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Program Manual for `LEA`

James J. Kelly
Department of Physics and Astronomy
University of Maryland, College Park, MD 20742
e-mail: kelly@enp.umd.edu

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Abstract

This report describes the program LEA, standing for *L*inear *E*xpansion *A*nalysis, designed to provide a flexible tool for the analysis of data for the scattering of nucleons by nuclei. The program can be used in a one-shot mode to calculate nucleon-scattering observables for a large variety of structure or interaction models. In this mode, many options are available for testing sensitivity to various aspects of the reaction model and to verify the internal consistency of the calculation by comparison with the plane-wave Born approximation. Alternatively, if a structure or interaction model can be expressed as a linear expansion, the coefficients can be fitted to a very large data set that may include many observables for several states and perhaps several energies simultaneously. The most important applications of these methods has been to extract the density dependence of an empirical effective interaction from inelastic scattering data for many states of several self-conjugate targets and then to use the fitted interaction to extract neutron transition densities for targets with a neutron excess.

Contents

1. INTRODUCTION

The original purpose of the `LEA` program was to apply *L*inear *E*xpansion *A*nalysis of the nucleon–nucleus scattering amplitude to models of either the effective interaction or neutron transition densities to data for proton inelastic scattering. However, during the subsequent evolution of the program, many other capabilities have been developed. The most important applications `LEA` are listed below.

- *DWA for nucleon–nucleus scattering.* Nucleon-nucleus elastic scattering, inelastic scattering, and charge exchange can be evaluated for a wide variety of models based upon the distorted–wave approximation (DWA). The detailed output and a very large variety of options allows one to thoroughly investigate many aspects the reaction.
  - *Optical potentials* can be produced either from folding models or from most standard nonrelativistic analyses. In addition, Schrödinger–equivalent potentials from Dirac phenomenoloy are available in a convenient form.
  - *Folding models* evaluate scattering potentials by folding the nucleon–nucleon effective interaction with nuclear transition densities. The interaction contains central, spin-orbit, and tensor components and may be density dependent. A wide variety of interaction models is available.
  - *Collective models* relate inelastic scattering potentials to variations of either the optical potential or of the ground–state density. Several deformation schemes are available.
  - *Born approximations* can be based upon the interaction, the scattering potential, or partial–wave expansions. Thus, three independent calculations can be used to verify the internal consistency of the code.
  - *Nonspherical potentials for elastic scattering* can be produced in folding or collective models and their contributions evaluated in first–order using the two–potential formula. This method can also be compared with a coupled–channels calculation truncated at first order.
- *Empirical effective interactions* (EEI) can be fitted to elastic and inelastic scatttering data for several states in several targets simultaneously. The density dependence of the nucleon–nucleon effective interaction in the nuclear medium is parametrized in a form guided by nuclear matter theory, but the coefficients can be varied to improve the fit to scattering data. Both elastic and inelastic scattering are described self consistently.
- *Neutron transition densities* can be fitted to nucleon scattering data, assuming that the proton transition densities are already known from electron scattering. The density is expanded in a complete set of radial basis functions to minimize model dependence. Error bands are produced which include statistical, normalization, and incompleteness errors. Data for several projectile energies can be fitted independently or simultaneously to assess residual errors due the reaction model.

- *Channel coupling for nucleon scattering* can be evaluated by the sequential iteration of coupled equations (SICE) method, based upon the ECIS algorithm of Raynal. The coupling potentials can be obtained either from folding (microscopic) models or collective (macroscopic) models.

- *Electromagnetically–induced single–nucleon knockout* reactions, namely $(e, e'N)$ or (γ, N) can be evaluated using final–state interactions (FSI) that include any of the options available to nucleon scattering, such as channel coupling based on density–dependent empirical effective interactions. Response functions and recoil polarization observables are evaluated.

- *Electron scattering form factors* can be evaluated in plane–wave approximation. This option is primarily intended to test the structure input for scattering calculations.

- *Nucleon–nucleon scattering* obseravables can also be calculated separately. This option is primarily intended to test models of the effective interaction.

In the folding model, the scattering amplitude for a direct reaction is described by the generic "$t\rho$" form representing the convolution of an effective interaction t with a transition density ρ. If either of the interaction or the structure factors is known, the unknown factor can be obtained by fitting data. For example, given that the electromagnetic interaction is known, extraordinarily precise nuclear charge and current densities are routinely unfolded from electron scattering data. The basic technique is to represent the target density as a linear expansion in a complete set of radial basis functions and to fit the coefficients to the data subject to appropriate constraints.

