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Integro-differential equations for light nuclei

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Abstract. Two methods of deriving the integro-differential equations for light nuclei are given. The resonating-group method of J. A. Wheeler is employed to construct the wave function and from the Schrödinger equation a set of simultaneous integro-differential equations is derived.

1. Introduction

The work of Hamada (1960, 1961), Hamada and Johnston (1962), Signell and Marshak (1957, 1958) and Gammel and Thaler (1957) has confirmed that nuclear forces consist of central, linear spin–orbit, tensor and quadratic spin–orbit forces. The theoretical work relating nucleon–nucleon forces to the properties of nuclei is very tedious even for light nuclei and prohibitive for medium and heavy nuclei.

Also in the method of resonating groups (Wheeler 1937) many types of direct and indirect terms, or potentials and kernels respectively, occur in the integro-differential equations describing a scattering or binding-energy problem. This arises even with central forces. When other type of forces are included many additional terms appear and further spin, isospin and orbital operator matrix elements have to be evaluated.

Hochberg (1967, unpublished) proposed two modifications in calculations based on the method of resonating groups which reduce the algebraic and numerical work while maintaining the accuracy. Moreover, the symmetry of the kernels is automatically ensured. The results for neutron–deuteron scattering in terms of phase shifts and cross sections have been published recently by Hochberg *et al.* (1968). Work on elastic neutron–triton and neutron–helium scattering problems is almost complete, and the results in terms of phase shifts and cross sections will be reported in a future publication.

2. Nucleon–nucleus scattering

Let $\Phi(\widetilde{123...A})$ be the total antisymmetric wave function of A nucleons. In Φ the total isospin T and its z component T_z will determine the nature of the target nucleus and projectile (nucleon), that is, its isobaric state. It is also characterized by the total angular momentum J, its z component J_z and the total spin S.

Let us consider

$$\begin{aligned}\Phi(\widetilde{12\ldots A}) = {} & F(1\text{–}23\ldots A)\Phi(1,\widetilde{23\ldots A}) \\ & -F(2\text{–}13\ldots A)\Phi(2,\widetilde{13\ldots A}) \\ & -F(3\text{–}21\ldots A)\Phi(3,\widetilde{21\ldots A}) \\ & -\ldots \qquad \text{(all exchanges of 1 with } 23\ldots A) \\ = {} & \tilde{\sum} F(1\text{–}23\ldots A)\Phi(1,\widetilde{23\ldots A}). \qquad (2.1)\end{aligned}$$

$F(1\text{–}23...A)$ denotes the space function of nucleon 1 relative to the centre of mass of $23...A$. $\Phi(1,\widetilde{23...A})$ is a function of space, spin and isospin variables of all nucleons $1, 2...A$ except the space variables of nucleon 1.

We define the kinetic energy operator

$$\begin{aligned} T_{123\ldots A} &= T_{1-23\ldots A}+T_{2-34\ldots A}+\ \ldots\ +T_{A-1,A} \\ &= T_{2-13\ldots A}+T_{1-34\ldots A}+\ \ldots\ +T_{A-1,A} \\ &= \ldots \qquad \text{(all other similar combinations)} \\ &= -\frac{\hbar^2}{2M}\left(\frac{A}{A-1}\nabla^2_{1-23\ldots A}+\frac{A-1}{A-2}\nabla^2_{2-34\ldots A}+\ \ldots\ +\frac{2}{1}\nabla^2_{A-1,A}\right) \\ &= -\frac{\hbar^2}{2M}\left(\frac{A}{A-1}\nabla^2_{2-13\ldots A}+\frac{A-1}{A-2}\nabla^2_{1-34\ldots A}+\ \ldots\ +\frac{2}{1}\nabla^2_{A-1,A}\right) \\ &= \ldots \qquad \text{(all other similar combinations).} \end{aligned} \tag{2.2}$$

All the operators are Hermitian which implies that any operator O can be expressed as

$$\mathrm{O} = \overrightarrow{\mathrm{O}}+\text{Hermitian conjugate.} \tag{2.3}$$

Thus we put

$$\begin{aligned} T &= \overrightarrow{T}+\overleftarrow{T} \\ &= -\frac{\hbar^2}{2M}(\overrightarrow{\nabla}^2+\overleftarrow{\nabla}^2). \end{aligned} \tag{2.4}$$

