Exact treatment of the Pauli principle in multiple scattering theory

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Exact equations for projectile-nucleus scattering are derived in which the effects of the Pauli principle are fully included. The resulting amplitude has two components; one resembles multiple scattering for distinguishable particles and the other describes distorted cluster exchange. The equations are simple to use and as such constitute an improvement over the present approximate schemes.

NUCLEAR REACTIONS Multiple scattering series, Pauli principle, cluster exchange, optical potential.

Different schemes for the inclusion of the Pauli principle in scattering involving identical particles have been proposed during the past 30 years.¹⁻⁴ Some give a formally correct treatment, but practical applications are often complicated. The simplest approximate treatment of this problem has been proposed by Takeda and Watson.²⁻⁴ In this treatment antisymmetrization is approximately achieved if in the multiple scattering series for a distinguishable projectile all elementary projectile-target particle scattering operators are antisymmetrized. Although this prescription has been justified only for high-energy small-angle scattering (where, in fact, the exchange effects are small) the Takeda and Watson prescription has been widely used under more general conditions. The Kerman, McManus, and Thaler (KMT) theory for the optical potential uses the same prescription.⁵

We now construct a *simple* way of including the Pauli principle in multiple scattering theories without any approximation. Our result is not significantly more complicated than the standard formalism for distinguishable particles. We present a detailed derivation for the simplest possible case, namely, proton-deuteron scattering. The result for scattering from more complex targets will be given without proof.

Consider, first, pd scattering for a distinguishable projectile 0 and target proton 1 (the neutron index is 2). The free wave function of the system is the product of a plane wave of momentum $\bar{k}, \chi_{\vec{k}}(0)$ (of a projectile) and a deuteron wave function $\phi_d(12)$. In general the wave function is given by

$$\psi_{\vec{k}}(012) = \chi_{\vec{k}}(0)\phi_d(12) + G(V_{01} + V_{02})\chi_{\vec{k}}(0)\phi_d(12).$$
(1)

Here G is the total Green's function

$$G = \left(E - \sum_{i=0}^{2} K_{i} - \sum_{i>j} V_{ij}\right)^{-1}$$
(2)

with K_i the kinetic energy operator for the *i*th nucleon and V_{ij} the two-body nucleon potential between nucleons ij.

The wave function of the system corresponding to (1), which is antisymmetric under interchange of two protons 0 and 1 is⁴

$$\psi_{\vec{k}}^{a}(012) = \frac{1}{\sqrt{2}} \{ [\chi_{\vec{k}}(0)\phi_{d}(12) - \chi_{\vec{k}}(1)\phi_{d}(02)] + G[(V_{01} + V_{02})\chi_{\vec{k}}(0)\phi_{d}(12) - (V_{12} + V_{01})\chi_{\vec{k}}(1)\phi_{d}(02)] \}.$$
 (3)

We now wish to extract the amplitude for scattering to a final pd (or ppn) state which is the coefficient of that state in the asymptotic form of the scattered wave in (3). We thus express G in (3) in terms of the channel Green's function G_0 = $(E - \sum_{i=0}^{2} K_i - V_{12})^{-1}$ which explicitly contains the required state in the asymptotic limit of spectral representation. Using the relation $G = G_0 + G_0(V_{01} + V_{02})G$ one finds⁴

$$\Psi_{\vec{k}}^{a}(012) = \frac{1}{\sqrt{2}} \left[\chi_{\vec{k}}(0)\phi_{d}(12) - \chi_{\vec{k}}(1)\phi_{d}(02) \right] \\ + \frac{1}{\sqrt{2}} G_{0}(V_{02} - V_{12})\chi_{\vec{k}}(1)\phi_{d}(02) \\ + G_{0}(V_{01} + V_{02})\psi_{\vec{k}}^{a}(012) .$$
(4)

