Translation invariance and antisymmetry in the theory of the nucleon optical model.∗

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The first step in any formalism that aims to connect a many-nucleon theory of nucleon-nucleus scattering and the concept of an optical model potential in the sense pioneered by Feshbach is to explain what is meant by the optical model wavefunction. By definition this is a function of a single space coordinate plus a set of single nucleon internal variables. This article gives a critique of the definition as it is frequently expressed in 2nd Quantisation language and suggest a new definition which is more consistent with the requirements of antisymmetry and translational invariance. A modification of the time-dependent Green’s function formalism is suggested.

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I. INTRODUCTION.

Theories devoted to calculating an optical potential that describes nucleon scattering from an A-nucleon target in terms of fundamental 2- and 3-body inter-nucleon interactions are of considerable current interest. For scattering from light nuclei fully antisymmetrised and translationally invariant resonating-group ab initio calculations have been successfully developed, see [1], [2] and references therein. For heavier targets a recent report by Idini, et al.,[3] references several approaches. They also report their own calculations of nucleon optical potentials based on a self-consistent Green’s function formalism (SCGF) which it is claimed is well suited to calculating optical potentials for medium mass targets.

Work on the fundamental definition of the optical model potential goes back to the pioneering work of Feshbach[4]. This work and subsequent work by Bell and Squires [5] and Capuzzi and Mahaux[6], as well as the more recent work reported in [7] and [3], all seek a function of one spatial coordinate and a set of single nucleon spin and iso-spin coordinates that can be identified as an optical model wave function. This is usually defined as the projection of the exact antisymmetrised many-body nucleon-A scattering wave function, |Ψ_E+⟩, onto the exact antisymmetrised target ground state, |Ψ_0⟩. It is standard to interpret this definition in 2nd Quantisation notation through the formula

$$\xi_E^+(r) = \langle \Psi_0 | \psi(r) | \Psi_E^+ \rangle.$$  

(1)

For a translationally invariant many-nucleon Hamiltonian the (A + 1)-nucleon scattering state |Ψ_E^+⟩ can be assumed to have a definite total momentum and in the c.m. system this momentum will be zero. Similarly, it can be assumed that the A-nucleon target ground |Ψ_0⟩ also has total momentum zero. Under these assumptions it will be shown that ξ_E^+(r) as defined in eq.(1) is independent of the space coordinate element of r and hence cannot possibly be an acceptable definition of the optical model wave function. It is the purpose of this paper to justify this statement and present a modified definition that corresponds more faithfully to the properties expected for the microscopic optical model. No new numerical calculations using the new definition are presented.

A. The case of single determinant states.

For medium and heavy targets all approaches have in common the use of a single particle mean-field basis in which nucleon antisymmetry is fully taken into account using second-quantisation techniques but introduces a violation of translation invariance very early in the development. To see how problems arise with this approach the mean-field limit is considered. In this limit the target ground state |Ψ_0⟩ is a single determinant of A bound single particle states in some potential well and |Ψ_E^+⟩ is a determinant of the same A states but with the extra nucleon in a continuum scattering state, u_k(r) in the same potential well.

In this special case the formula (1), \langle \Psi_0 | \psi(r) | \Psi_E^+ \rangle, gives precisely the scattering state u_k(r), so identifying the optical potential with the mean field, as expected. This result gives a false sense of security for the validity of formula

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Hence this integral is independent of \( r \) space:

Formally, this misleading result arises because determinants are not eigenstates of definite total momentum and hence the result outlined in the previous Section and proved in Section II does not apply. If one tried to improve the determinants for their violation of translation invariance by, \( e.g. \), projecting them on to their zero total momentum components and then using the formula (1) the result would be a function independent of \( r \) and certainly not acceptable.

II. WHY THE DEFINITION OF THE OPTICAL MODEL WAVE FUNCTION THROUGH EQ.(1) MUST BE REJECTED.

(i) The quantity \( \xi_{E^+}(r) \) from eq.(1) can be evaluated using the wave functions defining \( \Psi_0 \) and \( \Psi_{E^+} \) in configuration space:

\[
\xi_{E^+}(r) = \langle \Psi_0 | \psi(r) | \Psi_{E^+} \rangle = \sqrt{(A+1)} \int dr_1 \ldots dr_A \Psi_0^*(r_1, \ldots r_A) \times \Psi_{E^+}(r_1, \ldots r_A, r_{(A+1)} = r)
\]

\[
= \sqrt{(A+1)} \int dr_1 \ldots dr_A dr_{(A+1)} \Psi_0^*(r_1, \ldots r_A) \times \delta(r_{(A+1)} - r) \Psi_{E^+}(r_1, \ldots r_A, r_{(A+1)} - r).
\]

This integral is independent of \( r \). This can be seen by first translating the first \( A \) variables of integration by \( r \) to \( r'_i = r_i - r, \ i = 1, \ldots, A \), and using the fact that \( \Psi_0 \) and \( \Psi_{E^+} \) are zero-momentum states so that

\[
\Psi_0(r_1 + r, \ldots r_A + r) = \Psi_0(r_1, \ldots r_A),
\]

\[
\Psi_{E^+}(r'_1 + r, \ldots r'_A + r, r_{(A+1)}) = \Psi_{E^+}(r_1, \ldots r_A, r_{(A+1)} - r).
\]

Hence

\[
\xi_{E^+}(r) = \sqrt{(A+1)} \int dr'_1 \ldots dr'_A dr_{(A+1)} \Psi_0^*(r'_1 + r, \ldots r'_A + r) \times \delta(r_{(A+1)} - r) \Psi_{E^+}(r'_1, \ldots r'_A + r, r_{(A+1)} - r)
\]

\[
= \sqrt{(A+1)} \int dr'_1 \ldots dr'_A dr_{(A+1)} \Psi_0^*(r'_1, \ldots r'_A) \times \delta(r_{(A+1)} - r) \Psi_{E^+}(r'_1, \ldots r'_A, r_{(A+1)} - r)
\]

\[
= \sqrt{(A+1)} \int dr'_1 \ldots dr'_A \Psi_0^*(r'_1, \ldots r'_A) \times \Psi_{E^+}(r'_1, \ldots r'_A, r_{(A+1)} = 0),
\]

which is independent of \( r \).

