

# Translation invariance and antisymmetry in the theory of the nucleon optical model

R. C. Johnson\*

Department of Physics, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom

(Received 11 April 2017; published 13 June 2017)

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 wave function. 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 second quantization language and suggests 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.

DOI: [10.1103/PhysRevC.95.064610](https://doi.org/10.1103/PhysRevC.95.064610)

## I. INTRODUCTION

Theories devoted to calculating an optical potential that describes nucleon scattering from an  $A$ -nucleon target in terms of fundamental two- and three-body internucleon interactions are of considerable current interest. For scattering from light nuclei, fully antisymmetrized and translationally invariant resonating-group *ab initio* calculations have been successfully developed; see Refs. [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 is claimed to be well suited for 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 Refs. [3,7], all seek a function of one spatial coordinate and a set of single nucleon spin and isospin coordinates that can be identified as an optical model wave function. This is usually defined as the projection of the exact antisymmetrized many-body nucleon- $A$  scattering wave function,  $|\Psi_{E^+}\rangle$ , onto the exact antisymmetrized target ground state,  $|\Psi_0\rangle$ . It is standard to interpret this definition in second-quantization notation through the formula

$$\xi_{E^+}(\mathbf{r}) = \langle \Psi_0 | \psi(\mathbf{r}) | \Psi_{E^+} \rangle. \quad (1)$$

For a translationally invariant many-nucleon Hamiltonian, the  $(A+1)$ -nucleon scattering state  $|\Psi_{E^+}\rangle$  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  $|\Psi_0\rangle$  also has total momentum of zero. Under these assumptions, it will be shown that  $\xi_{E^+}(\mathbf{r})$  as defined in Eq. (1) is independent of the space coordinate element of  $\mathbf{r}$  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-quantization 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  $|\Psi_0\rangle$  is a single determinant of  $A$  bound single-particle states in some potential well and  $|\Psi_{E^+}\rangle$  is a determinant of the same  $A$  states but with the extra nucleon in a continuum scattering state,  $u_k(\mathbf{r})$  in the same potential well.

In this special case, the formula (1),  $\langle \Psi_0 | \psi(\mathbf{r}) | \Psi_{E^+} \rangle$ , gives precisely the scattering state  $u_k(\mathbf{r})$ , so identifying the optical potential with the mean field, as expected. This result gives a false sense of security for the validity of formula (1) because it fails to recognize the properties of this expression when exact, rather than model many-nucleon wave functions are used.

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 Sec. 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  $\mathbf{r}$  and certainly not acceptable.

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

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

$$\begin{aligned} \xi_{E^+}(\mathbf{r}) &= \langle \Psi_0 | \psi(\mathbf{r}) | \Psi_{E^+} \rangle \\ &= \sqrt{(A+1)} \int d\mathbf{r}_1 \dots d\mathbf{r}_A \Psi_0^*(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \Psi_{E^+}(\mathbf{r}_1, \dots, \mathbf{r}_A, \mathbf{r}_{(A+1)} = \mathbf{r}) \\ &= \sqrt{(A+1)} \int d\mathbf{r}_1 \dots d\mathbf{r}_A d\mathbf{r}_{(A+1)} \Psi_0^*(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \delta(\mathbf{r}_{(A+1)} - \mathbf{r}) \Psi_{E^+}(\mathbf{r}_1, \dots, \mathbf{r}_A, \mathbf{r}_{(A+1)}). \end{aligned} \quad (2)$$

\*R.Johnson@surrey.ac.uk

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

$$\begin{aligned} \Psi_0(\mathbf{r}_1 + \mathbf{r}, \dots, \mathbf{r}_A + \mathbf{r}) &= \Psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A), \\ \Psi_{E^+}(\mathbf{r}'_1 + \mathbf{r}, \dots, \mathbf{r}'_A + \mathbf{r}, \mathbf{r}_{(A+1)}) &= \Psi_{E^+}(\mathbf{r}_1, \dots, \\ &\quad \mathbf{r}_A, \mathbf{r}_{(A+1)} - \mathbf{r}). \end{aligned} \quad (3)$$

Hence,

$$\begin{aligned} \xi_{E^+}(\mathbf{r}) &= \sqrt{(A+1)} \int d\mathbf{r}'_1 \dots d\mathbf{r}'_A d\mathbf{r}_{(A+1)} \\ &\quad \times \Psi_0^*(\mathbf{r}'_1 + \mathbf{r}, \dots, \mathbf{r}'_A + \mathbf{r}) \\ &\quad \times \delta(\mathbf{r}_{(A+1)} - \mathbf{r}) \Psi_{E^+}(\mathbf{r}'_1 + \mathbf{r}, \dots, \mathbf{r}'_A + \mathbf{r}, \mathbf{r}_{(A+1)}) \\ &= \sqrt{(A+1)} \int d\mathbf{r}'_1 \dots d\mathbf{r}'_A d\mathbf{r}_{(A+1)} \Psi_0^*(\mathbf{r}'_1, \dots, \mathbf{r}'_A) \\ &\quad \times \delta(\mathbf{r}_{(A+1)} - \mathbf{r}) \Psi_{E^+}(\mathbf{r}'_1, \dots, \mathbf{r}'_A, \mathbf{r}_{(A+1)} - \mathbf{r}) \\ &= \sqrt{(A+1)} \int d\mathbf{r}'_1 \dots d\mathbf{r}'_A \Psi_0^*(\mathbf{r}'_1, \dots, \mathbf{r}'_A) \\ &\quad \times \Psi_{E^+}(\mathbf{r}'_1, \dots, \mathbf{r}'_A, \mathbf{r}_{(A+1)} = 0), \end{aligned} \quad (4)$$

which is independent of  $\mathbf{r}$ .

(ii) The same  $\mathbf{r}$ -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 isospin coordinates is omitted. The notation  $|\dots\rangle$  is used for vectors in Fock space.

