Nuclear-Structure Calculations in the Continuum—Application to Neutron-Carbon Scattering*

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An explicit method for calculating the scattering matrix from a given structure-model Hamiltonian is presented. The special technique adopted uses nonorthogonal eigenfunctions of the basic model Hamiltonian to represent the scattering wave functions in the interaction region. Application of this approach is mode to neutron scattering by ^{12}C. The weak-coupling particle-rotator model has been used for the positive-parity states of ^{13}C. The results obtained agree closely with the experimental total neutron cross section, both the background and resonant behavior being well reproduced by the theory.

I. INTRODUCTION

IN the paper by Lane and Robson,[1] it was demonstrated that a number of existing reaction theories could be derived from a common starting point. The purpose of this work is to present a method of calculating reaction properties which appears to be practical and which relates directly to nuclear-structure models. The methods used follow the Lane-Robson viewpoint.[2]

The theory to be discussed is of the R-matrix type, but, as indicated, it uses nuclear-structure considerations. A standard R-matrix reaction calculation which uses a model of the nucleus is possible in principle. However, such a calculation is not very practical because of the artificial boundary conditions imposed on the basis functions at the nuclear surface.[3] It would be very useful if basis functions appropriate to a structure calculation could be used in a reaction calculation.

Tobocman *et al.*[4] have given several prescriptions for using nuclear-structure states to calculate scattering cross sections in an R-matrix-type theory. The basic difficulty in the process is that of dealing with nonorthogonal functions, since the states which are used are not orthogonal in the radial coordinate over distances of the order of the nuclear radius.

The method described herein for relating structure states and scattering cross sections is conceptually the same as Tobocman's approach, but employs techniques used effectively by Lane and Robson.[1,2] The derivations and some applications were first presented by Adams.[5] Tests of the method have been made on simple exactly soluble cases[6] and the following conclusions have been reached.

(a) The R matrix defined and used below converges rapidly to the exact R matrix. Typically, four to six radial functions are needed to give essentially perfect agreement between the approximate cross section and the exact.

(b) Resonances and potential scattering are treated quite satisfactorily by the method.

(c) The scattering function within the nucleus is quite accurately represented by a few radial functions; moreover, the approximate function is very reliable at the matching radius and goes smoothly through the matching radius.

(d) The method works as well for higher partial waves as for s waves, and there are no apparent complications caused by the Coulomb force.

The object of this paper is to present the results of an application of the method to a physical case—that of neutron scattering by ^{12}C. The derivation of the basic equations is given in Sec. II. The model of the ^{13}C system which is to be used is discussed in Sec. III. The details of the calculation of the total neutron cross section of ^{12}C and the results are presented in Sec. IV.

II. THEORETICAL FORMULATION OF THE PROBLEM

In the following, only those systems will be of interest which conserve the total angular momentum J, the third component of the total angular momentum M, and the parity π. Hence, the states which are defined below—the basis states, scattering states, and surface functions—will have a definite J, M, and π, even though these additional labels will usually be dropped. The desired elements of the collision matrix are obtained for each J and π separately.

For definiteness, the procedure is presented for elastic and inelastic scattering of neutrons:

$$A+n\rightarrow B^*\rightarrow A+n$$
$$\rightarrow A^*+n'.$$

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The set of basis states $\{\Phi_i,\ i=1, 2, \ldots, N\}$ refer to the bound configurations which are to be used in describing the compound system B. This set might be part of a complete discrete set of states which are orthogonal over all space. The functions ϕ_c are channel or surface functions in the sense of Lane and Thomas[3] and are orthogonal with respect to integration over the intrinsic coordinates and relative angles:

$$(\phi_c \mid \phi_{c'}) = \delta_{cc'}.$$

The main quantity of interest is the scattering-wave function ψ_c which has the asymptotic form (for a given J, M, and π)

$$\psi_c \sim \sum_{c'} (I_c\phi_c\delta_{cc'} + S_{cc'}O_{c'}\phi_{c'}) \tag{1}$$

for separation distances between n and A (or n' and A^*, etc.) greater than the range of the nuclear force. The functions I_c and O_c are unit-flux ingoing and outgoing radial functions. Also included in the sum are the channels which are closed for energy reasons. In this case, the functions $(r\cdot O_c)$ are negative-energy neutron functions which become essentially decaying exponentials at large distances. The matching radius $r=a$ is taken to be that separation distance for which the above asymptotic form holds.

