{-7}$ sec), and 1543.1(3)− kev. The internal conversion data for Tm^{166} (7.7 hour) suggest levels in Er^{166} at 80.6(2+), 265.1(4+), 545.3(6+), 787.1(2+), 860.6(3+), and 957.2(4+) kev. with many more high lying levels. Energy level schemes are proposed for both Er^{168} and Er^{166}. The levels at 822, 897, and 996 kev in Er^{168} and 787, 861, and 957 kev in Er^{166} may possibly be associated with electric quadrupole (gamma) vibrations. Some general features regarding these vibrational levels are discussed and compared with available data on other even-even nuclei in the rare earth region.

I. INTRODUCTION

PRELIMINARY results of a survey of the radioactivities of neutron deficient rare earth isotopes have been reported previously.[1–5] This paper is concerned with a more detailed study of the energy levels of two even-even nuclei of this region, Er^{168} and Er^{166} which are reached by electron capture of the neutron deficient isotopes Tm^{168} and Tm^{166}, respectively. These nuclei are in the region where the nuclei are strongly deformed and have spheroidal equilibrium shape. According to the unified model[6–8] these are expected to exhibit energy levels which are collective in nature. This study was undertaken to obtain more data on such collective levels.

II. RELEVANT PREDICTIONS OF THE UNIFIED MODEL

The lowest modes of collective excitation of deformed nuclei correspond to rotations in which the nuclear shape remains unchanged. The resulting energy spectrum for a deformed even-even nucleus is given by

$$E_I=(\hbar^2/2\mathcal{I})I(I+1)+BI^2(I+1)^2, \qquad (1)$$

where $I=0, 2, 4\cdots$. The quantity $\mathcal{I}$ represents an effective moment of inertia. The second term in (1) is a correction term due to rotation-vibration interaction.[7] The quantity B is related to the vibrational quanta $\hbar\omega_\beta$ and $\hbar\omega_\gamma$ associated with the so called beta and gamma

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