The second term on the right-hand side of Eq. (4) is the so-called target exchange term and is neglected in the treatment of Takeda and Watson.^{2,4} We wish to retain this term in the definition of the (antisymmetrized) scattering operator T^a

$$T^{a}\chi_{\vec{k}}(0)\phi_{d}(12) = \frac{1}{\sqrt{2}}(V_{02} - V_{12})\chi_{\vec{k}}(1)\phi_{d}(02) + (V_{01} + V_{02})\Psi_{\vec{k}}^{a}.$$
 (5)

The corresponding amplitude for scattering to a

22

964

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state $\chi_{\mathbf{k}'}(0)\phi_{pn}(12)$ (where ϕ_{pn} is a general pn eigenstate) reads

$$F(E,\vec{\mathbf{k}},\vec{\mathbf{k}'}) = -4\pi^2 \frac{mM_d}{m+M_d} \langle \vec{\mathbf{k}'}, \phi_{pn} | T^a | \vec{\mathbf{k}}, \phi_d \rangle.$$
(6)

In the same way one could define the scattering operator for the channel with the final state projectile and target protons labels 0 and 1 interchanged, by rewriting Eq. (3) with the channel Green's function $G_1 = (E - \sum_{i=0}^2 K_i - V_{02})^{-1}$. The resulting scattering amplitude is the same as the one given by Eqs. (5) and (6). It is thus enough to consider one channel only. The incoherent contribution to the cross section from the second channel can be taken into account by adding a factor $\sqrt{2}$ in the normalization of the amplitude, Eq. (6).

In order to derive a Lippmann-Schwinger type of equation for the scattering operator T^{a} we introduce *exchange* potentials $V_{ij}^{a} \equiv V_{ij}P_{01}$, where P_{01} interchanges nucleons 0 and 1. Note that only the potential V_{01}^{ex} conserves the total momentum 01 and corresponds to the usual *pp* exchange potential. V_{12} and V_{02} act between three particles and thus do not conserve the total momentum of pairs 12, 02.

Using $V_{ij\chi\bar{k}}(1)\phi_d(02) = V_{ij\chi\bar{k}}^{ox}(0)\phi_d(12)$ we find from Eqs. (4) and (5) the desired Lippmann-Schwinger equation for T^a

$$T^{a} = \frac{1}{\sqrt{2}} (V_{01} + V_{02}) - \frac{1}{\sqrt{2}} (V_{01}^{ex} + V_{12}^{ex}) + (V_{01} + V_{02})G_{0}T^{a}.$$
 (7)

Introducing the "direct" scattering operator

$$T^{d} = (V_{01} + V_{02}) + T^{d}G_{0}(V_{01} + V_{02})$$
(8a)

and multiplying Eq. (7) by $(1 + T^{d}G_{0})$ we find that T^{a} can be represented as a sum of direct and exchange components

$$T^{a} = \frac{1}{\sqrt{2}} \left(T^{d} - T_{p}^{\text{ex}} - T_{n}^{\text{ex}} \right) \equiv \frac{1}{\sqrt{2}} \left(T_{\text{MS}}^{\prime} - T_{n}^{\text{ex}} \right), \qquad (8b)$$

 $T_{p}^{ex} = V_{01}^{ex} + T^{d}G_{0}V_{01}^{ex}, \qquad (8c)$

$$T_n^{e_x} = V_{12}^{e_x} + T^d G_0 V_{12}^{e_x} .$$
 (8d)

From its definition (8a) we see that T^{d} corresponds to the scattering of distinguishable nucleons and it can thus be expanded to a standard multiple scattering series⁴

$$T^{d} \equiv T^{d}_{MS} = \tau^{d}_{01} + \tau^{d}_{02} + \tau^{d}_{01}G_{0}\tau^{d}_{02} + \tau^{d}_{02}G_{0}\tau^{d}_{01} + \tau^{d}_{01}G_{0}\tau^{d}_{02}G_{0}\tau^{d}_{01} + \cdots$$
(9)

The operators τ_{01}^d and τ_{02}^d are the direct scattering operators of the projectile proton on the proton and neutron bound in the target and are given by

$$T_{0i}^{d} = V_{0i} + V_{0i} G_{0} \tau_{0i}^{d} .$$
 (10)