In the interior region where $r<a$ holds, the scattering function is to be expressed in terms of the set $\{\Phi_i\}$. One can start with the assumption that

$$\psi \equiv \psi_c = \sum_i c_i\Phi_i$$

and proceed carefully to evaluate the coefficients c_i.[5,6] Here, however, an alternative method[2] is followed. The equation which ψ satisfies is

$$(H-E)\psi = 0,$$

which, following Lane and Robson,[1] is modified to become

$$[H+\mathfrak{L}(b)-E]\psi = \mathfrak{L}(b)\psi. \tag{2}$$

The operator $\mathfrak{L}(b)$ is defined as

$$\mathfrak{L}(b) = \sum_{c'} \mid \phi_{c'}) \frac{\hbar^2}{2ma}\delta(r-a)\left(\frac{d}{dr}r - b_{c'}\right)(\phi_{c'} \mid, \tag{3}$$

where the constants b_c will be chosen later. From Eq. (2), ψ is obtained formally by operating with $[H+\mathfrak{L}(b)-E]^{-1}$:

$$\psi = [H+\mathfrak{L}(b)-E]^{-1}\mathfrak{L}(b)\psi. \tag{4}$$

There is good reason to believe[2] that the operator $[H+\mathfrak{L}(b)-E]^{-1}$ can be best represented over the region between $r=0$ and $r=a$ in terms of the set $\{\Phi_i,\ i=1, 2, \ldots, N\}$ as

$$[H+\mathfrak{L}(b)-E]^{-1} = \sum_{i,j} \mid \Phi_i\rangle A^{-1}{}_{ij}\langle\Phi_j \mid, \tag{5}$$

where $\mathbf{A}^{-1}$ is the inverse of the matrix $\mathbf{A}$ whose elements are

$$A_{ij} = \langle\Phi_i \mid H+\mathfrak{L}(b)-E \mid \Phi_j\rangle. \tag{6}$$

The integration in this matrix element and in the operator $\langle\Phi_j \mid$ is carried out over the full range of the angular and internal coordinates (represented by parentheses) and over the radial variable slightly beyond the distance $r=a$:

$$\langle\alpha \mid X \mid \beta\rangle = \lim_{\epsilon\to 0}\int_0^{a+\epsilon} r^2dr\,(\alpha \mid X \mid \beta).$$

In this way the delta function in the operator $\mathfrak{L}(b)$ is fully contained within the integration region.

With this representation for the inverse operator occurring in Eq. (4), ψ is given approximately by

$$\psi = \sum_{i,j} \Phi_i A^{-1}{}_{ij}\langle\Phi_j \mid \mathfrak{L}(b) \mid \psi\rangle. \tag{7}$$

The matrix element appearing on the right-hand side can be expanded as

$$\langle\Phi_j \mid \mathfrak{L}(b) \mid \psi\rangle = (\hbar^2a/2m)\sum_{c'}(\Phi_j \mid \phi_c)[(rI_c)'\delta_{cc'} + S_{cc'}(rO_{c'})' - b_{c'}(I_c\delta_{cc'} + S_{cc'}O_{c'})]_{r=a}. \tag{8}$$

A set of equations for the unknown elements $S_{cc'}$ of the collision matrix can be obtained by taking $r=a$ and using the asymptotic form of ψ in Eq. (1). Projecting the result onto the surface function $\phi_{c'}$ gives

$$I_c\delta_{cc'} + S_{cc'}O_{c'} = \sum_{i,j}(\phi_{c'} \mid \Phi_i)A^{-1}{}_{ij}\langle\Phi_j \mid \mathfrak{L}(b) \mid \psi\rangle. \tag{9}$$

Putting the results of Eq. (8) into Eq. (9) gives

$$I_c\delta_{cc'} + S_{cc'}O_{c'} = \sum_{c''} R_{c'c''}[(rI_c)'\delta_{cc''} + S_{cc''}(rO_{c''})' - b_{c''}(I_c\delta_{cc''} + S_{cc''}O_{c''})], \tag{10}$$

where

$$R_{c'c''} = (\hbar^2a/2m)\sum_{i,j}(\phi_{c'} \mid \Phi_i)A^{-1}{}_{ij}(\Phi_j \mid \phi_{c''}), \tag{11}$$

in which all radial functions are evaluated at $r=a$.