(ii) The same \( r \)-independent result is obtained when the right-hand-side of eq.(1) is evaluated using Fock-space formalism techniques. For simplicity explicit reference to spin and iso-spin coordinates is omitted. The notation \( | \ldots \rangle \) is used for vectors in Fock space.

The states \( | \Psi_{E^+} \rangle \) and \( | \Psi_0 \rangle \) are both eigenstates of the total momentum operator \( \hat{P} \) with eigenvalue zero, where

\[
\hat{P} = \int dk \ k a_k^\dagger a_k,
\]

and \( a_k^\dagger (a_k) \) creates (destroys) a nucleon in a single particle state with momentum \( k \).

In terms of state vectors and operators in Fock space

\[
\hat{P} \ | \Psi_0 \rangle = 0,
\]

\[
\hat{P} \ | \Psi_{E^+} \rangle = 0.
\]

It follows from from eq.(5) that

\[
[\hat{P}, \psi(r)]_- = i(\nabla_r \psi(r)),
\]
and hence
\[
\langle \nabla r \xi_{E^+}(r) \rangle = \langle \langle \Psi_0 | [\hat{P}, \psi(r)]_+ | \Psi_{E^+} \rangle \rangle \\
= \langle \langle \Psi_0 | (\hat{P} \psi(r) - \psi(r) \hat{P}) | \Psi_{E^+} \rangle \rangle \\
= 0. \tag{8}
\]

Hence, \( \xi_{E^+}(r) \) is independent of \( r \) and can not be the required optical model wave function. More generally, if \( | \Psi_1 \rangle \) and \( | \Psi_2 \rangle \) have momenta \( K_1 \) and \( K_2 \), respectively, then
\[
\langle \langle \Psi_1 | \psi(r) | \Psi_2 \rangle \rangle = \exp(iK_2 - K_1, r) \langle \langle \Psi_1 | \psi(0) | \Psi_2 \rangle \rangle. \tag{9}
\]

One comes to the same conclusion working in momentum space:
\[
\xi_{E^+}(r) = \langle \Psi_0 | \psi(r) | \Psi_{E^+} \rangle \\
= \int \frac{dk}{(2\pi)^{3/2}} \exp(ik \cdot r) \langle \Psi_0 | a_k | \Psi_{E^+} \rangle \\
= \int \frac{dk}{(2\pi)^{3/2}} \langle \Psi_0 | a_{k=0} | \Psi_{E^+} \rangle \delta(k) \\
= \frac{1}{(2\pi)^{3/2}} \langle \Psi_0 | a_{k=0} | \Psi_{E^+} \rangle. \tag{10}
\]

Again it seen that \( \xi_{E^+}(r) \) as defined by eq.(11) is independent of \( r \). The result (9) follows in a similar fashion.

III. DEFINITION OF THE OPTICAL MODEL WAVE FUNCTION.

The standard way of defining the type of \( A \)-nucleon, \((A+1)\)-nucleon overlap of which the optical model wave function is an example is to use a set of \( A-1 \) translationally invariant variables \( \chi_1, \ldots, \chi_{(A-1)} \) \((\text{e.g., Jacobi coordinates})\) that together with the \( A \)-nucleon c.m., \( R_A \), form a set of variables equivalent to the vectors \( r_1, \ldots, r_A \) describing the position of the nucleons relative to an arbitrary origin and have a transformation Jacobian equal to \(+1\). The variables \( \chi_1, \ldots, \chi_{(A-1)}, \chi_A \), together with the \( A+1 \)-nucleon c.m. \( R_{(A+1)} \), perform the same role for \( A+1 \) nucleons, where \( \chi_A \) is defined by
\[
\chi_A = r_{(A+1)} - R_A, \quad R_A = \left( \sum_{i=1}^{A} r_i \right)/A. \tag{11}
\]

In terms of these coordinates the relevant overlap is
\[
\xi_{E^+} (r) = (A+1) \int d\chi_1 \cdots d\chi_{(A-1)} | \Psi_0^+(\chi_1, \ldots, \chi_{(A-1)}) \times | \Psi_{E^+} (\chi_1, \ldots, \chi_{(A-1)}, \chi_A = r) \rangle. \tag{12}
\]

The zero momentum functions \( \Psi_{E^+} \) and \( \Psi_0 \) are independent of, respectively, \( R_{(A+1)} \) and \( R_A \).

The function defined in eq.(12) is certainly not generally independent of \( r \). From the definition of \( \chi_A \) it is clear the the meaning of \( r \) is the vector distance of the extra nucleon from the c.m. of the target.

Similar overlap functions are familiar from the study of the overlaps between bound state of the \( A \)- and \((A+1)\)-nucleon systems in the theory of \((d,p)\) and \((p,d)\) reactions. They have been shown to satisfy an inhomogeneous differential equation (the "source equation") in which the kinetic energy operator appears with the correct reduced mass and whose solutions have been extensively studied, see [3], [0].

The Jacobi coordinates do not lend themselves well to treating antisymmetrised functions. The 2nd Quantisation formalism is more attractive from this point of view. In the next Section a new formula is derived for the optical model wave function, and in fact for a general \( A \)-nucleon, \((A+1)\)-nucleon overlap, in terms of operators and states in Fock space by working directly from eq.(12).
IV. THE OPTICAL MODEL WAVE FUNCTION AS A MATRIX ELEMENT IN FOCK SPACE.

It is straightforward to convert the expression (12) to a relation between state vectors and creation and destruction operators acting in nucleon Fock space. Some key relevant formulae are gathered for convenience in Appendix A.

