

Totally microscopic description of n - ^{16}O elastic scattering

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An optical potential appropriate to elastic scattering of neutrons by oxygen is calculated with the starting point being the basic nucleon-nucleon interaction. A soft core force is employed so that matrix elements are finite and perturbation expansions are (apparently) convergent. All terms up to second order in the interaction are retained including correlation effects previously ignored. The calculations are carried out in a space large enough to minimize truncation effects. The resulting nonlocal energy dependent complex optical potential is used to calculate low energy s -wave phase shifts. These are compared with the results generated by an empirically fitted optical potential and with the results of previous calculations. The scattering length and effective range parameter are also calculated. Given the nature of the calculation, the results are quite encouraging.

[NUCLEAR REACTIONS n - ^{16}O , optical potential, approximate many-body scattering theory.]

I. INTRODUCTION

The problem of describing the scattering of a nucleon from a nucleus is one of the central problems in nuclear physics. Although there has been much effort and progress in the formulations and solution of models to describe the process, little progress has been made towards a complete *ab initio* description. This is not to say that there have not been advances made in the formal solution of the problem. Watson¹ more than 20 years ago showed how an optical potential, which describes nucleon-nucleus scattering, could be derived from the nucleon-nucleon interaction. The derivation begins with the construction of the two-body t matrix, or scattering operator, and the result, before approximations, is a set of coupled integral equations which can be treated in a number of ways.² Various perturbation expansions and different groupings of the different types of terms occurring in the infinite series have been developed which emphasize different aspects of the complicated process. Although these schemes are formally elegant, they do not permit one to proceed simply from the nucleon-nucleon force to an optical potential without numerous approximations. Not the least of the difficulties involves an adequate description of the target nucleus. The hard core nature of the two-body interaction also leads to considerable technical difficulties.

As a consequence of these difficulties many

model calculations have been performed which contain drastic, simplifying assumptions. One approach consists of using an effective interaction, fitted to bound state properties with a single determinantal wave function, for the scattering calculation.³ It is then asserted that because certain complexities have been incorporated into the force, only the lowest order terms in the optical potential expansion are sensible. Many other phenomenological models have been employed, such as using an effective local potential folded with an experimental density.⁴ In another model the nucleons are considered to form an inert core, as in the shell model, except for one active particle. The core, active particle and projectile are then treated as a three-body system.⁵

The approach taken here is to begin with a "realistic" potential, whose matrix elements in some convenient basis are all finite, and face the full complexity of the formal expansion of the optical potential. A similar approach has previously been taken by MacKellar *et al.* and by Sinha⁶ utilizing rather extreme approximations. Here every effort will be made to limit the approximations to the necessary truncation of the infinite perturbative series.

In the following section, the formulation of the scattering problem developed by Villars⁷ will be reviewed. Here complete antisymmetrization is retained throughout. The expansion for the optical potential in terms of the two body interaction will

be obtained and the terms evaluated, including all second order contributions, in the harmonic oscillator representation. The angular momentum algebra will then be performed for the special case of neutron scattering from a doubly closed shell nucleus ^{16}O and the method used for the numerical computation of the matrix elements of the optical potential summarized. Finally, the phase shifts resulting from this complex, non-local, energy dependent potential will be compared with those obtained from a phenomenological potential whose parameters have been fitted to the data and to the results of other calculations.

This comparison, for s-wave scattering, is sufficiently encouraging to warrant an extension to higher partial waves and heavier nuclei. These calculations are in progress.

II. VILLARS FORMULATION

In the second quantized representation the Hamiltonian is

$$H = \sum_{ij} \langle i | t | j \rangle a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle a_i^\dagger a_j^\dagger a_l a_k, \quad (1)$$

where t is the one-body, kinetic energy operator and V is the two-body nucleon-nucleon interaction. The states i, j are completely arbitrary and the creation and destruction operators a are defined relative to the true vacuum. Assuming that the nucleon-nucleon potential chosen does not have a hard core, one may carry out a Hartree-Fock calculation, thus determining a discrete set of single particle states, ϕ_λ , and energies ϵ_λ . The Schrödinger equation can be solved with the resulting Hartree-Fock potential, thus generating a set of continuum wave functions which, together with the bound ϕ_λ , form a complete set. The operators which create (or destroy) these states will be designated by $a^\dagger(k^*)$ [or $a(k^*)$], the k^* indicating a solution with out-going boundary conditions and energy $\hbar^2 k^2 / 2m = \epsilon_{k^*}$.

It is then convenient to use, as the vacuum, the Hartree-Fock determinant and define creation (and destruction) operators relative to this vacuum. We then define

$$b_\alpha^\dagger = a_\alpha \text{ for } \epsilon_\alpha < \epsilon_{\text{FERMI}}$$

and

$$b_\alpha^\dagger = a_\alpha^\dagger \text{ for } \epsilon_\alpha > \epsilon_{\text{FERMI}}.$$

Using the usual "dot" notation to represent normal products in terms of the b 's we then have

$$H = E_{\text{HF}} + \sum_\alpha \epsilon_\alpha : a_\alpha^\dagger a_\alpha : + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle : a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma :. \quad (3)$$

Here

$$E_{\text{HF}} = \sum_\lambda \langle \lambda | t | \lambda \rangle + \frac{1}{2} \sum_{\lambda\mu} \langle \lambda\mu | V_A | \lambda\mu \rangle, \quad (4)$$

$$\epsilon_\alpha = \langle \alpha | t | \alpha \rangle + \sum_\lambda \langle \alpha\lambda | V_A | \alpha\lambda \rangle$$

with the sums restricted to occupied levels.