It should be noted that the parameters b_c can be chosen in different ways. Lane and Robson[1] have shown that specific choices of these parameters can lead to different theories of the R-matrix type which occur in the literature. Also, the matrix $R_{c'c''}$ is different for different choices of the b_c. In any case, the above set of equations is to be solved simultaneously for the quantities $S_{cc'}$. The number of equations is the same as the number of open and closed channels being considered.

The bound-state problem is done analogously and offers an example of the flexibility in the choice of the parameters b_c. The approach used below follows that of Tobocman and Nagarajan[4] quite closely.

The bound-state eigenfunction ψ has the asumptotic form

$$\psi \sim \sum_c u_c\phi_c$$

for $r\geq a$, where u_c is the appropriately normalized negative-energy radial function corresponding to the

surface function ϕ_c. For bound states, it is convenient to choose the parameters b_c to be

$$b_c=[(ru_c)'/u_c]_{r=a}. \quad (12)$$

With this choice of b_c, one obtains the result

$$\langle\Phi_m \mid \mathfrak{L}(b) \mid \psi\rangle = (\hbar^2 a/2m)\sum_c (\Phi_m \mid \phi_c)[(ru_c)'-b_c u_c]_{r=a}=0. \quad (13)$$

For the situation $r<a$, the bound-state eigenfunction is expressed as a linear combination of the basis functions Φ_n:

$$\psi=\sum_n c_n\Phi_n.$$

Using this expansion together with Eq. (2) satisfied by ψ, and also the result in Eq. (13), gives

$$\langle\Phi_m \mid H+\mathfrak{L}(b)-E \mid \psi\rangle=\sum_n c_n\langle\Phi_m \mid H+\mathfrak{L}(b)-E \mid \Phi_n\rangle = \sum_n c_n A_{mn} = \langle\Phi_m \mid \mathfrak{L}(b) \mid \psi\rangle=0.$$

In order for this equation to be satisfied with nonzero coefficients, c_n the determinant of the matrix $\mathbf{A}$ must vanish. Hence, the equation which determines the eigenvalue $E=E_i$ corresponding to the eigenfunction $\psi=\psi_i$ is

$$\det(\mathbf{A})=0. \quad (14)$$

This method of getting eigenvalues was applied to neutrons in a cutoff harmonic-oscillator well by Adams.[5] He also solved for the expansion coefficients c_n and the logarithmic derivative of the eigenfunction ψ. The eigenvalues were found to be reliably given by using only three or four basis functions. The logarithmic derivative of ψ was found to approach the correct logarithmic derivative at the matching radius as the number of basis functions increased.

Note that the above results are unaffected by a unitary transformation of the basis functions. The R-matrix elements $R_{c'c''}$ and the determinant condition for bound states are unchanged by such a transformation.

III. APPLICATION TO NEUTRONS ON ^{12}C

The method described above has been applied to the calculation of the total neutron cross section of ^{12}C at energies up to $E=5$ MeV in the c.m. system.

The model to be used in the calculation can best be discussed in connection with Fig. 1. In the top part of the figure, the total neutron cross section is shown up to $E=5$ MeV. Below this curve and on the same scale, the energy levels of ^{13}C are shown. It is clear that the structure in the region shown is dominated by positive-parity states. Also, the background is undoubtedly s wave for the most part and

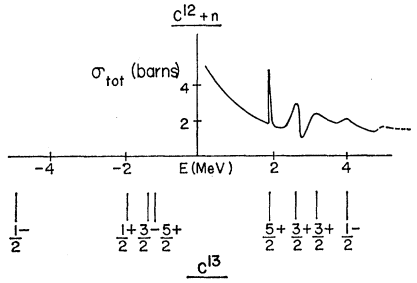

FIG. 1. Neutron cross section on ^{12}C and the ^{13}C spectrum. The energy scale applies to both parts of the figure. The results contained here are used to motivate the model used in the calculation.

therefore of positive parity. Note also the two positive-parity states at negative energies. It will be assumed that positive-parity states alone are sufficient to describe the cross section. This ignores the negative-parity states near the region of interest and the p-wave contribution to the background which comes in slowly with increasing energy.