We assume that $\Phi(1,\widetilde{23\ldots A})$ satisfies a Schrödinger equation

$$(\overrightarrow{T}_{234\ldots A}+\overrightarrow{V}_{234\ldots A}-E_{A-1})\Phi(1,\widetilde{234\ \ldots\ A}) = 0 \tag{2.5}$$

and also its adjoint equation

$$\Phi^*(1,\widetilde{234\ \ldots A})(\overleftarrow{T}_{234\ldots A}+\overleftarrow{V}_{234\ldots A}-E_{A-1}) = 0 \tag{2.6}$$

where

$$V_{234\ldots A} = V_{23}+V_{24}+\ \ldots\ +V_{A-1,A}. \tag{2.7}$$

V_{ij} is the interaction operator between particles i, j. The presence of the spin and isospin variables of nucleon 1 in $\Phi(1,\widetilde{23\ldots A})$ reminds us that Φ is not the ground-state wave function of the target nucleus consisting of $A-1$ nucleons $(23\ldots A)$ but some modification of it (a polarized state). If we choose $\Phi(1,\widetilde{23\ldots A})$ to have the correct total spin and isospin of the target nucleus $(23\ldots A)$ in its ground state, we can take as an approximation E_{A-1} to be the binding energy of this nucleus. The value of E_{A-1} has been obtained by several authors, including Sugie *et al.* (1957), Nagata *et al.* (1959), Hochberg *et al.* (1954) and Kanada *et al.* (1963), by a variational solution of equation (2.5). Since we assume an exact ground-state solution of equation (2.5) we can use the experimental value E_{A-1}. The validity of this approximation will be discussed at the end of § 3.

We now assume that $\Phi(1,\widetilde{23\ldots A})$ satisfies the Schrödinger equation

$$(T_{123\ldots A}+V_{123\ldots A}-E)\tilde{\sum} F(1\text{-}23\ \ldots\ A)\Phi(1,\widetilde{23\ \ldots\ A}) = 0 \tag{2.8}$$

where E is the total energy in the centre-of-mass system.

If we multiply the left-hand side of equation (2.8) by $\Phi^*(1, \widetilde{23\ldots A})$ and integrate and/or sum over all variables of particles $23\ldots A$, we obtain

$$\int d\tau_{234\ldots A}\Phi^*(1, \widetilde{23\ldots A})(T_{123\ldots A}+V_{123\ldots A}-E)\tilde{\sum} F(1\text{-}23\ldots A)\Phi(1, \widetilde{23\ldots A}) = 0. \quad (2.9)$$

Using equation (2.6) we can write equation (2.9) as

$$\int d\tau_{234\ldots A}\Phi^*(1, \widetilde{234\ldots A})(T_{1-23\ldots A}+V_{12}+V_{13}+\ldots V_{1A}-E_n)$$

$$\times F(1\text{-}23\ldots A)\Phi(1, \widetilde{23\ldots A}) - \int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})(T_{123\ldots A}+V_{123\ldots A})$$

$$\times \tilde{\sum_{i\neq 1}} F(i\text{-}123\ldots i-1, i+1, \ldots A)\Phi(i, \widetilde{123\ldots i-1, i+1, \ldots A}) = 0 \quad (2.10)$$

where we use

$$E = E_n + E_{A-1}\ldots \quad (2.11)$$

and E_n is the incident nucleon kinetic energy in the centre-of-mass system. Making use of symmetry properties of the integrals and variables of integration we can further modify the last equation to obtain

$$(T_{1-23\ldots A}-E_n)F(1\text{-}23\ldots A)+\{(A-1)$$

$$\times\int d\tau_{234\ldots A}\,\Phi^*(1, \widetilde{23\ldots A})V_{12}\Phi(1, \widetilde{23\ldots A})\}F(1\text{-}23\ldots A)$$

$$-(A-1)\int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})(T_{1-23\ldots A}+V_{12}+V_{13}$$

$$+\ldots+V_{1A}-E_n)\Phi(2, \widetilde{13\ldots A})F(2\text{-}13\ldots A) = 0. \quad (2.12)$$

This is the equation for the incident neutrons. A similar modification is required for the incident protons. The last integral can be written

$$-(A-1)\int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})\{T_{1-23\ldots A}+V_{12}$$

$$+(A-2)V_{13}-E_n\}\Phi(2, \widetilde{13\ldots A})F(2\text{-}13\ldots A).$$

Using equations (2.5) and (2.6) we can write

$$\int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})(T_{123\ldots A}+V_{123\ldots A}-E)\Phi(2, \widetilde{134\ldots A})F(2\text{-}134\ldots A)$$

$$= \int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})(T_{2-13\ldots A}+V_{21}+V_{23}$$

$$+\ldots+V_{2A}-E_n)\Phi(2, \widetilde{134\ldots A})F(2\text{-}134\ldots A)$$

$$= \int d\tau_{23\ldots A}\Phi^*(1, \widetilde{23\ldots A})(\tfrac{1}{2}T_{1-23\ldots A}+\tfrac{1}{2}T_{2-13\ldots A}+V_{12}$$

$$+\tfrac{1}{2}(A-2)(V_{13}+V_{23})-E_n)\Phi(2, \widetilde{13\ldots A})F(2\text{-}13\ldots A). \quad (2.13)$$