Consider next T_{p}^{ex} , the proton exchange part of the scattering operator T^{a} , Eq. (8c). When we substitute Eq. (9) into Eq. (8c) we find

$$T_{p}^{ex} = \tau_{01}^{ex} + \tau_{02}^{d}G_{0}\tau_{01}^{ex} + \tau_{01}^{d}G_{0}\tau_{02}^{d}G_{0}\tau_{01}^{ex} + \cdots, \qquad (11)$$

where $\tau_{01}^{ex} \equiv \tau_{pp}^{ex}$ is defined by

$$\Gamma_{01}^{\text{ex}} = V_{01}^{\text{ex}} + \tau_{01}^{d} G_0 V_{01}^{\text{ex}} \,. \tag{12}$$

Combining Eqs. (9) and (11) we obtain the $T'_{\rm MS}$ defined in (8b)

$$T'_{\rm MS} \equiv T^{d} - T^{ex}_{p}$$

= $\tau^{a}_{01} + \tau^{d}_{02} + \tau^{d}_{01}G_{0}\tau^{d}_{02} + \tau^{d}_{02}G_{0}\tau^{a}_{01}$
+ $\tau^{d}_{01}G_{0}\tau^{d}_{02}G_{0}\tau^{a}_{01} + \cdots, ,$ (13)

where

$$T^a_{01} \equiv \tau^a_{pp} = \tau^d_{pp} - \tau^{ex}_{pp}$$
(14)

is the antisymmetrized projectile proton-bound proton scattering operator. Equations (12) and (14) have the same form as for free proton-proton scattering including antisymmetrization.

We still need the component T_n in the exchange amplitude which is obtained by direct substitution of Eq. (9) into (8d)

$$T_{n}^{\text{ex}} = V_{12}^{\text{ex}} + (\tau_{01}^{d} + \tau_{02}^{d} + \tau_{01}^{d}G_{0}\tau_{02}^{d} + \tau_{02}^{d}G_{0}\tau_{01}^{d} + \cdots)G_{0}V_{12}^{\text{ex}}.$$
 (15)

Consider for instance the Born approximation to the elastic amplitude (in the overall c.m. frame) described by T_n^{ex} , Eq. (15).

$$\langle \bar{\mathbf{k}'}, \phi_d | V_{12}^{\text{ex}} | \phi_d, \bar{\mathbf{k}} \rangle = \langle \chi_{\bar{\mathbf{k}'}}(0) \phi_d(12)$$

$$\times V_{12} P_{01} \chi_{\bar{\mathbf{k}}}(0) \phi_d(12) \rangle.$$
(16a)

From the Schrödinger equation for ϕ_d we find

$$\langle \vec{\mathbf{k}}', \phi_{d} | V_{12} | \phi_{d}, \vec{\mathbf{k}} \rangle = -\langle \chi_{\vec{\mathbf{k}}'}(0)\phi_{d}(12) \\ \times [| \epsilon_{d} | + K_{12}^{\text{rel}}]\chi_{\vec{\mathbf{k}}}(1)\phi_{d}(02) \rangle$$

$$= -\left[|\epsilon_{d} | + \left(\vec{\mathbf{k}} + \frac{\vec{\mathbf{k}}'}{2}\right)^{2} \frac{1}{m} \right]$$

$$\times \phi_{d} \left(\vec{\mathbf{k}} + \frac{\vec{\mathbf{k}}'}{2}\right) \phi_{d} \left(\vec{\mathbf{k}}' + \frac{\vec{\mathbf{k}}}{2}\right), \quad (16b)$$

where $-|\epsilon_d|$ is the deuteron binding energy and K_{12}^{rel} is the kinetic energy of the relative pn motion. Equation (16b) apparently describes the undistorted single-neutron exchange amplitude, Fig. 1(a).

We thus find that the properly antisymmetrized pd amplitude can be written as a multiple scattering expansion with two components.

965



FIG. 1. Schematic representation of the Born term for neutron exchange (a), cluster exchange (b) in elastic scattering.