The following notation is then introduced: $|N_A\rangle$ represents the bound states of the A -particle system. They are exact solutions of the total Hamiltonian H and satisfy

$$H |N_A\rangle = E_{N_A} |N_A\rangle \quad (5)$$

with N_A being the appropriate set of quantum numbers. We can obtain a state which, in addition to the A , bound particles contains a particle in a scattering state (from the Hartree-Fock potential), with outgoing (or incoming) boundary conditions:

$$a^\dagger(k^*) |N_A\rangle \text{ or } a^\dagger(k^-) |N_A\rangle. \quad (6)$$

Such states should be distinguished from the true scattering states which will be designated by $|N_A, k^{(*)}\rangle$. These contain, in addition to the incoming wave incident on the target, an outgoing scattered wave. They are solutions to the full H with

$$(H - E_{N_A} - \epsilon_k) |N_A, k^{(*)}\rangle = 0. \quad (7)$$

In order to express these states in terms of the states $|N_A\rangle$ the operators J are introduced:

$$[H, a^\dagger(k^*)] = \epsilon_k a^\dagger(k^*) + J^\dagger(k^*), \quad (8)$$

$$[H, a(k^*)] = -\epsilon_k a(k^*) - J(k^*)$$

so that

$$J^\dagger(k^*) = \sum_{\alpha\beta\gamma} \langle \beta | V_A | k^* \delta \rangle : a_\alpha^\dagger a_\beta^\dagger a_\gamma :. \quad (9)$$

It then follows that

$$[H, a^\dagger(k^*)] |N_A\rangle = \epsilon_k a^\dagger(k^*) |N_A\rangle + J^\dagger(k^*) |N_A\rangle \quad (10)$$

and since, directly,

$$[H, a^\dagger(k^*)] |N_A\rangle = (H - E_{N_A}) a^\dagger(k^*) |N_A\rangle$$

we have

$$(H - E_{N_A} - \epsilon_k) a^\dagger(k^*) |N_A\rangle = J^\dagger(k^*) |N_A\rangle. \quad (11)$$

This equation is inverted to yield an equation for $a^\dagger(k^*) |N_A\rangle$ to which an (appropriate) amount of the solution of the homogeneous equation (7) is added:

$$a^\dagger(k^*) |N_A\rangle = |N_A, k^*\rangle + \frac{1}{H - E_{N_A} - \epsilon_k - i\eta} J^\dagger(k^*) |N_A\rangle$$

or, upon rearrangement,

$$|N_A, k^{(\pm)}\rangle = a^\dagger(k^\pm) |N_A\rangle + \frac{1}{E_{N_A} - \epsilon_k - H \pm i\eta} J^\dagger(k^\pm) |N_A\rangle. \quad (12)$$

This is, essentially, the desired result. The total scattering solution is expressed, in the second quantized representation, in terms of the bound state of the target and well-defined operators. (Note that the *incoming* wave representing the incident particle is contained in the first term, even though the scattered part of that term has outgoing boundary conditions.) The expression for the S matrix then follows directly, after some manipulation:

$$\begin{aligned} \langle N'k' | S | Nk \rangle &= \langle N'k' | S | Nk \rangle \\ &= \langle k' | s | k \rangle \delta_{N'N} - 2\pi i \delta(E_{N'} + \epsilon_{k'} - E_N - \epsilon_k) \\ &\quad \times \langle N' | J(k'^{(\pm)}) | Nk^{(\pm)} \rangle. \end{aligned} \quad (13)$$

Here $\langle k' | s | k \rangle$ is the one particle S matrix for scattering from the Hartree-Fock potential. In terms of the single particle t matrix this is

$$\langle k' | s | k \rangle = \delta(k' - k) - 2\pi i \delta(\epsilon_{k'} - \epsilon_k) \langle k' | t | k \rangle. \quad (14)$$

Then, since

$$\begin{aligned} \langle N'k' | S | Nk \rangle &= \langle k' | k \rangle \delta_{N'N} \\ &\quad - 2\pi i \delta(E_N + \epsilon_k - E_{N'} - \epsilon_{k'}) \langle N'k' | T | Nk \rangle \end{aligned} \quad (15)$$

we finally obtain

$$\langle N'k' | T | Nk \rangle = \langle k' | t | k \rangle \delta_{N'N} + \langle N' | J(k'^{(\pm)}) | Nk^{(\pm)} \rangle. \quad (16)$$

From this point, to obtain a general expression for the optical potential, Villars invokes the Lehmann-Zimmermann-Symanzik formalism and a linked-cluster expansion. A more direct—though far less elegant—procedure will be followed in the next section.