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

$$\hat{\mathbf{P}} = \int d\mathbf{k} \mathbf{k} a_k^\dagger a_k, \quad (5)$$

and  $a_k^\dagger(a_k)$  creates (destroys) a nucleon in a single-particle state with momentum  $\mathbf{k}$ .

In terms of state vectors and operators in Fock space,

$$\begin{aligned} \hat{\mathbf{P}}|\Psi_0\rangle &= 0, \\ \hat{\mathbf{P}}|\Psi_{E^+}\rangle &= 0. \end{aligned} \quad (6)$$

It follows from Eq. (5) that

$$[\hat{\mathbf{P}}, \psi(\mathbf{r})]_- = i[\nabla_r \psi(\mathbf{r})], \quad (7)$$

and hence

$$\begin{aligned} i[\nabla_r \xi_{E^+}(\mathbf{r})] &= \langle \langle \Psi_0 | [\hat{\mathbf{P}}, \psi(\mathbf{r})]_- | \Psi_{E^+} \rangle \rangle \\ &= \langle \langle \Psi_0 | (\hat{\mathbf{P}} \psi(\mathbf{r}) - \psi(\mathbf{r}) \hat{\mathbf{P}}) | \Psi_{E^+} \rangle \rangle \\ &= 0. \end{aligned} \quad (8)$$

Hence,  $\xi_{E^+}(\mathbf{r})$  is independent of  $\mathbf{r}$  and cannot be the required optical model wave function.

More generally, if  $|\Psi_1\rangle$  and  $|\Psi_2\rangle$  have momenta  $\mathbf{K}_1$  and  $\mathbf{K}_2$ , respectively, then

$$\langle \langle \Psi_1 | \psi(\mathbf{r}) | \Psi_2 \rangle \rangle = \exp(i(\mathbf{K}_2 - \mathbf{K}_1)\mathbf{r}) \langle \langle \Psi_1 | \psi(0) | \Psi_2 \rangle \rangle. \quad (9)$$

One comes to the same conclusion working in momentum space:

$$\begin{aligned} \xi_{E^+}(\mathbf{r}) &= \langle \Psi_0 | \psi(\mathbf{r}) | \Psi_{E^+} \rangle \\ &= \int d\mathbf{k} \frac{\exp(i\mathbf{k} \cdot \mathbf{r})}{(2\pi)^{3/2}} \langle \Psi_0 | a_{\mathbf{k}} | \Psi_{E^+} \rangle \\ &= \int d\mathbf{k} \frac{\exp(i\mathbf{k} \cdot \mathbf{r})}{(2\pi)^{3/2}} \langle \Psi_0 | a_{\mathbf{k}=0} | \Psi_{E^+} \rangle \delta(\mathbf{k}) \\ &= \frac{1}{(2\pi)^{3/2}} \langle \Psi_0 | a_{\mathbf{k}=0} | \Psi_{E^+} \rangle. \end{aligned} \quad (10)$$

Again, it seen that  $\xi_{E^+}(\mathbf{r})$  as defined by Eq. (1) is independent of  $\mathbf{r}$ . 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  $\chi_1, \dots, \chi_{(A-1)}$  (e.g., Jacobi coordinates) that together with the  $A$ -nucleon c.m.,  $\mathbf{R}_A$ , form a set of variables equivalent to the vectors  $\mathbf{r}_1, \dots, \mathbf{r}_A$  describing the position of the nucleons relative to an arbitrary origin and having a transformation Jacobian equal to  $+1$ . The variables  $\chi_1, \dots, \chi_{(A-1)}, \chi_A$ , together with the  $A+1$ -nucleon c.m.  $\mathbf{R}_{(A+1)}$ , perform the same role for  $A+1$  nucleons, where  $\chi_A$  is defined by

$$\chi_A = \mathbf{r}_{(A+1)} - \mathbf{R}_A, \quad \mathbf{R}_A = \left( \sum_{i=1}^{i=A} \mathbf{r}_i \right) / A. \quad (11)$$

In terms of these coordinates, the relevant overlap is

$$\begin{aligned} \xi_{E^+}(\mathbf{r}) &= \sqrt{(A+1)} \int d\chi_1 \dots d\chi_{(A-1)} \Psi_0^*(\chi_1, \dots, \chi_{(A-1)}) \\ &\quad \times \Psi_{E^+}(\chi_1, \dots, \chi_{(A-1)}, \chi_A = \mathbf{r}). \end{aligned} \quad (12)$$

The zero-momentum functions  $\Psi_{E^+}$  and  $\Psi_0$  are independent of, respectively,  $\mathbf{R}_{(A+1)}$  and  $\mathbf{R}_A$ .

The function defined in Eq. (12) is certainly not generally independent of  $\mathbf{r}$ . From the definition of  $\chi_A$ , it is clear that the meaning of  $\mathbf{r}$  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 states 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 Refs. [8,9].

The Jacobi coordinates do not lend themselves well to treating antisymmetrized functions. The second-quantization 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 formulas are gathered for convenience in Appendix A.

In general, the argument,  $\psi(\mathbf{r})$ , 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 one over  $3A$  independent variables by introducing an extra integration over  $\mathbf{R}_A$  in the form

$$\begin{aligned} \xi_{E^+}(\mathbf{r}) &= \sqrt{(A+1)} \int d\chi_1 \dots d\chi_{(A-1)} d\mathbf{R}_A \delta(\mathbf{R}_A) \\ &\quad \times \Psi_0^*(\chi_1, \dots, \chi_{(A-1)}) \\ &\quad \times \Psi_{E^+}(\chi_1, \dots, \chi_{(A-1)}, \chi_A = \mathbf{r}) \\ &= \sqrt{(A+1)} \int d\mathbf{r}_1 \dots d\mathbf{r}_{(A-1)} d\mathbf{r}_A \delta(\mathbf{R}_A) \Psi_0^*(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \Psi_{E^+}(\mathbf{r}_1, \dots, \mathbf{r}_A, \mathbf{r}_{(A+1)} = \mathbf{r}). \end{aligned} \quad (13)$$