Thus we can simplify equation (2.12) using equation (2.13) to obtain

$$(T_{1-23\dots A}-E_n)F(1\text{-}23\dots A)+(A-1)\left\{\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})V_{12}\Phi(1,\widetilde{23\dots A})\right\}$$
$$\times F(1\text{-}23\dots A)-(A-1)\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})$$
$$\times\{\tfrac{1}{2}T_{1-23\dots A}+\tfrac{1}{2}T_{2-13\dots A}+V_{12}+(A-2)(\tfrac{1}{2}V_{13}+\tfrac{1}{2}V_{23})-E_n\}$$
$$\times\Phi(2,\widetilde{13\dots A})F(2\text{-}13\dots A)=0. \tag{2.14}$$

This is the final integro-differential equation in the dependent variable F and the independent vector variable (1–23...A).

We now integrate and/or sum over all variables of nucleons except the radial component of the vector (1–23...A). This leads to a set of scalar equations in this radial component for given values of J, S and T. Therefore one type of potential and two types of kernel depend on the neutron–neutron interaction; all other terms in the equation merely depend on the number and type of nucleons (whether protons or neutrons) involved.

A further simplification is possible and this will now be discussed.

3. Alternative form of equation

We now make use of the following identity:

$$0=\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})(T_{134\dots A}+V_{13}+V_{14}+\dots$$
$$+V_{A-1,A}-E_{A-1})\Phi(2,\widetilde{134\dots A})$$
$$=\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})\{T_{134\dots A}+(A-2)V_{13}$$
$$+{}^{K}C_2V_{34}+{}^{z}C_2V_{56}-E_{A-1}\}\Phi(2,\widetilde{13\dots A}) \tag{3.1}$$

where

$$\left.\begin{aligned}{}^{K}C_2&={}^{A-2}C_2-{}^{z}C_2\\ {}^{A-2}C_2&\equiv\binom{A-2}{2}=\frac{(A-2)(A-3)}{1\times 2},\ \text{etc.}\end{aligned}\right\} \tag{3.2}$$

and z is the number of protons and 5,6 are a proton pair. This enables us to write equation (2.14) as

$$(T_{1-23\dots A}-E_n)F(1\text{-}23\dots A)+(A-1)\left\{\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})V_{12}\Phi(1,\widetilde{23\dots A})\right\}$$
$$\times F(1\text{-}23\dots A)-(A-q)\int d\tau_{23\dots A}\Phi^*(1,\widetilde{23\dots A})$$
$$\times(\tfrac{1}{2}T_{1-23\dots A}+\tfrac{1}{2}T_{2-13\dots A}+V_{12}-E_n-\tfrac{1}{2}T_{134\dots A}-\tfrac{1}{2}T_{234\dots A}$$
$$+E_{A-1}-{}^{K}C_2V_{34}-{}^{z}C_2V_{56})\Phi(2,\widetilde{134\dots A})F(2\text{-}134\dots A)=0 \tag{3.3}$$

where

$$q=z+1 \tag{3.4}$$

Equation (3.3) has the advantage that the kernel (i) is symmetric as before in equation (2.14), (ii) involves one term V_{12} which can be thought of as the interaction between the particles (1, 2) directly concerned in the scattering process, and (iii) involves two other terms V_{34} and V_{56} which describe the interaction between the particles of the target nucleus. The feature (iii) is particularly useful if one assumes all particle pairs to be in S states relative to each other. Consequently tensor, spin–orbit and quadratic spin–orbit forces will then give no contribution to the terms V_{34} and V_{56}.

We note that in equation (2.14) E_{A-1} does not appear explicitly and so the solution depends on choosing a reliable wave function Φ_{A-1} for nucleus $A-1$. This will be some modification of the bound-state functions Φ^b_{A-1} of nucleus $A-1$ owing to the proximity of the projectile nucleon.

To sum up, the simplifications are essentially based on the use of equation (2.5) and its adjoint (2.6) leading to two alternative forms of the linear integro-differential equations, namely equations (2.14) and (3.3). Equation (2.5) was previously used in scattering problems (see Sugie *et al.* 1957, van der Spuy 1956) and this reduced the algebra but led to symmetry difficulties which were eliminated by a second application of equation (2.5). The combined use of the equations (2.5) and (2.6) further reduces the algebraic and numerical work and avoids the symmetry difficulties.

We shall now give the results obtained for a few special cases. Let us consider the following two special cases.