(a) The first $T'_{\rm MS} = T^d - T^{\rm ex}_p$, Eq. (13), is identical to the expansion for distinguishable nucleons with one modification. In each term of the multiple scattering series the last (direct) scattering operator τ^d , whenever it describes the scattering of identical nucleons, is replaced by τ^a , Eq. (13). The latter properly describes the scattering of a proton from an identical target proton and has the same form as an operator for free pp scattering with antisymmetrization.

(b) The component T_n^{ex} describes neutron pickup. Notice [cf., Eq. (15)] that the distortion of simple pickup appears in terms of direct (nonantisymmetrized) scattering operators only and that distortion affects only the final state. (In an alternative derivation an expression for T^{ex} can be obtained with only the initial state being distorted.)

The derivation above deals with pd scattering but there are no essential complications in a generalization to the case of scattering from an arbitrary target of A particles. We give here only the final expressions for the exact scattering operator T_{pA}^a , where the projectile p is identical to N target constituents

$$T_{PA}^{a} = \frac{1}{\sqrt{N}} \left(T_{MS}^{\prime} - T^{\text{ex}} \right),$$
 (17a)

$$T'_{MS} = \sum_{i}^{a} \tau^{a}_{0i} + \sum_{i \neq j} \tau^{d}_{0i} G_{0} \tau^{a}_{0j} + \sum_{\substack{i \neq j \\ j \neq k}} \tau^{d}_{0i} G_{0} \tau^{d}_{0j} G_{0} \tau^{a}_{0k} + \cdots , \quad (17b)$$

$$T^{ex} = (1 + T^{d}_{MS} G_0) \sum_{j=1}^{N} \left(\sum_{i (\neq j)=1}^{A} V^{ex}_{ij} \right).$$
(17c)

The scattering amplitude is

$$F_{if}(E,\vec{\mathbf{k}},\vec{\mathbf{k}}') = -\frac{4\pi^2 m M_A N}{m+M_A} \langle \vec{\mathbf{k}}', \phi_A^f | T^a | \vec{\mathbf{k}}, \phi_A^i \rangle,$$
(17d)

where initial and final states are the (nonantisymmetrized) product of a projectile plane wave and the (antisymmetrized) wave function of the target. Again, the scattering matrix T^a_{PA} appears to have two components. The first one is the modified

multiple scattering series $T'_{\rm MS}$, Eq. (17b), which is the same as for $T_{\rm MS} \equiv T^{\rm M}_{\rm MS}$ (neglecting the symmetry between projectile and identical target particles) except for the last scattering operator τ in each term of this series. That operator must be replaced by its antisymmetrized counterpart $\tau^d - \tau^a = \tau^d - \tau^{\rm ex}$ whenever it describes the scattering of identical projectile and target nucleon. The operators $\tau_{\rm oi}$ are defined by Eqs. (10), (12), and (14) where the Green's function G_0 contains the full target Hamiltonian.

The second component T^{ex} , Eq. (17c), includes the exchange potential $V_{ij}^{\text{ex}} \equiv V_{ij}P_{0j}$, where P_{0j} interchanges the labels 0 and *j*. If the target wave function is a product of wave functions for the (A-1) particle core and for the relative core-particle motion, the Born term of T^{ex} describes core exchange [Fig. 1(b)]. The remaining terms describe distortion of that Born amplitude by $T_{\text{MS}}^d G_0$, i.e., in terms of the direct scattering operators τ^d , and these terms appear to affect only the final state.

We now emphasize the difference between our exact treatment and the approximation of Takeda and Watson.²⁻⁴ These authors obtain a multiple scattering series where *every* collision operator for identical particles is antisymmetrized. It differs from our result, Eq. (17b), where only the *last* operator τ is antisymmetrized. Moreover, the amplitude T^{ex} , Eq. (17c), describing the exchange of (A-1) target particles is neglected altogether by Takeda and Watson.