In the second equality, the variables of integration have been changed to  $\mathbf{r}_1, \dots, \mathbf{r}_A$  using the relation between these and the Jacobi coordinates for nucleons of the same mass:

$$\chi_i = \mathbf{r}_{(i+1)} - \mathbf{R}_i, \quad i = 1, \dots, A, \quad (14)$$

where  $\mathbf{R}_i$  is the c.m. coordinate of nucleons  $1, \dots, i$ . The inverse of these relations gives the set  $\mathbf{r}_1, \dots, \mathbf{r}_A$  as linear functions of the set  $\chi_1, \dots, \chi_{(A-1)}, \mathbf{R}_A$ . The coordinate  $\mathbf{r}_{(A+1)}$  is given by  $\chi_A + \mathbf{R}_A = \mathbf{r}$  under the integral sign. (In understanding these steps, it may be helpful to consider the  $A = 2$  case explicitly, with  $\chi_1 = (\mathbf{r}_2 - \mathbf{r}_1)$ ,  $\chi_2 = (\mathbf{r}_3 - \mathbf{R}_2)$ ,  $\mathbf{R}_2 = (\mathbf{r}_2 + \mathbf{r}_1)/2$ , and the inverse relations  $\mathbf{r}_3 = \mathbf{R}_3 + 2\chi_2/3$ ,  $\mathbf{r}_2 = \mathbf{R}_3 - \chi_2/3 + \chi_1/2$ ,  $\mathbf{r}_1 = \mathbf{R}_3 - \chi_2/3 - \chi_1/2$ .)

Note that strict notational conventions require the use of a different symbol for, e.g.,  $\Psi_0$ , considered as a function of  $\mathbf{r}_1, \dots, \mathbf{r}_A$  in the last line in Eq. (13). This step is avoided here by using the convention

$$\Psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A) = \Psi_0(\chi_1(\mathbf{r}_1, \dots, \mathbf{r}_A), \dots, \chi_{(A-1)}(\mathbf{r}_1, \dots, \mathbf{r}_A)), \quad (15)$$

where  $\chi_i(\mathbf{r}_1, \dots, \mathbf{r}_A)$ ,  $i = 1, \dots, (A-1)$  refers to the linear equations of the transformation between the two sets of variables.

The relation given in Eq. (A6) of the appendix enables the definition (13) to be written

$$\xi_{E^+}(\mathbf{r}) = \langle \langle \Psi(0, \mathbf{x} = 0) | \psi(\mathbf{r}) | \Psi_{E^+} \rangle \rangle. \quad (16)$$

where, for arbitrary  $\mathbf{x}$ ,

$$\begin{aligned} |\Psi(n, \mathbf{x})\rangle &= \frac{1}{\sqrt{A!}} \int d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_A \delta(\mathbf{R}_A - \mathbf{x}) \\ &\quad \times \Psi_n(\mathbf{r}_1, \dots, \mathbf{r}_A) \psi^\dagger(\mathbf{r}_A) \dots \psi^\dagger(\mathbf{r}_1) |0\rangle \end{aligned} \quad (17)$$

and

$$\begin{aligned} |\Psi_{E^+}\rangle &= \frac{1}{\sqrt{(A+1)!}} \int d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_{(A+1)} \\ &\quad \times \Psi_{E^+}(\mathbf{r}_1, \dots, \mathbf{r}_{(A+1)}) \psi^\dagger(\mathbf{r}_{(A+1)}) \dots \psi^\dagger(\mathbf{r}_1) |0\rangle. \end{aligned} \quad (18)$$

The kets  $|\Psi(n, \mathbf{x})\rangle$  form a complete set of antisymmetric  $A$ -nucleon states with an intrinsic state labeled by  $n$  and c.m. located at position  $\mathbf{x}$  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  $\mathbf{x}$  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 Sec. VI. 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,  $\psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$ , of the  $A$ -nucleon Hamiltonian with a total momentum  $\mathbf{K}'$ , and a single nucleon at a distance  $\mathbf{r}$  from the c.m. of the other  $A$  nucleons. This antisymmetric  $(A+1)$ -nucleon state is written as  $\Phi_{\mathbf{r}, 0, \mathbf{K}'}$ . Note that this definition means that  $\mathbf{r}$  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

$$\begin{aligned} \Phi_{\mathbf{r}, 0, \mathbf{K}'}(\mathbf{r}_1, \dots, \mathbf{r}_A, \mathbf{r}_{(A+1)}) &= \frac{1}{\sqrt{(A+1)!}} \left( 1 - \sum_{j=1}^A P_{((A+1), j)} \right) \delta(\mathbf{r}_{(A+1)} - \mathbf{R}_A - \mathbf{r}) \\ &\quad \times \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot \mathbf{K}') \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A), \end{aligned} \quad (19)$$

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

$$\mathbf{R}_A = \left( \sum_{i=1}^{i=A} \mathbf{r}_i \right) / A. \quad (20)$$

It is assumed that the many-nucleon Hamiltonian is translationally invariant and that the  $A$ -nucleon ground state  $\psi_0$  has total momentum of zero and is antisymmetrized 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 (A5) of the appendix gives the Fock space equivalent

$$\begin{aligned} |\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle &= \frac{1}{\sqrt{A!}} \int d\mathbf{r}_1 \dots d\mathbf{r}_A \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot \mathbf{K}') \\ &\quad \times \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A) \psi^\dagger(\mathbf{r} + \mathbf{R}_A) \psi^\dagger(\mathbf{r}_A) \dots \psi^\dagger(\mathbf{r}_1) |0\rangle. \end{aligned} \quad (21)$$

This state can be written in various ways.