In general the argument, \( \psi(r) \), of creation and destruction operators refers to the position of a nucleon relative to the origin of coordinates. It is therefore convenient to first change the integration in eq. (12) to over 3\( A \) independent variables by introducing an extra integration over \( R_A \) in the form

\[
\xi^{(+)}_E(r) = \sqrt{(A+1)} \int d\chi_1 \ldots d\chi_{(A-1)} dR_A \delta(R_A) \Psi_0^*(\chi_1, \ldots, \chi_{(A-1)}) \\
\quad \times \Psi^{(+)}_E(\chi_1, \ldots, \chi_{(A-1)}, x_A = r) \\
= \sqrt{(A+1)} \int dr_1 \ldots dr_{(A-1)} dr_A \delta(R_A) \Psi^*_0(r_1, \ldots, r_A) \\
\quad \times \Psi^{(+)}_E(r_1, \ldots, r_A, r_{(A+1)} = r).
\]

In the second equality the variables of integration have been changed to \( r_1, \ldots, r_A \) using the relation between these and the Jacobi coordinates for nucleons of the same mass,

\[
\chi_i = r_{(i+1)} - R_i, \quad i = 1, \ldots, A.
\]

The inverse of these relations gives the set \( r_1, \ldots, r_A \) as linear functions of the set \( \chi_1, \ldots, \chi_{(A-1)}, R_A \). The coordinate \( r_{(A+1)} \) is given by \( \chi_A + R_A = r \) under the integral sign. In understanding these steps it may be helpful to consider the \( A = 2 \) case explicitly, with \( \chi_1 = (r_2 - r_1), \chi_2 = (r_3 - R_2), \quad R_2 = (r_2 + r_1)/2, \) and the inverse relations \( r_3 = R_3 + 2\chi_2/3, \quad r_2 = R_3 - \chi_2/3 + \chi_1/2, \quad r_1 = R_3 - \chi_2/3 - \chi_1/2. \)

Note that strict notational conventions require the use of a different symbol for, e.g., \( \Psi_0 \), considered as a function of \( r_1, \ldots, r_A \) in the last line in eq. (13). This step is avoided here by using the convention

\[
\Psi_0(r_1, \ldots, r_A) = \Psi_0(\chi_1(r_1, \ldots, r_A), \ldots, \chi_{(A-1)}(r_1, \ldots, r_A)),
\]

where \( \chi_i(r_1, \ldots, r_A), \quad i = 1, \ldots, (A - 1) \) refers to the linear equations of the transformation between the two sets of variables.

The relation given in eq. (16) of Appendix A enables the definition (13) to be written

\[
\xi^{(+)}_E(r) = \langle \langle \Psi(0, x = 0) | \psi(r) | \Psi^{(+)}_E \rangle \rangle.
\]

where, for arbitrary \( x, \)

\[
| \Psi(n, x) \rangle = \frac{1}{\sqrt{A!}} \int dr_1 dr_2 \ldots dr_A \delta(R_A - x) \Psi_n(r_1, \ldots, r_A) \psi^\dagger(r_A) \psi^\dagger(r_1) | 0 \rangle.
\]

and

\[
| \Psi^{(+)}_E \rangle = \frac{1}{\sqrt{(A+1)!}} \int dr_1 dr_2 \ldots dr_{(A+1)} \psi^{(+)}(r_1, \ldots, r_{(A+1)}) \psi^\dagger(r_{(A+1)}) \psi^\dagger(r_1) | 0 \rangle.
\]

The kets \( | \Psi(n, x) \rangle \) form a complete set of antisymmetric \( A \)-nucleon states with an intrinsic state labelled by \( n \) and c.m. located at position \( x \) relative to an arbitrary origin. The bra in eq. (16) has the c.m. of the \( A \) target nucleons located at the origin, although in fact any value of \( x \) could have been chosen.

In this Section a general definition of an optical model wave function, eq. (16), has been obtained as the matrix element of a nucleon destruction operator between many-nucleon states in Fock space by starting from a standard translationally invariant definition in terms of many-body wave functions expressed in terms of Jacobi coordinates. In the next Section it is shown how the definition (16) can be derived from more basic physical ideas of what is meant by the optical model wave function.
A. Physical basis for the optical model wave function.

The precise definition of the \( A+1 \)-nucleon scattering state \( | \Psi_{E^+} \rangle \) will be discussed in Section VII. Leaving this aside for the present, a natural definition of the optical model wave function is the amplitude for finding in \( | \Psi_{E^+} \rangle \), \( A \) nucleons in the ground state, \( \psi_0(r_1, \ldots, r_A) \), of the \( A \)-nucleon Hamiltonian with a total momentum \( \mathbf{K}' \), and a single nucleon at a distance \( r \) from the c.m. of the other \( A \) nucleons. This antisymmetric \( A+1 \)-nucleon state is written \( \Phi_{\mathbf{r},0,\mathbf{K}'} \). Note that this definition means that \( r \) is not the eigenvalue of a single nucleon position operator because the positions of all \( A+1 \) nucleons are involved in its definition.

In configuration space the state \( \phi_{\mathbf{r},0,\mathbf{K}'} \) is described by the wave function

\[
\phi_{\mathbf{r},0,\mathbf{K}'}(r_1, \ldots, r_A, r_{(A+1)}) = \frac{1}{\sqrt{(A+1)!}} (1 - \sum_{j=1}^{A} P_{(i(A+1),j)} \delta(r_{(A+1)} - R_A - r) \times \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot \mathbf{K}') \psi_0(r_1, \ldots, r_A),
\]

(19)

where \( P_{(i,j)} \) interchanges the all the coordinates of nucleons \( i \) and \( j \), and

\[
R_A = (\sum_{i=1}^{i=A} r_i)/A.
\]

(20)

It is assumed that the many-nucleon Hamiltonian is translationally invariant and that the \( A \)-nucleon ground state \( \psi_0 \) has total momentum zero and is antisymmetrised in all nucleon coordinates. The factor \( 1/\sqrt{(A+1)!} \) has been chosen for later convenience.