In order to apply the exact equations (17a)– (17c) we must resort to approximations for the many body operators G_0 , τ_{01} . These could be impulse approximations, the so-called optimal approximations^{6,7} or others. The results of these approximations will be discussed elsewhere.^{7,8} Here we stress only that in order to use the Takeda and Watson *approximate* multiple scattering series similar approximations must be made. Therefore our *exact* multiple scattering series constitutes an improvement over the Takeda and Watson result.⁹

Next we consider a first order optical potential for pA elastic scattering as given by KMT.⁵ Assuming projectile and target nucleons to be distinguishable, a first order optical potential would be

$$U_{\rm opt}^{(1)}(\mathbf{\bar{p}},\mathbf{\bar{p}}') = (A-1)t_{PN}^{d}(\mathbf{\bar{p}},\mathbf{\bar{p}}')S_{0}(\mathbf{\bar{p}}-\mathbf{\bar{p}}'), \quad (18a)$$

with t_{pN}^{d} as the pN direct scattering amplitude and S_{0} the nuclear elastic form factor. In terms of the solution $T^{d'}$ of a Lippmann-Schwinger equation

$$T^{d'} = U_{\text{opt}}^{(1)} + U_{\text{opt}}^{(1)} \tilde{G}_0 T^{d'},$$
 (18b)

 $(\tilde{G}_0$ describes the propagation only in the nuclear

966

ground state) the actual elastic scattering amplitudes given by the first order optical potential is $T^{d} \equiv T_{MS}^{d} = (A/A - 1)T^{d'}$. Kerman, McManus, and Thaler follow the prescription of Takeda and Watson in order to obtain the elastic scattering amplitude T^{a} . Thus, in Eqs. (18a) and (18b),

they replace t_{pN}^{d} by t_{pN}^{a} (the properly antisymmetrized amplitude). Iterating these equations one gets

$$T^{a}_{\rm KMT} \equiv T^{a}_{\rm MS} = A\langle t^{a} \rangle + A(A-1)\langle t^{a} \rangle \tilde{G}_{0}\langle t^{a} \rangle + A(A-1)^{2} \langle t^{a} \rangle \tilde{G}_{0}\langle t^{a} \rangle \tilde{G}_{0}\langle t^{a} \rangle + \cdots .$$
(18c)

Our result differs from (18c). Using the same approximations of exact multiple scattering equations leading to the potential (18a) we obtain, by means of Eq. (18b), for the multiple scattering part of T^a [T^{ex} (Eq. 17c) is not present in KMT]

$$T_{MS}^{a} = A(t_{pN}^{a}S_{0} + T^{d}G_{0}^{a}t_{pN}^{a}S_{0})$$

$$= A\langle t^{a} \rangle + A\langle A - 1 \rangle \langle t^{d} \rangle \tilde{G}_{0} \langle t^{a} \rangle$$

$$+ A\langle A - 1 \rangle^{2} \langle t^{d} \rangle \tilde{G}_{0} \langle t^{d} \rangle \tilde{G}_{0} \langle t^{a} \rangle + \cdots .$$
(19)

Since the original *exact* expression for the antisymmetrized amplitude, Eq. (17b), differs es-

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sentially from the approximate prescription of Takeda and Watson, Eq. (19) constitutes an improvement over Eqs. (18b)-(18c).

Finally, it is of interest to compare the cluster exchange amplitude (17c) with a similar term appearing in the standard distorted wave theory for inelastic scattering.¹⁰ There one needs the exact final state Ψ^a as well as an initial state distorted by an optical potential, chosen to affect only the relative motion of the projectile and target. Equation (17c) contains an undistorted initial state and a final state $\Psi_k^d = (1 + G_0 T^d) | \mathbf{k}, A \rangle$ apparently distorted by scattering operators τ^d which are not antisymmetrized.

Detailed derivations of Eq. (17), as well as applications to large-angle elastic and inelastic p-nucleus scattering data, will be published elsewhere.^{7,8} This method can be generalized also for any type of nuclear reaction. It is shown in Ref. 7 that the analysis of data with our method is not more complicated than the use of standard methods which neglect antisymmetrization.

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