III. OPTICAL POTENTIAL FOR ELASTIC SCATTERING

We wish to obtain an expression for the optical potential U , which will reduce the many-body problem of the elastic scattering of a nucleon from a nucleus to the one-body problem of scattering from U . In other words we are looking for a U such that

$$\langle Nk' | T | Nk \rangle = \langle k' | U | k^{(\pm)} \rangle \quad (|k'| = |k|), \quad (17)$$

while the present result is

$$\langle Nk' | T | Nk \rangle = \langle k' | t | k \rangle + \langle N | J(k'^{(\pm)}) | Nk^{(\pm)} \rangle \quad (18)$$

with

$$J(k'^{(\pm)}) = \sum_{\beta\gamma\delta} \langle k'\beta | V | \gamma\delta \rangle : a_\beta^\dagger a_\delta a_\gamma : \quad (19)$$

and

$$|Nk^{(\pm)}\rangle = a^\dagger(k^\pm) |N\rangle + \frac{1}{E_N + \epsilon_k - H + i\eta} J^\dagger(k^{(\pm)}) |N\rangle. \quad (20)$$

Rather than trying to obtain a general expression for U , we will assume that an expansion of U in powers of V is rapidly convergent and obtain an expression for U which retains all terms up to third order. To this end we develop the perturbation expansion for the state $|N\rangle$, assumed to be the ground state of the target. The convergence of the perturbation expansion for the ground state has been demonstrated for the type of interaction to be utilized here.⁸

The Hamiltonian can be divided into two pieces, H_0 and H_1 , with

$$H_0 = E_{\text{HF}} + \sum_{\alpha} \epsilon_{\alpha} : a_{\alpha}^{\dagger} a_{\alpha} : \quad (21)$$

and

$$H_1 = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle : a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} : \quad (22)$$

The eigenstates of H_0 are simply the Hartree-Fock determinant and all multiparticle, multihole states that can be obtained from it. In terms of the b operators these states are

$$| \text{HF} \rangle, b_i^{\dagger} b_i^{\dagger} | \text{HF} \rangle, b_i^{\dagger} b_j^{\dagger} b_i^{\dagger} b_j^{\dagger} | \text{HF} \rangle, \text{ etc.}, \quad (23)$$

where i refers to a state below the Fermi level and j to one above. The corresponding eigenvalues are

$$E_{\text{HF}}, \quad E_{\text{HF}} + \epsilon_i - \epsilon_i, \quad E_{\text{HF}} + \epsilon_i + \epsilon_j - \epsilon_i - \epsilon_j. \quad (24)$$

In terms of these states, the solution of the Schrödinger equation with the total Hamiltonian H is given by

$$\begin{aligned} |N\rangle &= (1 + C_0) | \text{HF} \rangle \\ &\quad + \sum_{i < j} \sum_{KJ} \frac{\langle iJ | V_A | ij \rangle}{\epsilon_i + \epsilon_j - \epsilon_i - \epsilon_j} b_i^{\dagger} b_j^{\dagger} b_i^{\dagger} b_j^{\dagger} | \text{HF} \rangle, \end{aligned} \quad (25)$$

where C_0 is determined by normalization. Inserting this expression for $|N\rangle$ into (20) and (18) leads to first-order terms, containing

$$\langle \text{HF} | : a_{\beta}^{\dagger} a_{\delta} a_{\gamma} : a^{\dagger}(k^{\pm}) | \text{HF} \rangle \quad (26)$$

and two types of second order terms. One type of term comes from the second part of $|Nk^{(\pm)}\rangle$ taken with the HF component of $\langle N |$ and the other type comes from the first part of $|Nk^{(\pm)}\rangle$ taken with a two-particle-two-hole part for $\langle N |$.

The first order term (26) gives no contribution because there must be an equal number of b 's and b^\dagger 's to go from the "vacuum" back to the "vacuum." Thus the normal product has to contain two destruction operators and, since there is only one creation operator to the right, the result is zero.

The first kind of second order term arise from the excitations of the target during the scattering process, i.e., from the term

$$\langle \text{HF} | J(k'^{(-)}) \frac{1}{E_N + \epsilon_k - H_0 + i\eta} J^\dagger(k'^{(+)}) | \text{HF} \rangle. \quad (27)$$

(Note that to this order it is sufficient to replace H by H_0 in the propagator and that, to the same approximation E_N may be replaced by E_{HF} .)

$$\frac{1}{4} \sum_{\beta\gamma} \sum_{\mu\nu} \langle k'\beta | V_A | \gamma\delta \rangle \langle \mu\nu | V | k\sigma \rangle \times \langle \text{HF} | : a_\beta^\dagger a_\sigma a_\gamma : \frac{1}{E_{\text{HF}} + \epsilon_k - H_0 + i\eta} : a_\mu^\dagger a_\nu a_\nu : | \text{HF} \rangle = \frac{1}{2} \sum_{\beta\gamma} \frac{\langle k'\beta | V_A | \gamma\delta \rangle \langle \gamma\delta | V_A | k\beta \rangle}{\epsilon_k + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta + i\eta}, \quad (30)$$

The diagrammatic representation of these terms is given in Fig. 1.

This result may be written in the desired form by defining U^{ex} by

$$\langle k' | U^{\text{ex}} | k \rangle = \frac{1}{2} \sum_{\beta\gamma\delta} \frac{\langle k'\beta | V_A | \gamma\delta \rangle \langle \gamma\delta | V_A | k\beta \rangle}{\epsilon_k + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta + i\eta}. \quad (31)$$

It is this contribution to the optical potential which was calculated, in an approximate way, by MacKellar, Reading, and Kerman.⁶

There are other second order terms, however, arising from the two-particle-two-hole components of $|N\rangle$, i.e., from the correlations. These contain the factor

$$\langle \text{HF} | : a_\beta^\dagger a_\sigma a_\gamma : a^\dagger(k'^{+}) b_I^\dagger b_J^\dagger b_I^\dagger b_J^\dagger | \text{HF} \rangle \quad (32)$$

or the factor

$$\langle \text{HF} | b_j b_i b_J b_I : a_\beta^\dagger a_\sigma a_\gamma : a^\dagger(k'^{+}) | \text{HF} \rangle. \quad (33)$$

The first kind give zero contribution because k^*

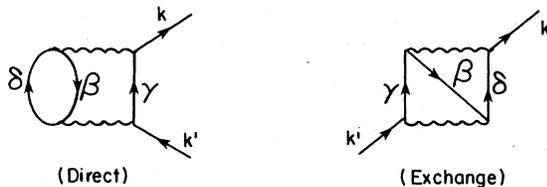


FIG. 1. The process leading to U^{ex} . Here the incoming particle excites the target into a two-particle-one-hole state.