The model of the positive-parity states of ^{13}C is the familiar one of a neutron weakly coupled to a deformed axially symmetric ^{12}C core.[7,8] The basis functions used for describing this bound system—and also used for the scattering system below—are constructed from the eigenfunctions of

$$H_0=H(^{12}\mathrm{C})+H_{\mathrm{sp}}.$$

Here $H(^{12}\mathrm{C})$ is the kinetic-energy operator of a rigid rotator which has eigenfunctions $N_{I_0}D_{M_0}{}^{I_0}{}_O$ for an axially symmetric rotator and eigenvalues proportional to $I_0(I_0+1)$. It is assumed for convenience that only the 0^+ and 2^+ states of ^{12}C are important and that these two states are at 0.0 and 4.43 MeV, respectively.

The operator H_{sp} is meant to be the energy operator of a single neutron in a spherically symmetric harmonic-oscillator potential. This operator is taken to have the form

$$H_{\mathrm{sp}}=T_{\mathrm{sp}}+\tfrac{1}{2}m\omega^2r^2+Cl(l+1)+D\mathbf{l}\cdot\mathbf{s}+V_0. \quad (15)$$

The third and fourth terms here are familiar and serve as a simple way of removing degeneracies between different values of l and $j=\pm\frac{1}{2}$. The last term is essentially a well-depth parameter which will be fixed by requiring that the bound states have the correct binding energies—all energies are measured from the ^{12}C$+n$ separation energy as indicated in Fig. 1.

The eigenfunctions of H_{sp} are

$$U_{jmln}=R_{nji}(r)[i^l Y_l\otimes\chi_{1/2}]_m{}^j = R_{nji}(r)\mathcal{Y}_m{}^{(l\frac{1}{2})j}, \quad (16)$$

[7] D. Kurath and R. D. Lawson, Nucl. Phys. **23**, 5 (1961).
[8] P. J. A. Buttle, Phys. Rev. **160**, 719 (1967).

where n and l are allowed to have the values

$$l=0, 2, 4, \ldots,$$
$$n=2, 3, 4, \ldots \quad \text{for} \quad l=0,$$
$$n=1, 2, 3, \ldots \quad \text{for} \quad l\neq 0.$$

Then $n=1$, $l=0$ function is eliminated as an approximate attempt to allow for the exclusion principle. The odd-l values are eliminated in accordance with the assumption of allowing for positive-parity states only. In the calculation to be described below, l values through $l=4$ were used and for each l value, up to six radial functions were used.

The eigenfunctions of H_0 are obtained by vector coupling the rotator and single-particle functions, i.e.,

$$\Phi_{I_0 j l n}{}^{JM}=N_{I_0}[D^{I_0}\otimes U_j]_M{}^J. \tag{17}$$

It is convenient to separate the radial function R_{njl} from the single-particle spin-angle coordinates and the core coordinates and to relabel the basis states as follows (dropping the labels J and M):

$$\Phi_i=\phi_c R_{ci}.$$

For example, the following channels exist within the model for $J^\pi=\frac{1}{2}^+$ states (I_0 is the core spin, l and j are the single-particle orbital and total angular momenta):

$$A: \quad I_0=0, \quad l=0, \quad j=\tfrac{1}{2};$$
$$B: \quad I_0=2, \quad l=2, \quad j=\tfrac{3}{2};$$
$$C: \quad I_0=2, \quad l=2, \quad j=\tfrac{5}{2}.$$

Channel A is open at all energies, while channels B and C are closed for energies less 4.43 MeV. The basis functions can be written and labeled as

$$\Phi_i(i=1, 4, 7, \cdots)=N_0[D^0\otimes \mathcal{Y}^{(0\,\frac{1}{2})\frac{1}{2}}]_m{}^{1/2}R_{n\frac{1}{2}0}, \quad (n=2, 3, 4, \ldots)$$

$$\Phi_i(i=2, 5, 8, \cdots)=N_2[D^2\otimes \mathcal{Y}^{(2\,\frac{1}{2})\frac{3}{2}}]_m{}^{1/2}R_{n\frac{3}{2}2}, \quad (n=1, 2, 3, \ldots)$$

$$\Phi_i(i=3, 6, 9, \cdots)=N_2[D^2\otimes \mathcal{Y}^{(2\,\frac{1}{2})\frac{5}{2}}]_m{}^{1/2}R_{n\frac{5}{2}2}, \quad (n=1, 2, 3, \ldots).$$

The quantities in front of the radial functions are the vector-coupled core and single-particle functions. These are the channel or surface functions ϕ_c with c corresponding to the A, B, and C channels above.