Using

$$\exp(+i\mathbf{R}_A \cdot \hat{\mathbf{P}})\psi^\dagger(\mathbf{r}_i)\exp(-i\mathbf{R}_A \cdot \hat{\mathbf{P}}) = \psi^\dagger(\mathbf{r}_i - \mathbf{R}_A), \quad (22)$$

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

$$\begin{aligned} & |\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle \\ &= \frac{1}{\sqrt{A!}} \int d\mathbf{r}_1 \dots d\mathbf{r}_A \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot (\mathbf{K}' - \hat{\mathbf{P}})) \\ &\quad \times \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}_A - \mathbf{R}_A) \dots \psi^\dagger(\mathbf{r}_1 - \mathbf{R}_A)|0\rangle\rangle. \quad (23) \end{aligned}$$

To exploit the fact that the ground state  $\psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$  has zero momentum, the integration variables in Eq. (23) are changed to the set of  $A - 1$  translationally invariant variables  $\chi_1, \dots, \chi_{(A-1)}$  introduced following Eq. (12) above. Together with  $\mathbf{R}_A$ , they form a set of variables equivalent to  $\mathbf{r}_1, \dots, \mathbf{r}_A$  and have a transformation Jacobian of  $+1$ . Under a translation of the coordinate system by  $\mathbf{x}$ , the  $\chi_1, \dots, \chi_{(A-1)}$  are unchanged and  $\mathbf{R}_A \rightarrow \mathbf{R}_A + \mathbf{x}$ .

The integral in Eq. (23) becomes

$$\begin{aligned} & |\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle \\ &= \frac{1}{\sqrt{A!}} \int d\chi_1 \dots d\chi_{(A-1)} d\mathbf{R}_A \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_A \cdot (\mathbf{K}' - \hat{\mathbf{P}}))\psi^\dagger(\mathbf{r})\psi^\dagger \\ &\quad \times (\mathbf{r}_A - \mathbf{R}_A) \dots \psi^\dagger(\mathbf{r}_1 - \mathbf{R}_A)|0\rangle\rangle. \quad (24) \end{aligned}$$

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  $\psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$ . Therefore, they can be expressed entirely in terms of the variables  $\chi_1, \dots, \chi_{(A-1)}$  and are independent of  $\mathbf{R}_A$ . The integral over  $\mathbf{R}_A$  can therefore be carried out to give

$$\begin{aligned} & |\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle \\ &= (2\pi)^{3/2} \delta(\mathbf{K}' - \hat{\mathbf{P}})\psi^\dagger(\mathbf{r}) \\ &\quad \times \left[ \frac{1}{\sqrt{A!}} \int d\chi_1 \dots d\chi_{(A-1)} \psi_0(\mathbf{r}_1, \dots, \right. \\ &\quad \left. \times \mathbf{r}_A)\psi^\dagger(\mathbf{r}_A - \mathbf{R}_A) \dots \psi^\dagger(\mathbf{r}_1 - \mathbf{R}_A)|0\rangle\rangle \right], \quad (25) \end{aligned}$$

where the translationally invariant combinations  $\mathbf{r}_i - \mathbf{R}_A$ ,  $i = 1 \dots A$ , 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  $\mathbf{r}_1, \dots, \mathbf{r}_A$  by introducing an extra integration over  $\mathbf{R}_A$  with a factor  $\delta(\mathbf{R}_A)$  in the integrand as in the discussion around Eq. (17). The quantity in square brackets in Eq. (25) can now be written as

$$\begin{aligned} |\Psi(0, \mathbf{x} = 0)\rangle\rangle &= \frac{1}{\sqrt{A!}} \int d\chi_1 \dots d\chi_{(A-1)} \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A) \\ &\quad \times \psi^\dagger(\mathbf{r}_A(\chi)) \dots \psi^\dagger(\mathbf{r}_1(\chi))|0\rangle\rangle \end{aligned}$$

$$\begin{aligned} &= \frac{1}{\sqrt{A!}} \int d\mathbf{r}_1 \dots d\mathbf{r}_A \delta(\mathbf{R}_A) \\ &\quad \times \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)\psi^\dagger(\mathbf{r}_A) \dots \psi^\dagger(\mathbf{r}_1)|0\rangle\rangle, \quad (26) \end{aligned}$$

In the first line,  $\mathbf{r}_i(\chi)$  means  $\mathbf{r}_i - \mathbf{R}_A$  expressed as a function of the  $(A - 1)$  coordinates  $\chi_i$ .

By comparing with Eq. (A5), it can be seen that this is just the formula for the Fock space equivalent to the  $A$ -nucleon wave function  $\delta(\mathbf{R}_A)\psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$ , with an internal state characterized 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  $|\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle$  needed to define the optical model wave function is therefore

$$|\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle = (2\pi)^{3/2} \delta(\mathbf{K}' - \hat{\mathbf{P}})\psi^\dagger(\mathbf{r})|\Psi(0, \mathbf{x} = 0)\rangle\rangle. \quad (27)$$

When these definitions are used, the result for the overlap of this state with an  $(A + 1)$  nucleon state  $|\Psi_{1, \mathbf{K}}\rangle\rangle$  with momentum  $\mathbf{K}$  is

$$\begin{aligned} \langle\langle \Phi(\mathbf{r}, 0, \mathbf{K}') | \Psi_{1, \mathbf{K}} \rangle\rangle &= (2\pi)^{3/2} \delta(\mathbf{K}' - \mathbf{K}) \langle\langle \Psi(0, \mathbf{x} = 0) | \\ &\quad \times \psi(\mathbf{r}) | \Psi_{1, \mathbf{K}} \rangle\rangle, \quad (28) \end{aligned}$$

where  $|\Psi(0, \mathbf{x} = 0)\rangle\rangle$  is defined in Eq. (26).