For the wave function given in (19) the relation (A4) of Appendix A gives the Fock space equivalent

\[
| \Phi(\mathbf{r}, 0, \mathbf{K}') \rangle = \frac{1}{\sqrt{A!}} \int dr_1 \ldots dr_A \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot \mathbf{K}') \psi_0(r_1, \ldots, r_A) \times \psi^\dagger(\mathbf{r} + \mathbf{R}_A) \psi^\dagger(\mathbf{r}_A) \ldots \psi^\dagger(\mathbf{r}_1) | 0 \rangle.
\]

(21)

This state can be written in various ways.

Using

\[
\exp(+i\mathbf{R}_A \cdot \hat{\mathbf{P}}) \psi^\dagger(\mathbf{r}_i) \exp(-i\mathbf{R}_A \cdot \hat{\mathbf{P}}) = \psi^\dagger(\mathbf{r}_i - \mathbf{R}_A),
\]

(22)

and \( \hat{\mathbf{P}} | 0 \rangle = 0 \), eq.(21) can be written

\[
| \Phi(\mathbf{r}, 0, \mathbf{K}') \rangle = \frac{1}{\sqrt{A!}} \int dr_1 \ldots dr_A \psi_0(r_1, \ldots, r_A) \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot (\mathbf{K}' - \hat{\mathbf{P}})) \times \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}_A - \mathbf{R}_A) \ldots \psi^\dagger(\mathbf{r}_1 - \mathbf{R}_A) | 0 \rangle.
\]

(23)

To exploit the fact that the ground state \( \psi_0(r_1, \ldots, r_A) \) has zero momentum the integration variables in eq.(23) are changed to the set of \( A-1 \) translationally invariant variables \( \chi_1, \ldots, \chi_{(A-1)} \) introduced following eq.(14) above. Together with \( \mathbf{R}_A \) they form a set of variables equivalent to \( r_1, \ldots, r_A \) and have a transformation Jacobian of +1. Under a translation of the coordinate system by \( \mathbf{x} \) the \( \chi_1, \ldots, \chi_{(A-1)} \) are unchanged and \( \mathbf{R}_A \rightarrow \mathbf{R}_A + \mathbf{x} \).

The integral in eq.(23) becomes

\[
| \Phi(\mathbf{r}, 0, \mathbf{K}') \rangle = \frac{1}{\sqrt{A!}} \int d\chi_1 \ldots d\chi_{(A-1)} d\mathbf{R}_A \psi_0(r_1, \ldots, r_A) \times \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot (\mathbf{K}' - \hat{\mathbf{P}})) \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}_A - \mathbf{R}_A) \ldots \psi^\dagger(\mathbf{r}_1 - \mathbf{R}_A) | 0 \rangle.
\]

(24)

Note that in eq.(24) the functional convention introduced in eq.(15) is used.

The combinations \( \mathbf{r}_i - \mathbf{R} \) that appear as arguments of the creation operators in eq.(24) are all translationally invariant, as is \( \psi_0(r_1, \ldots, r_A) \). Therefore, they can be expressed entirely in terms of the variables \( \chi_1, \ldots, \chi_{(A-1)} \) and
are independent of $R_A$. The integral over $R_A$ can therefore be carried out to give
\[
|\Phi(r, 0, K')\rangle = (2\pi)^{3/2} \delta(K' - \vec{P}) \psi^\dagger(r) \times \left[ \frac{1}{\sqrt{A!}} \int d\chi_1 \cdots d\chi_{(A-1)} \psi_0(r_1, \ldots, r_A) \psi^\dagger(r_A - R_A) \cdots \psi^\dagger(r_1 - R_A) | 0 \rangle \right],
\]
(25)
where the translationally invariant combinations $r_i - R_A$, $i = 1 \ldots A$, and the arguments of $\psi_0$ are functions of the $(A - 1)$ coordinates $\chi_i$ only.

The quantity in square brackets in eq. (25) can be rewritten in terms of an integral over the $A$ coordinates $r_1, \ldots, r_A$ by introducing an extra integration over $R_A$ with a factor $\delta(R_A)$ in the integrand as in the discussion around eq. (17). The quantity in square brackets in eq. (25) can now be written
\[
|\Psi(0, x = 0)\rangle = \frac{1}{\sqrt{A!}} \int d\chi_1 \cdots d\chi_{(A-1)} \psi_0(r_1, \ldots, r_A) \psi^\dagger(r_A(\chi)) \cdots \psi^\dagger(r_1(\chi)) | 0 \rangle
\]
= \frac{1}{\sqrt{A!}} \int dr_1 \cdots dr_A \delta(R_A) \psi_0(r_1, \ldots, r_A) \psi^\dagger(r_A) \cdots \psi^\dagger(r_1) | 0 \rangle,
\]
(26)
In the first line $r_i(\chi)$ means $r_i - R_A$ expressed as a function of the $(A - 1)$ coordinates $\chi_i$.

Comparing with eq. (25) it can be seen that this is just the formula for the Fock space equivalent to the $A$-nucleon wave function $\delta(R_A) \psi_0(r_1, \ldots, r_A)$, with an internal state characterised by the index "0" and zero momentum and with its c.m. located with certainty at the origin of coordinates.

The final expression for the state $|\Phi(r, 0, K')\rangle$ needed to define the optical model wave function is therefore
\[
|\Phi(r, 0, K')\rangle = (2\pi)^{3/2} \delta(K' - K) \langle \Psi(0, x = 0) | \psi(r) | \Psi_1(K) \rangle,
\]
(27)
Using these definitions the result for the overlap of this state with an $(A + 1)$ nucleon state $|\Psi_1(K)\rangle$ with momentum $K$ is
\[
\langle \Phi(r, 0, K') | \Psi_1(K) \rangle = (2\pi)^{3/2} \delta(K' - K) \langle \Psi(0, x = 0) | \psi(r) | \Psi_1(K) \rangle,
\]
(28)
where $|\Psi(0, x = 0)\rangle$ is defined in eq. (26).