4. Neutron–deuteron scattering problems

Let $\Psi(\widetilde{12}, 3)$ be the resonating-group wave function where particles 1, 2 are neutrons and 3 is a proton. The formulation without isospin as mentioned earlier in this paper is shortened for practical calculations.

The basic Schrödinger equation is

$$(T_{123}-E+V_{12}+V_{13}+V_{23})\{\Phi(\overline{23})F(1\text{–}23)-\Phi(\overline{13})F(2\text{–}13)\} = 0 \qquad (4.1)$$

where we have written

$$\Psi(\widetilde{12}, 3) = \Phi(\overline{23})F(1\text{–}23)-\Phi(\overline{13})F(2\text{–}13) \qquad (4.2)$$

and $\Phi(\overline{23})$, etc., are symmetric in interchange of 2 and 3. T is the kinetic-energy operator. E is the total energy of the system and the V_{ij}'s are the interactions between particles i and j. We now use the deuteron equation

$$(T_{23}+V_{23}-E_{\mathrm{D}})\Phi(\overline{23}) = 0 \qquad (4.3)$$

and its complex conjugate

$$\Phi^*(\overline{23})(T_{23}+V_{23}-E_{\mathrm{D}}) = 0 \qquad (4.4)$$

where

$$E = E_{\mathrm{n}}+E_{\mathrm{D}} \qquad (4.5)$$

E_{D} and E_{n} being the deuteron binding energy and the incident neutron energy respectively (centre-of-mass units).

Following the simplifications outlined in § 3, the equivalent of equation (3.3) is

$$\begin{aligned}\Big\{-\frac{\hbar^2}{2M}\Big(\frac{3}{2}\nabla_r{}^2\Big)-E_{\mathrm{n}}\Big\}F(r)+\sum_{\mathrm{spin}}\int d^3\boldsymbol{u}\,\Phi^*(\overline{23})(|\boldsymbol{u}|)2V_{12}(|\boldsymbol{u}|)\Phi(\overline{23})(|\boldsymbol{u}|)F(r)\\ =\Big(\frac{4}{3}\Big)^3\sum_{\mathrm{spin}}\int d^3\boldsymbol{r}'\Phi^*(\overline{23})(|\boldsymbol{u}|)V_{12}(|\boldsymbol{u}-\boldsymbol{v}|)\Phi(\overline{13})(|\boldsymbol{v}|)F(r')\\ +\Big(\frac{4}{3}\Big)^3\sum_{\mathrm{spin}}\int d^3\boldsymbol{r}'\Phi^*(\overline{23})(|\boldsymbol{u}|)\Big[E_{\mathrm{D}}-E_{\mathrm{n}}-\frac{\hbar^2}{2M}\Big\{\frac{2}{3}\Big(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\Big)+\frac{8}{3}\frac{\partial}{\partial \boldsymbol{u}}\cdot\frac{\partial}{\partial \boldsymbol{v}}\Big\}\Big]\\ \times\Phi(\overline{13})(|\boldsymbol{v}|)F(r')\end{aligned} \qquad (4.6)$$

where

$$\left.\begin{aligned}\boldsymbol{u} &= \tfrac{4}{3}\boldsymbol{r}'+\tfrac{2}{3}\boldsymbol{r}\\ \boldsymbol{v} &= \tfrac{2}{3}\boldsymbol{r}'+\tfrac{4}{3}\boldsymbol{r}\end{aligned}\right\} \qquad (4.7)$$

and $\boldsymbol{r}$, $\boldsymbol{r}'$ are the centre-of-mass coordinates of particles 1 and 2 respectively. The scalar linear integro-differential equations are obtained by multiplying equation (4.6) on the left by $Y^{JS}(1)$ which is the eigenfunction of 1 having given eigenvalues J and S (total angular momentum and total spin respectively) and summing and integrating over all variables except the radial component of $\boldsymbol{r}$.

5. Neutron–triton scattering problems

Let 1, 2, 3 be the neutrons and 4 the proton. Then, by a procedure similar to that of § 4, the final equation for the neutron–triton scattering can be written as

$$\left\{\int \Phi^*(-1)(T_{1\text{-}234}-E_{\mathrm{n}}+3V_{12})\Phi(-1)\,\mathrm{d}\tau_{234}\right\}F(1)$$

$$-2\int \mathrm{d}\tau_{234}\Phi^*(-1)(T_{1\text{-}234}-T_{1\text{-}34}-T_{34}+E_{\mathrm{T}}-E_{\mathrm{n}}+V_{12}-V_{34})\Phi(-2)F(2) = 0 \qquad (5.1)$$

where $\Phi^*(-1)$ is $\Phi(\widetilde{234})$, etc., and E_{T} is the triton binding energy. It should be noted that we have applied equation (3.3) to the two special cases considered above.

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