Inserting the expressions for J and J^\dagger , and using the fact that the states created by having a 's and a^\dagger 's act on the vacuum are eigenstates of H_0 , leads to the factor

$$\langle \text{HF} | : a_\beta^\dagger a_\sigma a_\gamma : : a_\mu^\dagger a_\nu a_\nu : | \text{HF} \rangle. \quad (28)$$

In order to contribute we must have

$$\epsilon_\sigma, \epsilon_\beta < \epsilon_{\text{FERMI}}, \text{ and } \epsilon_\delta, \epsilon_\gamma, \epsilon_\mu, \epsilon_\nu > \epsilon_{\text{FERMI}},$$

in which case the factor becomes

$$\delta_{\beta,\sigma} (\delta_{\gamma\mu} \delta_{\delta\nu} - \delta_{\gamma\nu} \delta_{\delta\mu}). \quad (29)$$

The contribution from these terms can then be written as

is an unoccupied state and thus $a_k^\dagger = b_k^\dagger$. The second type of factor, (28), yields zero unless β is above the Fermi level and δ and γ are below. Thus

$$\langle \text{HF} | b_j b_i b_J b_I : a_\beta^\dagger a_\sigma a_\gamma : a^\dagger(k'^{+}) | \text{HF} \rangle = (\delta_{i\delta} \delta_{j\gamma} - \delta_{i\gamma} \delta_{j\delta}) \times (\delta_{I\beta} \delta_{Jk} - \delta_{I\beta} \delta_{J\beta}). \quad (34)$$

Thus, to the second order, the "correlation" contribution is

$$\frac{1}{2} \sum_{i < j} \sum_{I < J} \sum_{\beta\gamma\delta} \langle k'\beta | V_A | \gamma\delta \rangle \times \frac{(\delta_{i\delta} \delta_{j\gamma} - \delta_{i\gamma} \delta_{j\delta}) (\delta_{I\beta} \delta_{Jk} - \delta_{I\beta} \delta_{J\beta})}{\epsilon_I + \epsilon_J - \epsilon_i - \epsilon_j} \times \langle IJ | V_A | ij \rangle = \frac{1}{2} \sum_{\beta\gamma\delta} \frac{\langle k'\beta | V_A | \gamma\delta \rangle \langle \gamma\delta | V_A | k\beta \rangle}{\epsilon_k + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta} \quad (35)$$

with the prime on the sum indicating that the sum is restricted to states such that

$$\epsilon_\beta > \epsilon_{\text{FERMI}} \text{ and } \epsilon_\gamma, \epsilon_\delta < \epsilon_{\text{FERMI}}.$$

We may also write this result in the desired form by defining U^{cor} via

$$\langle k' | U^{\text{cor}} | k \rangle = \frac{1}{2} \sum_{\beta\gamma\delta} \frac{\langle k'\beta | V_A | \gamma\delta \rangle \langle \gamma\delta | V_A | k\beta \rangle}{\epsilon_k - \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta}. \quad (36)$$

The diagrammatic representation of these terms

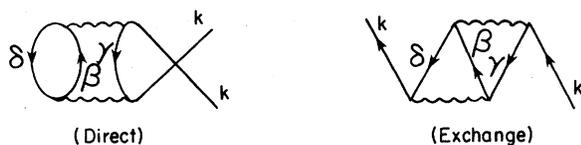


FIG. 2. The process leading to U^{cor} . Here the incoming particle interacts with a two-particle-two-hole component of the target's wave function.

is given in Fig. 2.

With these definitions Eq. (18) can now be written, up to second order, as

$$\begin{aligned} \langle Nk' | T | Nk \rangle &= \langle k' | t | k \rangle + \langle k' | U^{\text{cor}} + U^{\text{ex}} | k \rangle \\ &= \langle k' | t + U^{\text{cor}} + U^{\text{ex}} | k \rangle, \end{aligned}$$

where, again, t is the scattering matrix for the

$$\langle i | U_k^{\text{ex}} | j \rangle = \sum_{\lambda} \int \frac{d^3 k_a}{(2\pi)^3} \int \frac{d^3 k_b}{(2\pi)^3} \frac{\langle i\lambda | V_A | k_a k_b \rangle \langle k_a k_b | V_A | j\lambda \rangle}{\epsilon_k + \epsilon_{\lambda} - \epsilon_a - \epsilon_b + i\eta}, \quad (38)$$

where k_a, k_b are scattering states from the Hartree-Fock potential with outgoing boundary conditions and energies ϵ_a, ϵ_b . The subscript k on U^{ex} is used to indicate that the scattering energy is $(\hbar^2 k^2 / 2m)$. (Bound, but unoccupied, levels are implicitly included in the integrals on k_a, k_b). Only one such state exists for the nucleus considered and it, being at almost zero energy, has been incorporated into the continuum.