The expression  $\langle\langle \Psi(0, \mathbf{x} = 0) | \psi(\mathbf{r}) | \Psi_{1, \mathbf{K}} \rangle\rangle$  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  $|\Psi(0, \mathbf{x} = 0)\rangle\rangle$  does not have definite momentum. In fact, the  $\delta(\mathbf{R}_A)$  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  $\delta(\mathbf{K}' - \hat{\mathbf{P}})$  in the ket  $|\Phi(\mathbf{r}, 0, \mathbf{K}')\rangle\rangle$  given in Eq. (25) projects out a component of momentum  $\mathbf{K}'$  from any state it acts on and hence gives rise to the momentum-conserving  $\delta$  function  $\delta(\mathbf{K}' - \hat{\mathbf{K}})$  in the complete overlap  $\langle\langle \Phi_{\mathbf{r}, 0, \mathbf{K}'} | \Psi_{1, \mathbf{K}} \rangle\rangle$  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  $|\Psi_{1, \mathbf{K}}\rangle\rangle$  has the form

$$\begin{aligned} \langle\langle \mathbf{r}_1, \dots, \mathbf{r}_{(A+1)} | \Psi_{1, \mathbf{K}} \rangle\rangle &= \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{R}_{(A+1)} \cdot \mathbf{K}) \\ &\quad \times \Psi_1(\mathbf{r}_1, \dots, \mathbf{r}_{(A+1)}), \quad (29) \end{aligned}$$

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,  $\mathbf{K} = \mathbf{K}' = 0$  is assumed and any reference to these quantities is omitted in the notation. The quantity defined by

$$\xi_{0,1}(\mathbf{r}) = \langle\langle \Psi(0, \mathbf{x} = 0) | \psi(\mathbf{r}) | \Psi_1 \rangle\rangle \quad (30)$$

coincides with that introduced in Sec. IV, Eq. (16).

It can be checked that if the overlap  $\langle\langle \Phi(\mathbf{r}, 0, \mathbf{K}') | \Psi_{1, \mathbf{K}} \rangle\rangle$  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  $\mathbf{K}$  and  $\mathbf{K}'$  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 $\xi_{0,1}(\mathbf{r})$ .

It is assumed that  $\psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$  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

$$[\hat{H} - (\hat{\mathbf{P}})^2/(2Am)]|\Psi(0, \mathbf{x} = 0)\rangle = E_0|\Psi(0, \mathbf{x} = 0)\rangle \quad (31)$$

is a valid Fock-space equation where  $\hat{H}$  and  $\hat{\mathbf{P}}$  are Fock-space operators and  $|\Psi(0, \mathbf{x} = 0)\rangle$  is the state defined in Eq. (26).

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  $\hat{\mathbf{P}}|\Psi_1\rangle = 0$ :

$$[\hat{H} - (\hat{\mathbf{P}})^2/(2Am)]|\Psi_1\rangle = E_1|\Psi_1\rangle. \quad (32)$$

It follows that

$$\begin{aligned} (E_0 - E_1)\xi_{0,1}(\mathbf{r}) &= \langle\langle\Psi(0, \mathbf{x} = 0) | (\hat{H} - (\hat{\mathbf{P}})^2/(2Am))\psi(\mathbf{r}) | \Psi_1\rangle\rangle \\ &\quad - \langle\langle\Psi(0, \mathbf{x} = 0) | \psi(\mathbf{r})(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)) | \Psi_1\rangle\rangle \\ &= \langle\langle\Psi(0, \mathbf{x} = 0) | [(\hat{H} - (\hat{\mathbf{P}})^2/(2Am)), \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle. \end{aligned} \quad (33)$$

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

$$\hat{H} = \hat{T} + \hat{V}, \quad (34)$$

where

$$\hat{T} = -\frac{\hbar^2}{2m} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}') (\nabla_{\mathbf{r}'}^2 \psi(\mathbf{r}')), \quad (35)$$

and hence

$$[\hat{T}, \psi^\dagger(\mathbf{r})]_- = -\frac{\hbar^2}{2m} (\nabla_{\mathbf{r}}^2 \psi^\dagger(\mathbf{r})) \quad (36)$$

and

$$[\hat{T}, \psi(\mathbf{r})]_- = +\frac{\hbar^2}{2m} (\nabla_{\mathbf{r}}^2 \psi(\mathbf{r})). \quad (37)$$

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

$$\begin{aligned} (E_0 - E_1)\xi_{0,1}(\mathbf{r}) &= \langle\langle\Psi(0, \mathbf{x} = 0) | [\hat{T}, \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle \\ &\quad + \langle\langle\Psi(0, \mathbf{x} = 0) | [\hat{V}, \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle \\ &\quad - \langle\langle\Psi(0, \mathbf{x} = 0) | [(\hat{\mathbf{P}})^2/(2Am), \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle \\ &= \langle\langle\Psi(0, \mathbf{x} = 0) | \frac{\hbar^2}{2m} (\nabla_{\mathbf{r}}^2 \psi(\mathbf{r})) | \Psi_1\rangle\rangle \\ &\quad + \langle\langle\Psi(0, \mathbf{x} = 0) | [\hat{V}, \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle \\ &\quad - \langle\langle\Psi(0, \mathbf{x} = 0) | \frac{-\hbar^2}{2mA} (\nabla_{\mathbf{r}}^2 \psi(\mathbf{r})) | \Psi_1\rangle\rangle \end{aligned}$$

$$\begin{aligned} &= \left(1 + \frac{1}{A}\right) \left(\frac{\hbar^2}{2m}\right) \nabla_{\mathbf{r}}^2 \xi_{0,1}(\mathbf{r}) \\ &\quad + \langle\langle\Psi(0, \mathbf{x} = 0) | [\hat{V}, \psi(\mathbf{r})]_- | \Psi_1\rangle\rangle. \end{aligned} \quad (38)$$

Hence,

$$\begin{aligned} &\left[-\frac{\hbar^2}{2\mu_{mA}} \nabla_{\mathbf{r}}^2 - (E_1 - E_0)\right] \xi_{0,1}(\mathbf{r}) \\ &= \langle\langle\Psi(0, \mathbf{x} = 0) | [\psi(\mathbf{r}), V]_- | \Psi_1\rangle\rangle, \end{aligned} \quad (39)$$

where

$$\mu_{mA} = \frac{A}{(A + 1)} m \quad (40)$$

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

$$E_1 = E_0 + \frac{\hbar^2 k_1^2}{2\mu_{mA}}, \quad (41)$$

where  $\mathbf{k}_1$  is the incident nucleon momentum in the c.m. system.