The expression $\langle \Psi(0, x = 0) | \psi(r) | \Psi_1(K) \rangle$ that appears on the right-hand-side of eq. (28) is a more general example of the overlap introduced earlier in eq. (16). Note that $|\Psi(0, x = 0)\rangle$ does not have definite momentum. In fact the $\delta(R_A)$ factor in eq. (26) means that in this state all values of the total momentum of the $A$-nucleons are equally probable. On the other hand the operator $\delta(K' - \vec{P})$ in the ket $|\Phi(r, 0, K')\rangle$ given in eq. (25) projects out a component of momentum $K'$ from any state it acts on and hence gives rise to the momentum conserving delta function $\delta(K' - K)$ in the complete overlap $\langle \Phi(r, 0, K') | \Psi_1(K) \rangle$ given in eq. (28). This delta function would be integrated over a narrow wave packet in momentum space in any complete scattering theory. The other factors on the right-hand-side of eq. (28) are the main focus of interest.

For translationally invariant Hamiltonians it can be assumed that $|\Psi_1(K)\rangle$ has the form
\[
\langle r_1, \ldots, r_{(A+1)} | \Psi_1(K) \rangle = \frac{1}{(2\pi)^{3/2}} \exp(iR_{(A+1)}.K) \Psi_1(r_1, \ldots, r_{(A+1)}),
\]
(29)
where $\Psi_1$ is an intrinsic state of zero momentum.

Scattering theories are usually expressed in terms of overall c.m. system quantities. In the following therefore $K = K' = 0$ is assumed and any reference to these quantities is omitted in the notation. The quantity defined by
\[
\xi_{0,1}(r) = \langle \Psi(0, x = 0) | \psi(r) | \Psi_1 \rangle,
\]
(30)
coincides with that introduced in Section 11, eq. (16).

It can be checked that if the overlap $\langle \Phi(r, 0, K') | \Psi_1(K) \rangle$ is calculated directly using the configuration space wave functions (19) and (29) one obtains the result corresponding to (12) after a momentum conserving delta function is removed and $K$ and $K'$ are set equal to zero.

In the next Section it will be shown that when $\Psi_0$ and $\Psi_1$ are associated with the same Hamiltonian operator in Fock space, $\xi_{0,1}$ satisfies an inhomogeneous differential equation ("source equation") with a kinetic energy term that carries the correct reduced mass for motion of one nucleon relative to the c.m. of the other $A$ nucleons.
V. SOURCE EQUATION FOR $\xi_{0,1}(r)$.

It is assumed that $\psi_0(r_1, \ldots, r_A)$ is an eigenstate of the $A$-nucleon intrinsic Hamiltonian $H = (\mathbf{P})^2/(2Am)$ with eigenvalue $E_0$, where $\mathbf{P}$ is the $A$-nucleon total momentum operator. By construction the intrinsic Hamiltonian operator commutes with the c.m. coordinate $\mathbf{R}_A$ and hence

\[
(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)) | \Psi(0, x = 0)\rangle = E_0 | \Psi(0, x = 0)\rangle.
\]

is a valid Fock-space equation where $\hat{H}$ and $\hat{\mathbf{P}}$ are Fock-space operators and $| \Psi(0, x = 0)\rangle$ is the state defined in eq. (23).

If $\Psi_1$ is an $(A+1)$, zero momentum, eigenstate of $H$ with eigenvalue $E_1$ it is also an eigenstate of the Fock-space operator $(\hat{H} - (\hat{\mathbf{P}})^2/(2Am))$ because $\hat{\mathbf{P}} | \Psi_1\rangle = 0$.

\[
(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)) | \Psi_1\rangle = E_1 | \Psi_1\rangle.
\]

It follows that

\[
(E_0 - E_1)\xi_{0,1}(r) = \langle \langle \Psi(0, x = 0) | (\hat{H} - (\hat{\mathbf{P}})^2/(2Am))\psi(r) | \Psi_1\rangle \rangle
- \langle \langle \Psi(0, x = 0) | \psi(r)(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)) | \Psi_1\rangle \rangle
= \langle \langle \Psi(0, x = 0) | [(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)), \psi(r)]_- | \Psi_1\rangle \rangle.
\]

It is assumed that $\hat{H}$ can be written as the sum of a kinetic energy term $\hat{T}$ and a potential energy term $\hat{V}$:

\[
\hat{H} = \hat{T} + \hat{V},
\]

where

\[
\hat{T} = -\frac{\hbar^2}{2m} \int dr' \psi^\dagger(r')(\nabla^2_{\mathbf{r'}}\psi(r')),
\]

and hence

\[
[\hat{T}, \psi^\dagger(r)]_- = \frac{\hbar^2}{2m}(\nabla^2_{\mathbf{r}}\psi(r)),
\]

and

\[
[\hat{T}, \psi(r)]_- = +\frac{\hbar^2}{2m}(\nabla^2_{\mathbf{r}}\psi(r)).
\]

Using these commutators and the results (7) in eq. (33)

gives

\[
(E_0 - E_1)\xi_{0,1}(r) = \langle \langle \Psi(0, x = 0) | [\hat{T}, \psi(r)]_- | \Psi_1\rangle \rangle + \langle \langle \Psi(0, x = 0) | [\hat{V}, \psi(r)]_- | \Psi_1\rangle \rangle
- \langle \langle \Psi(0, x = 0) | [\hat{\mathbf{P}}^2/(2Am), \psi(r)]_- | \Psi_1\rangle \rangle
= \langle \langle \Psi(0, x = 0) | \frac{\hbar^2}{2m}(\nabla^2_{\mathbf{r}}\psi(r)) | \Psi_1\rangle \rangle + \langle \langle \Psi(0, x = 0) | [\hat{V}, \psi(r)]_- | \Psi_1\rangle \rangle
- \langle \langle \Psi(0, x = 0) | -\frac{\hbar^2}{2mA}(\nabla^2_{\mathbf{r}}\psi(r)) | \Psi_1\rangle \rangle
= (1 + \frac{1}{A}(\frac{\hbar^2}{2mA}\nabla^2_{\mathbf{r}}])\xi_{0,1}(r) + \langle \langle \Psi(0, x = 0) | [\hat{V}, \psi(r)]_- | \Psi_1\rangle \rangle.
\]

Hence

\[
(-\frac{\hbar^2}{2\mu_mA}\nabla^2_{\mathbf{r}} - (E_1 - E_0))\xi_{0,1}(r) = \langle \langle \Psi(0, x = 0) | [\psi(r), \hat{V}]_- | \Psi_1\rangle \rangle,
\]

where

\[
\mu_mA = \frac{A}{(A + 1)^m},
\]
is the nucleon-\(A\) reduced mass.