For $J=\frac{3}{2}$ and $\frac{5}{2}$, there are five and six surface functions, respectively, and l has the values 0, 2, and 4.

As indicated above, the interaction which couples the rotational states of the ^{12}C core and the single-neutron states is taken to be that due to the deformed part of the harmonic-oscillator well. The deformation is assumed to be weak, axially symmetric and, prolate; the coupling interaction is

$$H_I=|\beta|\, m\omega^2 r^2 Y_2{}^0(\theta', \phi'). \tag{18}$$

The primes indicate that the angles are measured in the body system. The deformation parameter β is negative and presumed small.

If the ^{13}C system were taken to be a completely bound system at all energies, the eigenvalues and eigenfunctions would be found by computing the matrix elements (using the set Φ_i) of

$$H(^{13}\mathrm{C})=H_0+H_I=H(^{12}\mathrm{C})+H_{\mathrm{sp}}+H_I \tag{19}$$

and diagonalizing the resulting matrix. The ^{13}C system is not bound for all energies, however, and this fact should be accounted for.

To include the fact that the neutron channel is open at energies greater than zero, it must be recognized that the force binding the neutron to the ^{12}C core is of finite range, and a reaction Hamiltonian must be accordingly constructed. Since this study is meant more to emphasize a particular calculational method for reactions than to be a serious study of the structure of ^{13}C, the following simple assumption is made for the reaction Hamiltonian:

$$H(\text{reaction})=H(^{13}\mathrm{C}) \quad \text{for} \quad r<a$$
$$=H(^{12}\mathrm{C})+T_{\mathrm{sp}} \quad \text{for} \quad r>a. \tag{20}$$

The radius $r=a$ beyond which the nuclear interaction between the ^{12}C core and the neutron vanishes is a parameter of this reaction model, but it clearly has a fairly definite physical meaning and its numerical value is known approximately from other studies such as optical-model analyses.

In order to use directly the results of Sec. II, the states Φ_i and ϕ_c of this section are identified with the basis vectors and surface functions of Sec. II. The quantities in parentheses in Eq. (11) are the radial harmonic-oscillator function at $r=a$:

$$(\phi_c\,|\,\Phi_i)=R_{ci}(a). \tag{21}$$

One might be tempted to diagonalize $H(^{13}\mathrm{C})$ over all space and use the new basis states instead of the Φ_i used here. However, as noted at the end of Sec. II, the results which are of interest here are unchanged by such a transformation.

The set of boundary parameters b_c are chosen to be zero in determining the scattering matrix;

$$b_c=0.$$

This choice of values for b_c corresponds to the choice of boundary condition $(r\Psi)'=0$ sometimes used to define the basis functions in the Wigner-Eisenbud R-matrix theory.

The matrix elements A_{ij} can be written out as

$$A_{ij}=\langle\Phi_i \mid H+\mathfrak{L}(0)-E \mid \Phi_j\rangle$$
$$=(E_i^0-E)\langle\Phi_i \mid \Phi_j\rangle+\langle\Phi_i \mid H_I \mid \Phi_j\rangle$$
$$+\langle\Phi_i \mid \mathfrak{L}(0) \mid \Phi_j\rangle. \quad (22)$$

The quantities in angular brackets occurring here are simply evaluated:

$$\langle\Phi_i \mid \Phi_j\rangle=\delta_{cc'}\int_0^a r^2dr\, R_{ci}R_{c'j}, \quad (23a)$$

$$\langle\Phi_i \mid H_I \mid \Phi_j\rangle=\mid\beta\mid m\omega^2(\phi_c \mid Y_2^0 \mid \phi_{c'})$$
$$\times\int_0^a r^2dr\, R_{ci}r^2R_{c'j}, \quad (23b)$$

$$\langle\Phi_i \mid \mathfrak{L}(0) \mid \Phi_j\rangle=(\hbar^2a/2m)\delta_{cc'}[R_{ci}(rR_{c'j})']_{r=a}. \quad (23c)$$