Equation (39) can now be written

$$\begin{aligned} &\left(-\frac{\hbar^2}{2\mu_{mA}} \nabla_{\mathbf{r}}^2 - \frac{\hbar^2 k_1^2}{2\mu_{mA}}\right) \xi_{0,1}(\mathbf{r}) \\ &= \langle\langle\Psi(0, \mathbf{x} = 0) | [\psi(\mathbf{r}), V]_- | \Psi_1\rangle\rangle. \end{aligned} \quad (42)$$

Many techniques have been developed to deal with the source term  $[\psi(\mathbf{r}), V]_-$ , including work dedicated to expressing the source term as an operator in single nucleon degrees of freedom acting on  $\xi_{0,1}(\mathbf{r})$  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. Like Refs. [5] and [6] the authors of Ref. [7] 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  $\epsilon \rightarrow 0^+$  of the state

$$|\Psi_1^\epsilon\rangle = \frac{i\epsilon}{E_1 - H + i\epsilon} (2\pi)^{3/2} a_{k_1}^\dagger |-\mathbf{k}_1, \psi_0\rangle, \quad (43)$$

where  $(2\pi)^{3/2} a_{k_1}^\dagger |-\mathbf{k}_1, \psi_0\rangle$  describes the incident channel in which the incident nucleon has momentum  $\mathbf{k}_1$  and the target has a total momentum  $-\mathbf{k}_1$ . In configuration space, this incident channel state is the antisymmetrized version of

$$\begin{aligned} & \exp(i\mathbf{k}_1 \cdot \mathbf{X}_A) \psi_0(\mathbf{X}_1, \dots, \mathbf{X}_{(A-1)}) \\ & = \exp(i\mathbf{k}_1 \cdot \mathbf{r}_{(A+1)}) \exp(-i\mathbf{k}_1 \cdot \mathbf{R}_A) \psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A). \end{aligned} \quad (44)$$

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

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

$$\frac{i\epsilon}{(E_1 + i\epsilon - H)} = \epsilon \int_{-\infty}^0 dt \exp(-i(E_1 + i\epsilon - H)t). \quad (45)$$

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

$$\begin{aligned} |\Psi_1^\epsilon\rangle & = \epsilon \int_{-\infty}^0 dt \exp(-i(E_1 + i\epsilon - H)t) \\ & \times (2\pi)^{3/2} a_{k_1}^\dagger |-\mathbf{k}_1, \psi_0\rangle, \end{aligned} \quad (46)$$

and from Eq. (30) the optical model overlap is

$$\begin{aligned} \xi_{0,1}^\epsilon(\mathbf{r}) & = \langle \langle \Psi(0, \mathbf{x} = 0) | \psi(\mathbf{r}, \epsilon) \int_{-\infty}^0 dt \\ & \times \exp(-i(E_1 + i\epsilon - H)t) (2\pi)^{3/2} a_{k_1}^\dagger |-\mathbf{k}_1, \psi_0\rangle \rangle. \end{aligned} \quad (47)$$

This expression can be written in terms of the Heisenberg operators

$$\begin{aligned} \Psi(\mathbf{r}, t) & = \exp(iHt) \psi(\mathbf{r}) \exp(-iHt), \\ \Psi^\dagger(\mathbf{r}, t) & = \exp(iHt) \psi^\dagger(\mathbf{r}) \exp(-iHt), \\ A_{k_1}^\dagger(t) & = \exp(iHt) a_{k_1}^\dagger \exp(-iHt). \end{aligned} \quad (48)$$

In terms of these, Eq. (47) becomes

$$\begin{aligned} \xi_{0,1}^\epsilon(\mathbf{r}) & = \langle \langle \Psi(0, \mathbf{x} = 0) | \epsilon \int_{-\infty}^0 dt \exp(-i(E_1 + i\epsilon)t) \\ & \times (2\pi)^{3/2} \exp(iHt) a_{k_1}^\dagger \exp(-iHt) \\ & \times \exp(+iHt) |-\mathbf{k}_1, \psi_0\rangle \rangle \\ & = \langle \langle \Psi(0, \mathbf{x} = 0) | \epsilon \int_{-\infty}^0 dt \Psi(\mathbf{r}, t = 0) \\ & \times \exp(-i(E_1 + i\epsilon)t) \\ & \times (2\pi)^{3/2} A_{k_1}^\dagger(t) \exp(i(E_0 + E_{1A})t) |-\mathbf{k}_1, \psi_0\rangle \rangle \\ & = \langle \langle \Psi(0, \mathbf{x} = 0) | \epsilon \int_{-\infty}^0 dt \Psi(\mathbf{r}, t = 0) \end{aligned}$$

$$\begin{aligned} & \times \exp(-i(\epsilon_{k_1} + i\epsilon)t) \\ & \times (2\pi)^{3/2} A_{k_1}^\dagger(t) |-\mathbf{k}_1, \psi_0\rangle \rangle. \end{aligned} \quad (49)$$