In the case that \(\Psi_1\) describes a scattering state in the overall c.m. system corresponding to elastic scattering of a nucleon by an \(A\)-nucleon in its ground state \(\Psi_0\), the eigenvalue \(E_1\) is

\[
E_1 = E_0 + \frac{\hbar^2 k_1^2}{2\mu_mA},
\]

where \(k_1\) is the incident nucleon momentum in the c.m. system.

Eq. (39) can now be written

\[
(-\frac{\hbar^2}{2\mu_mA} \nabla^2 - \frac{\hbar^2 k_1^2}{2\mu_mA})\xi_{0,1}(r) = \langle\langle \Psi(0, x = 0) | [\psi(r), V]_- | \Psi_1 \rangle\rangle,
\]

(42)

Many techniques have been developed to deal with the source term \([\psi(r), V]_-\), including work dedicated to expressing the source term as an operator in single nucleon degrees of freedom acting on \(\xi_{0,1}(r)\) and hence providing a microscopic basis for the optical model. The aim of much of this work is to link up with standard many-body theories of nuclear structure which exploit a basis of determinants of single nucleon states in a potential fixed relative to the origin of coordinates and hence introduce a violation of translation invariance very early in the development. For example, this is true of the work of Bell and Squires [5] and Capuzzi and Mahaux [6], as well as the more recent work [7] cited in the Introduction. In common with references [5], Capuzzi and [6], and [7] they use a definition of the optical model wave function based eq. (1) instead of eq. (30). This is at least formally unacceptable. Further work is needed to assess any quantitative consequences.

As a first step to carrying forward an approach based on eq. (42), the next Section shows how the modified definition of the optical model wave function given in eqs. (16) and (30) can be expressed in terms of a time dependent one-body Green’s function. It was mentioned in the Introduction that time dependent Green’s function methods are believed to be the way forward for medium and heavy targets.

VI. THE OPTICAL MODEL WAVE FUNCTION IN TERMS OF A TIME DEPENDENT GREEN’S FUNCTION.

\(\Psi_1\) describes a scattering state with a plane wave nucleon incident on an \(A\)-nucleon ground state \(\psi_0\) as the incident channel and outgoing waves in all other channels. In the overall c.m. system this state is the limit as \(\epsilon \to 0\) of the state

\[
| \Psi_1^* \rangle = \frac{i\epsilon}{E_1 - H + i\epsilon} (2\pi)^{3/2} a_{k_1}^\dagger | -k_1, \psi_0 \rangle,
\]

(43)

where \((2\pi)^{3/2} a_{k_1}^\dagger | -k_1, \psi_0 \rangle\) describes the incident channel in which the incident nucleon has momentum \(k_1\) and the target has a total momentum \(-k_1\). In configuration space this incident channel state is the antisymmetrised version of

\[
\exp(ik_1 \cdot x_A)\psi_0(x_1, \ldots, x_{(A-1)}) = \exp(ik_1 \cdot r_{(A+1)}) \exp(-i k_1 \cdot R_A)\psi_0(r_1, \ldots, r_A).
\]

(44)

The expression (43) is the generalisation to include c.m. degrees of freedom explicitly of the formulation of collision theory described in [6], their eq.(4.19), and [10].

In order to make a connection with time-dependent Green functions a time variable is introduced via the identity \((\hbar = 1)\)

\[
\frac{i\epsilon}{E_1 + i\epsilon - H} = \epsilon \int_{-\infty}^{0} dt \exp(-i(E_1 + i\epsilon - H)t).
\]

(45)

The scattering state defined in eq. (43) can now be written

\[
| \Psi_1^* \rangle = \epsilon \int_{-\infty}^{0} dt \exp(-i(E_1 + i\epsilon - H)t) \times (2\pi)^{3/2} a_{k_1}^\dagger | -k_1, \psi_0 \rangle,
\]

(46)
and from eq. (30) the optical model overlap is
\[ \xi_{0,1}(r) = \langle \langle \Psi(0, x=0) \mid \psi(r) \epsilon \int_{-\infty}^{0} dt \exp(-i(E_1 + i\epsilon - H)t) \times (2\pi)^{3/2}a_{k_1}^\dagger \mid -k_1, \psi_0) \rangle \].

This expression can be written in terms of the Heisenberg operators
\[ \Psi(r, t) = \exp(iHt)\psi(r) \exp(-iHt) \]
\[ \Psi^\dagger(r, t) = \exp(iHt)\psi^\dagger(r) \exp(-iHt) \]
\[ A_{k_1}^\dagger(t) = \exp(iHt)a_{k_1}^\dagger \exp(-iHt). \]

In terms of these eq. (47 becomes
\[ \xi_{0,1}(r) = \langle \langle \Psi(0, x=0) \mid \epsilon \int_{-\infty}^{0} dt \Psi(r, t=0) \exp(-i(E_1 + i\epsilon)t) \times (2\pi)^{3/2}a_{k_1}^\dagger \mid -k_1, \psi_0) \rangle \]
\[ \times \langle \langle -k_1, \psi_0 \rangle \rangle. \]