Standard techniques can be used to evaluate the angle matrix element occurring in Eq. (23b). The radial integrals are done numerically. Only a finite number N of basis states Φ_i will be used in practice. The matrix **A**, whose elements are given above, is real, symmetric, and of order N. Standard matrix-inversion techniques are used to obtain $\mathbf{A}^{-1}$. Once $\mathbf{A}^{-1}$ is obtained, $R_{c'c''}$ is calculated from Eq. (11), and the elements of the collision matrix are found by appropriately solving the set of equations in Eq. (10). The quantity of interest here is the total neutron cross section, which involves only certain diagonal elements $S_{cc'}$. For the special case of $^{12}C+n$, the maximum number of channels of a given angular momentum and parity is six. In this work, the necessary diagonal elements of the collision matrix were found by using Cramer's rule, the determinants being at most 6×6 in size.

The problem of alignment of the $H(^{13}C)$ energy scale and the H (reaction) energy scale is still to be faced. Saying the same thing in another way, the parameter V_0 in the single-particle Hamiltonian in Eq. (15) must be determined.

One alternative is to let the joining radius $r=a$ go to infinity and then to diagonalize the matrix of $H(^{13}C)$. The value of V_0 could then be found which aligns an appropriate one of the eigenvalues thus obtained with a corresponding negative-energy state in the observed spectrum of ^{13}C. However, this approach uses a different model for the bound states from the model used for the scattering states.

A more consistent approach is to follow the procedure for bound states given in Sec. II and equate a bound state obtained by this method with the known physical state to obtain a value for V_0. The procedure used here is to assume first that both the $\frac{1}{2}^+$ state of ^{13}C at -1.86 MeV and the $\frac{5}{2}^+$ state at -1.10 MeV are adequately described by the model. The boundary-condition parameters b_c are then calculated from Eq. (12) using the experimental binding energies. (These parameters are different for different choices of the radius $r=a$.) Then, a search is made for the value of V_0 for which the determinant of **A** vanishes. Because of the different angular momenta involved, the two determinations of V_0 from the two states are independent. Not surprisingly, it was necessary to adjust the radius $r=a$ somewhat in order to get the two values to agree. It should be noted that any changes in the other parameters such as C and D of Eq. (15) make a redetermination of V_0 necessary. Also, it should be noted that changes in the radius $r=a$ constitute changes in the reaction model and do not represent a dependence of the reaction theory on this radius. As indicated in the Introduction, experience with simple models shows that changing the matching radius while holding the model fixed only weakly affects the rate of convergence.

IV. CALCULATIONS AND RESULTS

Initial values of the parameters used in the scattering-cross-section calculation were obtained by structure considerations of ^{13}C.

The structure calculation which was most closely followed is the weak-coupling calculation for mass-13 nuclei done by Kurath and Lawson.[7] Their calculation was repeated for orientation purposes and as a check on the matrix elements involved. As in their work, the eigenvalues of the uncoupled Hamiltonian H_0 [and therefore the values of C and D in Eq. (15)] were fixed by requiring that the splitting between the $1d_{5/2}$ and the $1d_{3/2}$ levels is 5.0 MeV, and between the $2s_{1/2}$ and $1d_{5/2}$ levels is 0.30 MeV. Actually, these authors were less explicit than the model described in Sec. III in the radial dependence occurring in H_I and in the form of the radial single-particle functions. They simply replaced all radial integrals by a constant.

The model described in Sec. III uses an explicit r^2 dependence in H_I and includes a number of harmonic-oscillator radial functions. As expected, a repeat of the Kurath-Lawson work with these changes makes little difference in the lower eigenvalues when the coupling strength β is small in magnitude.

A value of $\hbar\omega=15$ MeV has been used in this calculation. This value is considered to be a reasonable compromise between the usual prescription of $\hbar\omega\approx 41/A^{1/3}\approx17$ MeV and a value of about 8 MeV, which corresponds to the value of the harmonic-oscillator parameter given by Kurath and Lawson.

The deformation parameter β can be obtained from the optimum value of the coupling parameter given by Kurath and Lawson and the above value of $\hbar\omega$. The value $\mid\beta\mid=0.15$ is obtained in this way.

To complete the determination of the parameters, the bound $\frac{1}{2}^+$ and $\frac{5}{2}^+$ states are required to have the observed negative energies, and Eq. (14) was required to be approximately satisfied for each case. In this way it was determined that the matching radius $r=a=5.7$ F and the well depth $V_0=-53$ MeV.