The derivation of the last line of Eq. (49) has used

$$H |-\mathbf{k}_1, \psi_0\rangle = (E_0 + E_{1A}) |-\mathbf{k}_1, \psi_0\rangle, \quad (50)$$

where  $E_0$  is the ground-state energy of the target and  $E_{1A}$  is the incident target c.m. kinetic energy

$$E_{1A} = \frac{\hbar^2 k_1^2}{2Am}. \quad (51)$$

$E_1 - E_0 - E_{1A}$  is therefore the incident nucleon kinetic energy

$$\epsilon_{k_1} = \frac{\hbar^2 k_1^2}{2m}. \quad (52)$$

The expression (49) for the optical model wave function can be written in terms of a Green's function by using

$$a_k^\dagger = \int d\mathbf{r}' \frac{\exp(i\mathbf{k} \cdot \mathbf{r}')}{(2\pi)^{3/2}} \psi^\dagger(\mathbf{r}'). \quad (53)$$

It follows from this that

$$\begin{aligned} a_{k_1}^\dagger & = \int d\mathbf{k}' \delta(\mathbf{k}_1 - \mathbf{k}') a_{k'}^\dagger \\ & = \int d\mathbf{k}' \left[ \int d\mathbf{r}' \frac{\exp(i(\mathbf{k}_1 - \mathbf{k}') \cdot \mathbf{r}')}{(2\pi)^3} \right] a_{k'}^\dagger \\ & = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}_1 \cdot \mathbf{r}')}{(2\pi)^{3/2}} \int d\mathbf{k}' \frac{\exp(-i\mathbf{k}' \cdot \mathbf{r}')}{(2\pi)^{3/2}} a_{k'}^\dagger \\ & = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}_1 \cdot \mathbf{r}')}{(2\pi)^{3/2}} \psi^\dagger(\mathbf{r}'), \end{aligned} \quad (54)$$

and hence

$$\begin{aligned} A_{k_1}^\dagger(t) & = \exp(iHt) a_{k_1}^\dagger \exp(-iHt) \\ & = \int d\mathbf{r}' \frac{\exp(i\mathbf{k}_1 \cdot \mathbf{r}')}{(2\pi)^{3/2}} \Psi^\dagger(\mathbf{r}', t). \end{aligned} \quad (55)$$

It follows from Eqs. (49) and (55) that

$$\begin{aligned} \xi_{0,1}^\epsilon(\mathbf{r}) & = \langle \langle \Psi(0, \mathbf{x} = 0) | \epsilon \int_{-\infty}^0 dt \Psi(\mathbf{r}, t = 0) \\ & \times \exp(-i(\epsilon_{k_1} + i\epsilon)t) (2\pi)^{3/2} A_{k_1}^\dagger(t) |-\mathbf{k}_1, \psi_0\rangle \rangle, \\ & = \epsilon \int_{-\infty}^0 dt \int d\mathbf{r}' \exp(-i(\epsilon_{k_1} + i\epsilon)t) \\ & \times \exp(i\mathbf{k}_1 \cdot \mathbf{r}') \langle \langle \Psi(0, \mathbf{x} = 0) | \\ & \times \mathcal{T} \{ \Psi(\mathbf{r}, 0) \Psi^\dagger(\mathbf{r}', t) \} |-\mathbf{k}_1, \psi_0\rangle \rangle. \end{aligned} \quad (56)$$

The time-ordering operator  $\mathcal{T}$  can be introduced without error because all values of  $t$  in the integral satisfy  $t < 0$ .

Equation (56) can be written

$$\begin{aligned} \xi_{0,k_1}^\epsilon(\mathbf{r}) & = \epsilon \int_{-\infty}^0 dt \int d\mathbf{r}' \exp(i(\mathbf{k}_1 \cdot \mathbf{r}' - (\epsilon_{k_1} + i\epsilon)t)) \\ & \times G(\mathbf{r}, t = 0; \mathbf{r}', t), \end{aligned} \quad (57)$$

where the Green's function is given by

$$G(\mathbf{r}, t; \mathbf{r}', t') = \langle \Psi(0, \mathbf{x} = 0) | \mathcal{T} \{ \Psi(\mathbf{r}, t) \times \Psi^\dagger(\mathbf{r}', t') \} | -\mathbf{k}_1, \psi_0 \rangle. \quad (58)$$

This differs from the usual ground-state-ground-state one-nucleon Green's function in that in the bra the ground state has a c.m. localized at the origin and in the ket the ground state has the total momentum  $-\mathbf{k}_1$ , i.e., opposite to the incident nucleon momentum in the overall c.m. system. It would be interesting to explore how far this differences leads to significant quantitative effects on the calculation of microscopic optical potentials.

Equation (57) differs from the expression for the optical model wave function given by Bell and Squires [5]. 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 energy by integrating over all times. The scattering state (43) is based on a physically transparent and well-understood limiting process. The state  $|\Psi_k^{(\epsilon)}\rangle$  defined in Eq. (43) is the state at time  $t = 0$  that evolves from a state in the remote past with energy  $E$  with a spread of  $\epsilon$  (see Gellman and Goldberger [11]). It is not clear at this time how these two different ways of handling the time affect the resulting theoretical optical potentials. They clearly involve two different time orderings in the Green's function (58) and this may alter the diagrams appearing in the perturbation expansion of the Green's function.

Extensive quantitative comparisons of translational invariant and noninvariant 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. (42) within the fully antisymmetrized translationally invariant oscillator shell model and use a formulation of the overlap function in terms of Jacobi coordinates as defined in Eq. (12) of Sec. III. Therefore, they do not suffer from the definition difficulties set out in Sec. II.

Of particular relevance are the results obtained in Ref. [8] for asymptotic normalization 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. Reference [8], Table I, quotes c.m. corrections to squared ANCs 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 Secs. V and VI for the case of nucleon-nucleus scattering.

## VII. CONCLUSIONS

A new, fully antisymmetrized, 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 wave function 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.

## ACKNOWLEDGMENTS

This work has benefited from discussions with several members of the Surrey Nuclear Theory Group: C. Barbieri, A. Idini, P. D. Stevenson, and N. K. Timofeyuk. Support from the UK Science and Technology Facilities Council through Grant STFC ST/000051/1 is acknowledged.