The derivation of the last line of eq. (49) has used
\[ H \mid -k_1, \psi_0) = (E_0 + E_{1A}) \mid -k_1, \psi_0) \]
where \( E_0 \) is the ground state energy of the target and \( E_{1A} \) is the incident target c.m. kinetic energy
\[ E_{1A} = \frac{\hbar^2k_1^2}{2Am}. \]

\( E_1 - E_0 - E_{1A} \) is therefore the incident nucleon kinetic energy
\[ \epsilon_{k_1} = \frac{\hbar^2k_1^2}{2m}. \]

The expression (49) for the optical model wavefunction can be written in terms of a Green function by using
\[ a_{k_1}^\dagger = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}\cdot\mathbf{r}')}{(2\pi)^{3/2}} \psi^\dagger(\mathbf{r}'). \]

It follows from this that
\[ a_{k_1}^\dagger = \int d\mathbf{k}' \delta(k_1 - k')a_{k'}^\dagger \]
\[ = \int d\mathbf{k}' \left( \int d\mathbf{r}' \frac{\exp(i(\mathbf{k}_1 - \mathbf{k}')\cdot\mathbf{r}')}{(2\pi)^{3/2}} \right) a_{k'}^\dagger \]
\[ = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}_1\cdot\mathbf{r}')}{(2\pi)^{3/2}} \int d\mathbf{k}' \frac{\exp(-i\mathbf{k}'\cdot\mathbf{r}')}{(2\pi)^{3/2}} a_{k'}^\dagger \]
\[ = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}_1\cdot\mathbf{r}')}{(2\pi)^{3/2}} \psi^\dagger(\mathbf{r}'). \]
and hence
\[
A_{k_1}^\dagger(t) = \exp(iHt)\phi_{k_1}^\dagger \exp(-iHt) = \int dr' \exp(i\mathbf{k}_1 \cdot \mathbf{r}') \frac{\Psi^\dagger(r', t)}{(2\pi)^{3/2}}.
\] (55)

It follows from eqs. (19) and (55) that
\[
\xi_{0,1}(r) = \langle \langle \Psi(0, \mathbf{x} = 0) | e^{i0} \int_{-\infty}^{0} dt \Psi(r, t = 0) \exp(-i(\mathbf{e}_{k_1} + \mathbf{e}) t) 
\times (2\pi)^{3/2}A_{k_1}^\dagger(t) | -k_1, \psi_0 \rangle \rangle,
\]
\[
= e^{i0} \int_{-\infty}^{0} dt \int dr' \exp(-i(\mathbf{e}_{k_1} + \mathbf{e}) t)) \times \exp(i\mathbf{k}_1 \cdot \mathbf{r}') \langle \langle \Psi(0, \mathbf{x} = 0) | \mathcal{T}\{\Psi(r, 0) \Psi^\dagger(r', t)\} | -k_1, \psi_0 \rangle \rangle.
\] (56)

The time ordering operator \( \mathcal{T} \) can be introduced without error because all values of \( t \) in the integral satisfy \( t < 0 \). Eq. (56) can be written
\[
\xi_{0,k_1}(r) = e^{i0} \int_{-\infty}^{0} dt \int dr' \exp(i(\mathbf{k}_1 \cdot \mathbf{r}' - (\mathbf{e}_{k_1} + \mathbf{e}) t)) \times G(r, t = 0; r', t)
\] (57)

where the Green function is given by
\[
G(r, t; r', t') = \langle \langle \Psi(0, \mathbf{x} = 0) | \mathcal{T}\{\Psi(r, t) \Psi^\dagger(r', t')\} | -k_1, \psi_0 \rangle \rangle.
\] (58)

This differs from the usual groundstate-groundstate one-nucleon Green function in that the bra the groundstate has a c.m. localised at the origin and the ket the ground state has the total momentum \( -k_1 \), i.e., opposite to the incident nucleon momentum in the overall c.m. system. It would be interesting to explore how far these differences leads to significant quantitative effects on the calculation of microscopic optical potentials.

Eq. (57) differs from the expression for the optical model wavefunction given by Bell and Squires. These differences appear to come from the way boundary conditions are handled. Bell and Squires introduce an unusual asymptotic condition which specifies a point source of particles at a large distance. They then project out a state with definite incident nucleon momentum in the overall c.m. system. It would be interesting to explore how far this differences leads to similar quantitative effects. Bell and Squires mention that the differences in Eq. (57) may alter the diagrams appearing in the perturbation expansion of the Green function.

Extensive quantitative comparisons of translational invariant and non-invariant calculations of overlap functions of bound state wave functions ("center-of-mass corrections") have been published in Ref. [8], and references therein. These calculations evaluate the source term in eq. (12) within the fully antisymmetrised translationally invariant oscillator shell-model and use a formulation of the overlap function in terms of Jacobi coordinates as defined in eq. (12) of Section III. Therefore, they do not suffer from the definition difficulties set out in Section III.

Of particular relevance are the results obtained in Ref. [8] for Asymptotic Normalisation Coefficients (ANCs), which determine the amplitude of the overlap function in the region outside the \( A \)-nucleon nucleus and which one might expect are influenced by similar considerations as the optical model scattering amplitude in the case of an optical model overlap. Ref. [8], Table 1, quotes c.m. corrections to squared ANC of 15.5% even for the \( ^{40}\text{Ca} - ^{41}\text{Ca} \) overlap with \( A \) as large as 40. According to ref. [8] these corrections are much larger than one would expect simply from the use of the correct reduced mass in the kinetic energy term in the source equation and scaling corrections deduced from the harmonic oscillator model. This suggests that similar quantitative effects may arise from c.m. corrections incorporated in the new formalism developed in Sections V and VI for the case of nucleon-nucleus scattering.

VII. CONCLUSIONS

A new fully antisymmetrised, translationally invariant definition of the nucleon-nucleus optical model wave function in terms of many-nucleon scattering wave function has been introduced. It has been shown that this wavefunction
satisfies a differential equation in which the kinematically correct kinetic energy operator appears. It has also been shown how this wave function can be related to a modified definition of a one-nucleon time-dependent Green’s function.