TABLE I. Values of the parameters used in the calculation of the total neutron cross section.

	C (MeV)	D (MeV)	V_0 (MeV)	a (F)	$\lvert\beta\rvert$
Set 1	0.38	−2.0	−53	5.7	0.15
Set 2	0.28	−2.5	−49	5.0	0.45

Calculation of the cross section can now be carried out *with no further undetermined parameters*. The order of the approximation depends on the number of basis functions being used. From Eq. (17) and the discussion following it, it is established that the number of basis functions depends on the number of surface functions or channels, which is fixed for each J value, and on the number of radial functions being used with each channel. It is convenient to keep the number N_r of radial functions the same for each channel and for each J value and to use this number as a measure of the order of approximation. The angular momentum states used were $J=\frac{1}{2}, \frac{3}{2}$, and $\frac{5}{2}$ (and, as indicated above, only positive parities were considered). With the ^{12}C model discussed earlier, only $l=0$, 2, and 4 partial waves are involved.

For each angular momentum, the matrix **A**, whose elements are given by Eqs. (22) and (23), is computed and numerically inverted. The R-matrix elements $R_{c'c''}$ are then obtained from Eqs. (11) and (21), and the desired elements of the collision matrix are obtained from the set of equations in Eq. (10).

An approximation to the total neutron cross section is given by

$$\sigma=(\pi/k_0^2)[2\times\mathrm{Re}(1-S_{00}^{+\frac{1}{2}})+4\times\mathrm{Re}(1-S_{00}^{\frac{3}{2}+})+6\times\mathrm{Re}(1-S_{00}^{\frac{1}{2}+})],$$

where S_{00}^{J+} is the collision-matrix element corresponding to the target and residual nuclei being in the

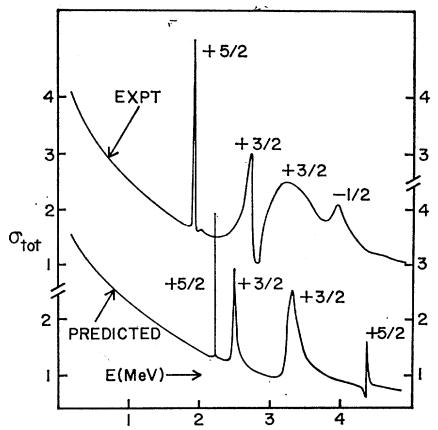

FIG. 2. Neutron cross section on ^{12}C. The upper curve and scale show the experimental total neutron cross section. The lower curve and scale show the results obtained by calculation using the first set of parameters in Table I.

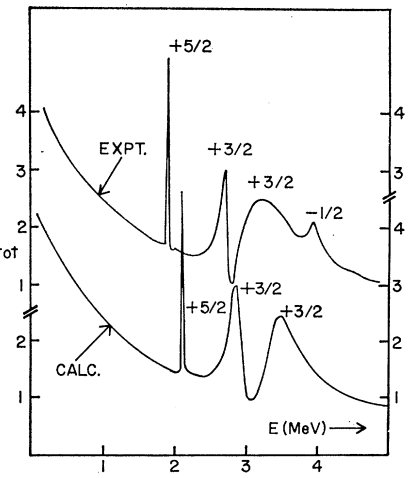

FIG. 3. Neutron cross section on ^{12}C. Same as in Fig. 2 except that the second set of parameters in Table I is used.

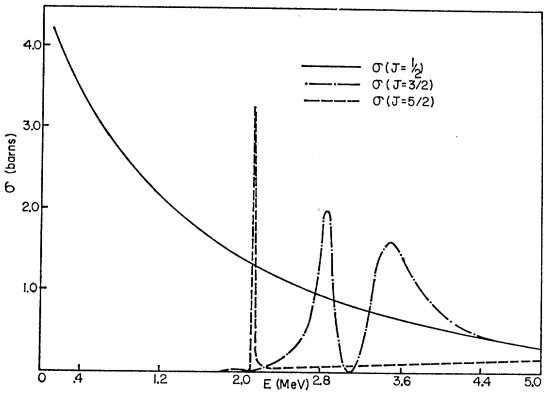

FIG. 4. Partial cross sections. The sum of the three curves add up to the lower curve of Fig. 3.