The continuum states should, in principle, be obtained numerically for each scattering energy. In coordinate space they are given by

$$\begin{aligned} \langle r | k \rangle &= \sum_{j m l m_l} 4\pi i^l e^{i\phi_{lj}(k)} R_{lj}(k, r) Y_{lm_l}(\hat{k}) Y_{ljm}(\hat{r}) \\ &\quad \times \langle l m_l \frac{1}{2} m_s | j m \rangle \tau_z, \end{aligned} \quad (39)$$

where

$$Y_{ljm}(\hat{r}) = \sum_{m_l m_s} \langle l m_l \frac{1}{2} m_s | j m \rangle Y_{lm_l}(\hat{r}) \chi_{1/2 m_s}.$$

The functions $R_{lj}(k, r)$ are the source of the difficulty being the solutions of the radial part of the Schrödinger equation with the Hartree-Fock potential. In order to reduce the calculation to a realistic size it is necessary to approximate these functions by something simpler. A viable approx-

Hartree-Fock potential. This is the desired expression.

IV. A CALCULABLE FORM FOR THE OPTICAL POTENTIAL

The expression obtained for the second order optical potential is not readily amenable to calculation. To obtain a more suitable form it is convenient to work in the harmonic oscillator representation. The basis states $|i\rangle$ are then characterized by the quantum numbers n, l, j, m , and τ_z . For spherical nuclei, which are the only ones considered here, the occupied orbitals have sharp values of l, j, m , and τ_z and thus an occupied state $|\lambda\rangle$ is given by

$$|\lambda\rangle = \sum_n c_{\lambda}^n |nljm\tau_z\rangle. \quad (37)$$

In this representation U^{ex} has the form

imation scheme has been developed⁹ in which the functions R are expanded in terms of the discrete set of orbitals obtained by diagonalizing the Hartree-Fock matrix in some truncated, harmonic oscillator basis. This expansion has been shown to be quite accurate for those values of r which are significant for integrals containing the potential. According to this approximation

$$R_{ij}(k, r) \approx \sum_{\mu} D_{\mu}(k) N_{ij}(k) \phi_{\mu}(r), \quad (40)$$

where the function $\phi_{\mu}(r)$ is the radial part of an eigenfunction of the Hartree-Fock matrix. The D 's are energy dependent expansion coefficients and N is a normalization factor.

The resulting expression for the states k_a, k_b can be substituted into U^{ex} and the integrations over the angles \hat{k}_a and \hat{k}_b can readily be performed. Sums on magnetic quantum numbers of products of Clebsch-Gordan coefficients can also be easily carried out, further simplifying the quantity to be calculated. Since all the states are now expressed in terms of harmonic oscillator states, the calculation of U^{ex} consists merely of summing products of readily calculable matrix elements multiplied by functions of the Hartree-Fock expansion coefficients and energies. Specifically,

$$\langle i | U^{\text{ex}} | j \rangle = \sum \frac{(2T+1)(2J+1)}{\pi^2} \int k_a^2 dk_a \int k_b^2 dk_b F_1(\mu_1 \mu_3 k_a) F_1(\mu_2 \mu_4 k_b) \frac{F_2(\mu_1 \mu_2 \lambda i J T) F_2(\mu_3 \mu_4 \lambda j J T)}{\epsilon_a + \epsilon_\lambda - \epsilon_a - \epsilon_b}, \quad (41)$$

where the summation is over the occupied orbitals λ , all the Hartree-Fock states μ , and a coupled angular momentum and isospin, J and T . The functions F_1 and F_2 are given by

$$F_1(\mu_1 \mu_3 k_a) = D_{\mu_1}(k_a) N_{i_1 j_1}(k_a) D_{\mu_3}(k_a) N_{i_3 j_3}(k_a),$$

$$F_2(\mu_1 \mu_2 \lambda i J T) = \sum_{n_1 n_2 n} C_{\mu_1}^{n_1} C_{\mu_2}^{n_2} C_{\lambda}^{n_3} \langle n_1 l_1 j_1, n_2 l_2 j_2 | V_A | n_1 l_1 j_1, n_2 l_2 j_2 \rangle_{JT}. \quad (42)$$

In a similar way one may obtain a simplified expression for the correlation contribution to the optical potential,

$$\langle i | U^{\text{cor}} | j \rangle = \sum \frac{(2T+1)(2J+1)}{4\pi} \int k_a^2 dk_a G_1(\nu_1, k_a) G_1(\nu_2, k_a) \frac{G_2(\nu_1 \lambda \mu i J T) G_2(\nu_2 \lambda \mu j J T)}{\epsilon_a + \epsilon_a - \epsilon_\lambda - \epsilon_\mu} \quad (43)$$

where

$$G_1(\nu_1, k_a) = D_{\nu_1}(k_a) N_{i_1 j_1}(k_a)$$

and

$$G_2(\nu \lambda \mu i J T) = \sum_{n_1 n_2 n} C_{\mu_1}^{n_1} C_{\mu_2}^{n_2} C_{\nu}^{n_3} \langle n_1 l_1 j_1, n_2 l_2 j_2 | V_A | n_1 l_1 j_1, n_2 l_2 j_2 \rangle_{JT}. \quad (44)$$

These two expressions, U^{cor} and U^{ex} , constitute the starting point for the present calculation.

V. DETAILS OF THE CALCULATION

The present calculation utilizes the Hartree-Fock results¹⁰ obtained for ^{16}O using the Tabakin nucleon-nucleon interaction.¹¹ Although this interaction has certain deficiencies it does contain all of the qualitative features of the forces which give better fits to the two-body data. It has the virtue that, not having a hard core, one may calculate its matrix elements and thus avoid a G -matrix calculation. Further, the Tabakin interaction has been used in perturbation calculations¹² which apparently converge quite rapidly to a reasonable binding energy for ^{16}O .