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Appendix A: Brief notes on 2nd Quantisation.

Many-body theory can be formulated in a new space (Fock space) in which states exist that have components in different orthogonal sub-spaces, each of which corresponds to a different number of particles (nucleons in the present case), including one component with zero particles, the vacuum. The Fock space concept allows the introduction of operators, such as creation and destruction operators that act in Fock space and connect sub-spaces with different numbers of particles. The nuclear states dealt with here usually have a definite number of particles and hence only one component in Fock space, and Hamiltonians that do not connect states with different numbers of particles, but in handling antisymmetry requirements Fock space ideas frequently simplify calculations considerably. In BCS pairing theory one actually does deal with states that do not have a definite number of nucleons and therefore have non-zero components in orthogonal parts of Fock space.

A general state vector, $|A\rangle\rangle$, in Fock space has the form

$$|A\rangle\rangle = \begin{cases} A_0 \\ |A_1\rangle_{(1)} \\ |A_2\rangle_{(1)(2)} \\ . \\ |A_n\rangle_{(1)(2)...(n)} \\ . \end{cases} \text{,} \quad (A1)$$

where the number $A_0$ is the amplitude for finding the system in a state with zero nucleons. The state with zero nucleons is called the vacuum and has a zero in every row except the first, i.e.

$$|0\rangle = \begin{cases} 1 \\ 0 \\ . \end{cases} \text{.} \quad (A2)$$
In eqs. (A1) the quantity $| A_j \rangle_{(1)}$ is a state vector in the single nucleon subspace of nucleon labelled "1", $| A_2 \rangle_{(1)(2)}$ is an antisymmetrized state in the 2-nucleon subspace of nucleons "1" and "2", and, in the row labelled $n$, $| A_n \rangle_{(1)(2)...(n)}$ is an antisymmetrized state in the $n$-nucleon subspace of nucleons "1" to "$n$".

Note that the rows of $| A \rangle$ are labelled with the integers 0, 1, 2, ..., starting with row "0" which contains the vacuum amplitude $A_0$.

In general a double right-angle bracket, $| ... \rangle \rangle$, is used to denote state vectors in Fock space and the usual single right-hand bracket, $| ... \rangle$, to denote a state with a definite number of nucleons.

1. **Definition of creation and destruction operators.**

The complete definition of the creation and destruction operators acting on a general ket $| A \rangle \rangle$ in Fock space as ($x$ signifies a set of commuting nucleonic dynamic variables for space, spin and isospin)

$$
\psi^\dagger(x_0 \mid A \rangle \rangle) = \begin{cases}
0 \\
\frac{1}{\sqrt{2}} A_0 \mid x_0 \rangle_{(1)} \\
\frac{1}{\sqrt{2}} A_{1(2)} \mid x_0 \rangle_{(1)} \mid A_1 \rangle_{(2)} \\
\frac{1}{\sqrt{n}} A_{1(2...n)} \mid x_0 \rangle_{(1)} \mid A_{n-1} \rangle_{(2)...(n)} \\
\vdots
\end{cases},
$$

$$
\psi(x_0 \mid A \rangle \rangle) = \begin{cases}
\langle x_0 \mid A_1 \rangle \\
\sqrt{2} \int dx_2 \mid x_2 \rangle_{(1)} \langle x_0, x_2 \mid A_2 \rangle \\
\vdots
\sqrt{(n+1)} \int dx_2 \ldots dx_{n+1} \mid x_2, \ldots x_{n+1} \rangle_{(1)...(n)} \langle x_0, x_2, \ldots x_{n+1} \mid A_{n+1} \rangle \\
\vdots
\end{cases}.
$$

(A3)

Here $A_{1(2...n)}$ acts on the labels of nucleons 1, 2, ..., $n$, and is defined by

$$
A_{1(2...n)} = 1 - \sum_{j=2}^{n} P_{(1,j)},
$$

(A4)

where $P_{(1,j)}$ interchanges the labels of nucleons 1 and $j$.

2. **Connection between a state in Fock space with a definite number of nucleons and a many-body wave function**

An $A$-nucleon state with wave function $\phi_S(x_1, x_2 \ldots x_A)$ is described in Fock space by a vector $| \Phi_S \rangle \rangle$ given by

$$
| \Phi_S \rangle \rangle = \frac{1}{\sqrt{A!}} \int dx_1 dx_2 \ldots dx_A \phi_S(x_1, \ldots x_A) \psi^\dagger(x_A) \ldots \psi^\dagger(x_1) | 0 \rangle \rangle.
$$

(A5)

The notation used is $x_1 = r_1, s_z, \tau_3$, etc., and the integral signs include a summation over $s_z = \pm 1/2, \tau_3 = \pm 1/2$.

The inverse of (A3) is

$$
\phi_S(x_1, \ldots x_A) = \frac{1}{\sqrt{A!}} \langle 0 \mid \psi(x_1) \ldots \psi(x_A) | \Phi_S \rangle \rangle.
$$

(A6)

The operator $\psi^\dagger(x_0)$ creates a particle at $x_0$. Its adjoint $\psi(x_0)$ destroys a particle at point $x_0$. A formal definition of what these statements mean in terms of the action of these operators on an arbitrary Fock state is given in eqs. (A3).
above; however, these definitions are rarely needed in practice and all one invariably has to use is the anti-commutation relations that can be derived from the definitions:

\[
\begin{align*}
\psi(x_0)\psi(x_0') + \psi(x_0')\psi(x_0) &= 0, \quad \psi(x_0)\psi(x_0') = 0, \\
\psi(x_0)\psi(x_0') + \psi(x_0')\psi(x_0) &= 0, \quad \psi(x_0)\psi(x_0') = 0, \\
\psi(x_0)\psi(x_0') + \psi(x_0')\psi(x_0) &= \delta(x_0 - x_0').
\end{align*}
\] (A7)