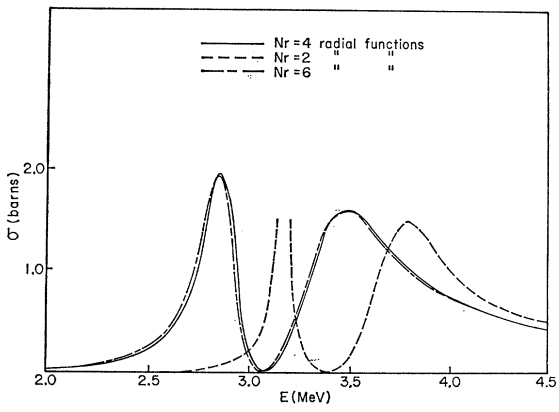

FIG. 5. Convergence of calculated cross section. The position and widths of the resonances change some when N_r is increased from 2 to 4, but change very little when N_r is increased from 4 to 6.

ground state. For example, for the $J=\frac{1}{2}$ case discussed earlier, the A channel there is the channel here labeled O. Also, k_0 is the wave number of the incident neutrons, and the notation Re means that the real part of the quantity in parentheses is to be taken.

The results of a calculation of σ using the first set of parameters summarized in Table I is shown in Fig. 2 along with the experimentally determined total neutron cross section. The two curves have been drawn separately with separate scales for clarity. The calculation has $N_r=4$ radial functions per channel (i.e., there are 3×4 basis functions for $J=\frac{1}{2}$, 5×4 basis functions for $J=\frac{3}{2}$, and 6×4 basis functions for $J=\frac{5}{2}$). The over-all calculated results are qualitatively correct. However, there is an unseen $\frac{5}{2}^+$ resonance predicted at about $E=4$ MeV, and the widths are much too small. Calculations done allowing N_r to increase show that the results given in Fig. 2 are essentially the converged cross section. (An example is shown below.)

In order to increase the widths of calculated resonances, the deformation parameter was increased in magnitude. This change made necessary some adjustments of the other parameters in order to preserve the observed ordering and spacing of the resonances and maintain the positions of the bound states. While no extensive parameter search was attempted, the second set of parameters given in Table I was found to give the results shown in Fig. 3. Here again, the results are essentially the converged results obtained using $N_r=4$ radial functions per channel. The improvement is very noticeable, and the results are quite acceptable both in magnitude and structure, considering the crudeness of the reaction model. The fact that the calculated background becomes somewhat low at higher energies is probably due to the neglect of the p-wave contribution to the cross section.

The contributions of each angular momentum to the total cross section are shown in Fig. 4. As in Fig. 3, $N_r=4$ radial functions per channel were used.

The process of convergence is shown for the $J=\frac{3}{2}$ cross section in Fig. 5. It is clear that even for $N_r=2$ radial functions, the results are quite reasonable and that going beyond $N_r=4$ to $N_r=6$ has very little effect on the results.

V. CONCLUSIONS

It should perhaps be repeated that the calculation just described is meant to serve as an introduction to and an application of a particular method of calculating properties of a reaction. It is quite conceivable that improvements in the model would lead to improved results. Particularly, the restriction to positive-parity states is a rather unsatisfactory one, as is also the truncation of target states to just the 0^+ and 2^+ states.

The main conclusion which can be drawn is that it is possible to start with a physical structure model and use the basis functions appropriate to that model and proceed in a straightforward way to obtain integrated cross sections. Since the elements of the collision matrix are obtained, there appears to be no reason why differential cross sections, polarizations, etc., could not also be obtained.

The results of this more physical test case are consistent with the simpler cases referred to in the Introduction, in that a relatively small number of radial functions are sufficient to insure that convergence has taken place.

Finally, it should be emphasized that the present calculations do not require the introduction of an optical potential or the inclusion of distant levels.[8] This appears to be an advantageous feature of using nonorthogonal basis functions.

Lovas[9] has done a somewhat similar calculation to the one just discussed. He also calculated the total neutron cross section of ^{12}C, but he used both a different structure model and a different reaction theory. Hence comparisons between the two sets of results are not very meaningful.

ACKNOWLEDGMENTS

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[9] I. Lovas, Nucl. Phys. **81**, 353 (1966).