Since the space of harmonic oscillator states used in the Hartree-Fock calculation contains six s states, only a 6×6 Hartree-Fock potential is available for s -wave scattering and, therefore, $\langle i | U^{\text{ex}} | j \rangle$ and $\langle i | U^{\text{cor}} | j \rangle$ will be limited to 6×6 matrices for this case. A second truncation is necessary in the expansion of the scattering states, k_a , in terms of partial waves. In this calculation only the $s_{1/2}$, $p_{1/2}$, $p_{3/2}$, $d_{5/2}$, and $d_{3/2}$ contributions will be considered—the error due to neglecting higher partial waves will be small for a number of reasons, including the relative size

of the corresponding two-body matrix elements for s -wave scattering and their small amplitude at modest energies.

Even with these truncations the calculation of U^{ex} and U^{cor} require rather sophisticated computer programming. For example, the F_2 array which enters into the calculation of U^{ex} has just under 200 000 entries and each entry requires the calculation of about 200 matrix elements of the potential. A large number of these matrix elements are trivially zero by parity or angular momentum considerations but, nonetheless, the number of necessary matrix elements is extremely large.¹³

In addition to the difficulties associated with the large numbers of calculations, care must also be taken in the integration on k_a and k_b because the denominator in U^{ex} can vanish. The denominator in U^{cor} cannot vanish because ϵ_λ and ϵ_μ are negative and therefore U^{cor} is totally real. U^{ex} , however, has a real and imaginary part. This problem is treated by using Simpson's rule for the integration and choosing the points so that the poles are at mesh points. In the evaluation one then tests whether the denominator is zero and, if so, there is no contribution to the integral from this point. In addition the contributions from the immediately preceding and following points are multiplied by 1.5. This properly takes care of the residue of the integral if it is linear in the region of a pole. Further accuracy, although possible, was not found to be necessary. In this way, the integrals were found to converge if the number of points considered was 22–24 for each variable. The calculation of the imaginary part of U^{ex} is straightforward, being only a single integration with no singularities.

Thus the calculation of $\langle i | U^{\text{cor}} + U^{\text{ex}} | j \rangle$ is reduced to taking a matrix product of rather large matrices and integrating the result using Simpson's

rule. Because a large space was used to minimize truncation effects the calculations still are quite time consuming. Given the matrix elements of the two-body interaction, stored in a particularly convenient way, the calculation of the 36 complex elements of $\langle i | U_k^{\text{ex}} + U_k^{\text{cor}} | j \rangle$, for a single energy, takes about 12 minutes on an IBM 370.

MacKellar *et al.*⁶ circumvented most of the difficulty in calculating U^{ex} by making some rather extreme approximations. In the expression (38), ϵ_λ was replaced by a constant Δ , independent of the state λ . Also the states k_a , k_b were replaced by plane wave states and thus ϵ_a , ϵ_b by the appropriate $\hbar^2 k^2/2m$. The integrals on k_a and k_b can then be performed directly. The resulting U^{ex} is purely real and somewhat devoid of structure but, nonetheless, it was the success of these calculations which helped to motivate the present work.

VI. CALCULATION OF PHASE SHIFTS

The optical potential obtained in the preceding section is energy dependent, complex, and non-local. Having obtained the matrix elements in only a finite dimensional, harmonic oscillator representation the potential is automatically in the form of a sum over a small number of separable terms, i.e.,

$$\langle \vec{r} | U_{\text{opt}} | \vec{r}' \rangle = \sum_{i,j=1}^N \langle \vec{r} | i \rangle \langle i | U_{\text{opt}} | j \rangle \langle j | \vec{r}' \rangle, \quad (45)$$

where

$$\langle \vec{r} | i \rangle = Y_{l_j m}(\hat{r}) R_{n_l}(r).$$

One can thus obtain the phase shifts exactly by matrix inversion of an N by N matrix rather than solving an integrodifferential equation by some numerical approximation.

Briefly, one begins with the T -matrix equation,

$$\langle \vec{k} | T(E) | \vec{k}' \rangle = \langle \vec{k} | U_{\text{opt}} | \vec{k}' \rangle - \int \frac{d^3 q}{(2\pi)^3} \langle \vec{k} | U_{\text{opt}} | \vec{q} \rangle \langle \vec{q} | (H_0 - E - i\eta)^{-1} | \vec{q} \rangle \langle \vec{q} | T(E) | \vec{k}' \rangle, \quad (46)$$

where H_0 is the kinetic energy operator and spin indices have been suppressed. Writing

$$\langle \vec{k} | T(E) | \vec{k}' \rangle = \sum_{ij} T_{ij}(k, k', E) \sum_m Y_{l_j m}(\hat{k}) Y_{l_j m}^*(\hat{k}') \quad (47)$$

and substituting this, and the Fourier transform of $\langle \vec{r} | U_{\text{opt}} | \vec{r}' \rangle$, into (46) leads to

$$T_{ij}(k, k', E) = \sum_{nn'} \bar{R}_{n_l}(k) \langle n l_j | U_{\text{opt}} | n' l_j \rangle \bar{R}_{n'_l}(k) - \frac{1}{4\pi} \sum_{nn'} \int \frac{q^2 dq}{2\pi^2} \bar{R}_{n_l}(k) \langle n l_j | U_{\text{opt}} | n' l_j \rangle \bar{R}_{n'_l}(q) g_0(q, E) T_{ij}(q, k', E), \quad (48)$$