## APPENDIX: BRIEF NOTES ON SECOND QUANTIZATION

Many-body theory can be formulated in a new space (Fock space) in which states exist that have components in different orthogonal subspaces, 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 subspaces 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 nonzero components in orthogonal parts of Fock space.

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

$$|A\rangle\rangle = \begin{Bmatrix} A_0 \\ |A_1\rangle_{(1)} \\ |A_2\rangle_{(1)(2)} \\ \vdots \\ |A_n\rangle_{(1)(2)\dots(n)} \\ \vdots \end{Bmatrix}, \quad (A1)$$

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.,

$$|0\rangle\rangle = \begin{Bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{Bmatrix}. \quad (A2)$$

In Eq. (A1) the quantity  $|A_1\rangle_{(1)}$  is a state vector in the single nucleon subspace of nucleon labeled "1,"  $|A_2\rangle_{(1)(2)}$  is an antisymmetrized state in the 2-nucleon subspace of nucleons 1 and 2, and, in the row labeled  $n$ ,  $|A_n\rangle_{(1)(2)\dots(n)}$  is an antisymmetrized state in the  $n$ -nucleon subspace of nucleons 1 to  $n$ .

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

In general, a double right-angle bracket,  $|\dots\rangle\rangle$ , is used to denote state vectors in Fock space and the usual single

right-hand bracket,  $|\dots\rangle$ , is used 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 is ( $x$  signifies a set of commuting nucleonic dynamic variables for space, spin, and isospin)

$$\psi^\dagger(x_0)|A\rangle\rangle = \left\{ \begin{array}{c} 0 \\ A_0|x_0\rangle_{(1)} \\ \frac{1}{\sqrt{2}}\mathcal{A}_{1(2)}[|x_0\rangle_{(1)}|A_1\rangle_{(2)}] \\ \vdots \\ \frac{1}{\sqrt{n}}\mathcal{A}_{1(2\dots n)}[|x_0\rangle_{(1)}|A_{n-1}\rangle_{(2)\dots(n)}] \\ \vdots \\ \vdots \end{array} \right\},$$

$$\psi(x_0)|A\rangle\rangle = \left\{ \begin{array}{c} \langle x_0|A_1\rangle \\ \sqrt{2} \int dx_2|x_2\rangle_{(1)}\langle x_0,x_2|A_2\rangle \\ \vdots \\ \sqrt{(n+1)} \int dx_2 \dots dx_{n+1}|x_2, \dots, x_{n+1}\rangle_{(1)\dots(n)}\langle x_0,x_2, \dots, x_{n+1}|A_{n+1}\rangle \\ \vdots \\ \vdots \end{array} \right\}. \quad (\text{A3})$$

Here,  $\mathcal{A}_{1(2\dots n)}$  acts on the labels of nucleons  $1, 2, \dots, n$ , and is defined by

$$\mathcal{A}_{1(2\dots n)} = 1 - \sum_{j=2}^{j=n} P_{(1,j)}, \quad (\text{A4})$$

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  $\phi_S(x_1, x_2, \dots, x_A)$  is described in Fock space by a vector  $|\Phi_S\rangle\rangle$  given by

$$|\Phi_S\rangle\rangle = \frac{1}{\sqrt{A!}} \int dx_1 dx_2 \dots dx_A \phi_S(x_1, \dots, x_A) \psi^\dagger(x_A) \dots \psi^\dagger(x_1)|0\rangle\rangle. \quad (\text{A5})$$

The notation used is  $x_1 = \mathbf{r}_1, s_z, \tau_3$ , etc., and the integral signs include a summation over  $s_z = \pm 1/2, \tau_3 = \pm 1/2$ .

The inverse of (A5) is

$$\phi_S(x_1, \dots, x_A) = \frac{1}{\sqrt{A!}} \langle\langle 0|\psi(x_1) \dots \psi(x_A)|\Phi_S\rangle\rangle. \quad (\text{A6})$$

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 anticommutation relations that can be derived from the definitions:

$$\begin{aligned} \psi^\dagger(x_0)\psi^\dagger(x'_0) + \psi^\dagger(x'_0)\psi^\dagger(x_0) &= 0, & \psi^\dagger(x_0)\psi^\dagger(x_0) &= 0, \\ \psi(x_0)\psi(x'_0) + \psi(x'_0)\psi(x_0) &= 0, & \psi(x_0)\psi(x_0) &= 0, \\ \psi(x_0)\psi^\dagger(x'_0) + \psi^\dagger(x'_0)\psi(x_0) &= \delta(x_0 - x'_0). \end{aligned} \quad (\text{A7})$$

[1] C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, *Phys. Rev. Lett.* **113**, 032503 (2014).

[2] P. Navrátil and S. Quaglioni, *Phys. Rev. Lett.* **108**, 042503 (2012).

[3] A. Idini, C. Barbieri, and P. Navrátil, *Acta Phys. Pol. B* **48**, 273 (2017).

[4] H. Feshbach, *Ann. Phys.* **5**, 357 (1958).

[5] J. Bell and E. Squires, *Phys. Rev. Lett.* **3**, 96 (1959).



- [6] F. Capuzzi and C. Mahaux, *Ann. Phys. (N.Y.)* **239**, 57 (1995).
- [7] J. Rotureau, P. Danielewicz, G. Hagen, F. M. Nunes, and T. Papenbrock, *Phys. Rev. C* **95**, 024315 (2017).
- [8] N. K. Timofeyuk, *Phys. Rev. C* **84**, 054313 (2011).
- [9] N. K. Timofeyuk, *J. Phys. G: Nucl. Part. Phys.* **41**, 094008 (2014).
- [10] F. Villars, Collision Theory, in *Fundamentals in Nuclear Theory*, edited by A. de-Shalit and C. Villi (International Atomic Energy Agency, Vienna, 1967), pp. 260–333.
- [11] M. L. Goldberger and K. M. Watson, *Collision Theory* (Dover, New York, 2004).