where

$$g_0(q, E) = \left(\frac{\hbar^2 q^2}{2m} - E - i\eta \right)^{-1}. \quad (49)$$

and

$$\bar{R}_{n_l}(k) = 4\pi \int_0^\infty r^2 dr j_l(kr) R_{n_l}(r). \quad (50)$$

One then defines $F_{n_l j}(k, E)$ via

$$T_{ij}(k, k', E) = \sum_n \bar{R}_{n_l}(k) F_{n_l j}(k', E) \quad (51)$$

and substituting into (48) leads to the matrix equation

$$F_{n_l j}(k', E) = \sum_{n''} D_{nn''}^{-1}(l_j E) \langle n' l_j | U_{\text{opt}} | n'' l_j \rangle \bar{R}_{n''_l}(k'), \quad (52)$$

where

$$D_{nn'}(l_j E) = \delta_{nn'} + \frac{1}{4} \sum_{n''} \langle n l_j | U_{\text{opt}} | n'' l_j \rangle \times \int_0^\infty \frac{q^2 dq}{2\pi^2} R_{n''_l}(q) g_0(q, E) R_{n'_l}(q). \quad (53)$$

The problem of determining T then reduces to that of inverting the $N \times N$ matrix D . The phase shifts then follow from the relation

$$T_{ij}\left(k, k, \frac{\hbar^2 k^2}{2m}\right) = -\frac{\hbar^2}{2mk} (4\pi)^2 e^{i\delta_{ij}(k)} \sin \delta_{ij}(k). \quad (54)$$

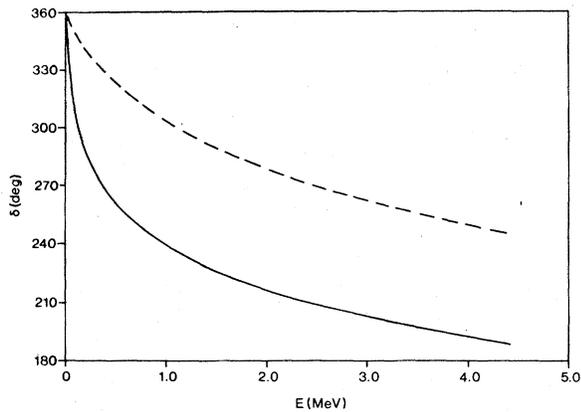


FIG. 3. S-wave phase shifts. The dotted line is the experimentally fitted phase shift and the solid line is the phase shift resulting from the total optical potential calculated here. At these energies the optical potential, and thus the phase shift, are calculated to be purely real.

VII. RESULTS

The s-wave phase shifts for low energy neutrons, elastically scattered from O^{16} , are shown in Fig. 3. The experimentally determined phase shifts are given by the dotted curve¹⁴ and the results of the present calculation are the solid curve. The theoretical results are determined, to a large extent, by the Hartree-Fock potential itself, as shown in Fig. 4. The dashed curve is the result using only the Hartree-Fock potential and the solid curves are obtained with the full U_{opt} . Since U^{cor} and U^{ex} are of opposite signs, they tend to cancel and since they are of the same order of magnitude, the net effect on the phase shifts is small. It had been previously stated⁶ that part of the "large difference between the first- and second-order calculations is consistent with the fact that the second order has the 1s and 2s states bound in approximately the right place, whereas the first order has the 2s unbound." In fact, as has been discussed elsewhere,¹⁵ the 2s state is bound already in the Hartree-Fock field. Thus the dashed curve must also start at 2π for zero energy, in order to satisfy Levinson's theorem, if $\delta(E \rightarrow \infty) = 0$.

In Fig. 5 the results of the present calculation are compared with the results of previous calculations. In these calculations the oxygen target is assumed to remain in its Hartree-Fock determinantal state, which is obtained using some effective interaction. The curve labeled DKB is obtained using the Nestor potential¹⁶ and those labeled S use two versions of the Skyrme¹⁷ interaction. It should be emphasized that the previous calculations are quite different from the the present one in that

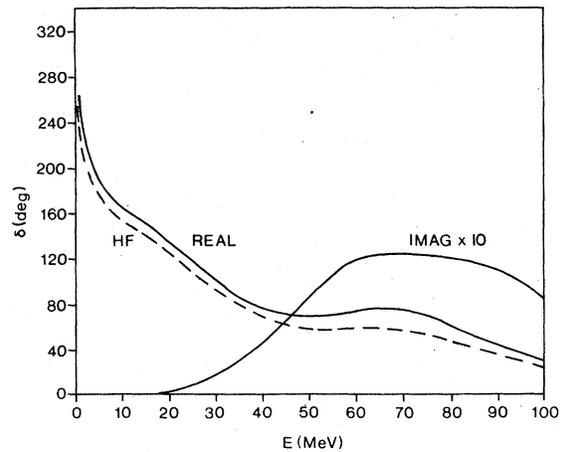


FIG. 4. Effect of the second order correction. The dashed curve is obtained by solving the scattering problem with just the Hartree-Fock potential. The result when the total optical potential is used is a complex phase shift whose real and imaginary parts are shown. Note the imaginary part has been multiplied by a large factor for display purposes. These phase shifts are not intended to be meaningful over such a wide energy region but are shown just to illustrate the second order contribution.

their ansatz is that the wave function is a single determinant and an interaction is employed whose parameters are fitted to many-body properties. In the present calculation the interaction is fitted to two-body data and the wave function is not restricted.

Another measure of the effect of the higher order

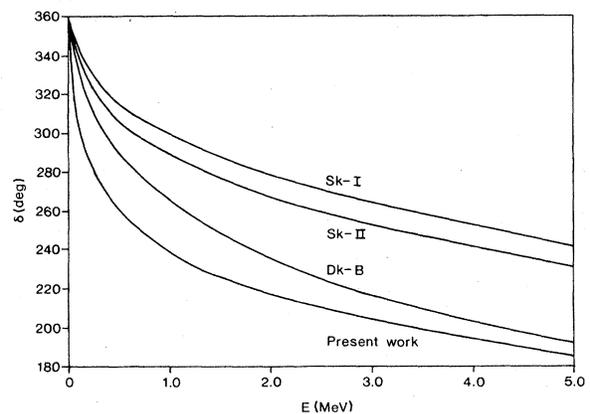


FIG. 5. Results of previous calculations. The curves labeled Sk-I, Sk-II, and DKB are obtained by scattering from the Hartree-Fock potentials alone, using various effective interactions. The parameters of these interactions are fitted to many-body properties, such as ground state energy and rms radius. The present calculation uses an interaction which is fitted to two-body data and more general a wave function.

corrections on scattering phenomena is the scattering length and effective range. One defines the scattering length a_0 by

$$-\frac{1}{a_0} = \lim_{k \rightarrow 0} k \cot \delta.$$

Evaluating this for the Hartree-Fock potential alone yields $a_0 = 33.66$ fm. If one used, instead, the optical potential including U^{ex} , but not U^{cor} , the result is 11.95 fm. Using the full optical potential yields $a_0 = 15.48$ fm. The experimental value of a_0 obtained from the coherent scattering of thermal neutrons is about 5.8 fm.¹⁸ Given the sensitivity of a_0 to small changes in the potential, the theoretical value is quite reasonable.

One may also define the effective range parameter r_0 by the expansion

$$k \cot \delta = \frac{-1}{a_0} + \frac{1}{2} r_0 k^2.$$

This parameter is not determined experimentally, because of the complexity of the low energy cross section as a function of energy. It may, however, be calculated using the various calculated phase shifts. For the Hartree-Fock potential alone, the effective range is calculated to be 8 fm. If U^{ex} is included one finds $r_0 = 6$ fm and if the full optical potential is used, $r_0 = 6.6$ fm.

It is of some interest to consider the energy dependence of the various components of the optical potential responsible for these results. Since the potentials are nonlocal they are not amenable to simple graphical representation. Thus, to illus-

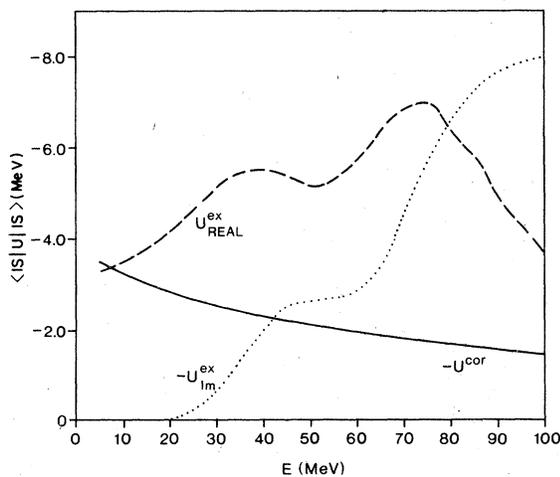


FIG. 6. Illustration of energy dependence. Because the second order contributions to the optical potential are nonlocal, the dependence on energy is illustrated by simply the largest matrix element. Of particular importance is the fact that U^{ex} and U^{cor} are of opposite sign and nearly equal magnitude at low energies.

trate the energy dependence, the diagonal matrix element corresponding the lowest s state is shown, in Fig. 6, as a function of energy. (This is always the largest matrix element.) The solid line is $\langle 1s | U^{\text{cor}} | 1s \rangle$, the dashed line is the real part of $\langle 1s | U^{\text{ex}} | 1s \rangle$, and the dotted line is its imaginary part.

VIII. CONCLUSIONS

The results reported here are the product of an attempt at a totally microscopic description of the nucleon-nucleus scattering process. Beginning with a soft-core, nucleon-nucleon potential which is fitted, albeit rather poorly, to two-body scattering data, one proceeds to solve the quantum mechanical, many-body problem with the appropriate boundary conditions. The only assumptions have to do with the truncation of spaces, which can be checked by increasing the size of the basis, and the convergence of the perturbation expansion, which can be checked by calculating higher order terms.

Because the nucleon-nucleon potential does not quantitatively agree with experimental predictions it is not expected to fit all aspects of the scattering data. Certain aspects of the data, on the other hand, should be correctly represented because the quantum mechanical treatment is correct.

The results are quite encouraging. Although the experiments indicate the presence of a "compound elastic resonance" in the s -wave phase shifts which the calculations do not reproduce, the other features of this phase shift, as a function of energy, are given quite well. (This failure to produce a resonance is not due to the nucleon-nucleon potential but rather to the cutoff of the perturbation expansion since, presumably, the incoming neutron shares its energy with the entire ^{16}O nucleus at this energy.)

In subsequent calculations the higher partial wave phase shifts for n - ^{16}O will be considered so that the total elastic cross section can be computed. Also being undertaken is a study of the sensitivity of the results to the details of the nucleon-nucleon interaction.

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