For classes of transitions for which electron scattering determines all aspects of the nuclear structure relevant to excitation of the same transition by nucleons, the effective interaction can be extracted from proton scattering data with little residual uncertainty due to the structure. It is known that this interaction depends strongly upon the density within the interaction region. Medium modifications can then be described by the local density approximation (LDA). If the LDA is sound, the effective interaction should depend only upon density and be independent of state and target. Therefore, medium modifications should be fitted to data for many states and several targets simultaneously. States whose transition densities have strong interior contributions provide sensitivity to the high–density properties of the effective interaction, whereas surface–peaked transition densities provide sensitivity to the low–density properties of the interaction. Furthermore, self–consistency between inelastic scattering potentials and elastic optical potentials calculated from the same effective interaction ensures accuracy of the interior wave function required for inelastic scattering or for knockout reactions. The `LEA` program performs this analysis.

Once the interaction is established, nucleon scattering can be exploited to study nuclear structure. For transitions dominated by the matter densities, the neutron transition density can be fitted to proton scattering data provided that the proton transition density is already known from electron scattering. We have shown that the intrinsic sensitivity of nucleon scattering to the radial neutron density is competitive with the sensitivity of electron scattering to the charge density. Therefore, if the residual errors in the reaction model can be controlled, neutron densities can be measured with good accuracy.

One way to test the importance of errors in the reaction model is to deduce the neutron density for a particular state using several widely separated proton energies. The `LEA` program can fit the density to data for each energy separately or several energies simultaneously. The stability of the result is then a measure of the systematic errors.

Of course, the program can also perform routine calculations for general transitions without fitting. In this mode, distorted-wave calculations can be compared with two independent plane-wave calculations. If the distorting potentials are null and the interaction is density independent, all three calculations should give precisely the same results. Thus, `LEA` provides rigorous tests of internal consistency. More importantly, the plane-wave calculations decompose the scattering amplitudes in several informative representations that can provide considerable physical insight.

The `LEA` program is based upon a nonrelativistic Schrödinger formalism and uses local approximations for exchange. However, the LEA method itself is more general and may be applied to any direct reaction model for which the scattering amplitude can be linearized with respect to the parameters of interest. The methods can be applied to Dirac models or to calculations that compute knock-on exchange exactly. Our choice of formalism is based upon considerations of economy and transparency. At the present time, the nonrelativistic model is more fully developed and does not require as many inaccessible interaction and structure amplitudes as do current versions of the relativistic model. The connections between electron scattering, proton scattering, and structure models are more transparent and better understood for local nonrelativistic calculations. Furthermore, much of the difference between the Dirac and Schrödinger models is due to virtual-pair contributions which can be parametrized by an effective density dependence and used in nonrelativistic LDA calculations. Similarly, the exchange terms can be developed as an short-range expansion involving current operators with higher powers of the gradient. Thus, a local calculation can reproduce nonlocal exchange effects quite accurately. Therefore, if it becomes necessary, methods to improve the present approximations without altering the fundamental structure of the program already exist.

This document outlines the input needed to use `LEA`. Several publications reporting representative applications are available.

2. FORMALISM FOR NUCLEON–NUCLEUS SCATTERING

In this section we outline the basic formalism used for the most important models of nucleon–nucleus scattering that are implemented in the `LEA` program. Although we do not present detailed derivations, we do attempt to provide descriptions that are sufficiently complete to define the available options. Wherever possible, the program input employs similar acronyms.

2.1. Schrödinger Equation

The nucleon–nucleus scattering calculations are all based upon a form of the Schrödinger equation in which relativistic kinematics are included. Optical potentials from Dirac phenomenology may also be included using transformations of the Dirac equation to

Schrödinger–equivalent forms, as described in Sec. 2.2.2. The optical potential and scattering potentials are treated as local operators in coordinate space. The operators may include angular momentum or derivative couplings. Models based upon the nucleon–nucleon interaction use short–range exchange approximations to reduce the exchange contributions to local form.

Distorted waves, χ are obtained from a Schrödinger equation of the form

$$\left[\nabla^2 + k^2 - 2\mu U\right]\chi = 0 \tag{1}$$

where

$$U(r) = U^Z(r) + U^C(r) + U^{LS}\boldsymbol{L}\cdot\boldsymbol{\sigma} \tag{2}$$

is a spherical optical potential containing Coulomb (U^Z), central (U^C), and spin–orbit (U^{LS}) components. In many models, the spin–orbit potential naturally assumes a derivative form,

$$U^{LS} = \frac{1}{r}\frac{\partial F^{LS}}{\partial r} \tag{3}$$

where F^{LS} is a form factor whose shape is similar to that of the central potential. Relativistic kinematics are incorporated by using the exact relativistic wave number k and by replacing the reduced mass with the reduced energy

$$\mu = \frac{E_N E_{A-1}}{E_N + E_{A-1}} \tag{4}$$

where E_N and E_{A-1} are the relativistic total energies of the ejectile and the residual nucleus in the nucleon–nucleus (NA) center–of–mass frame.

2.2. Optical Potentials

Optical potentials may be obtained from fits to elastic scattering data, performed either with the Schrödinger or with the Dirac equation followed by transformation to an equivalent Schrödinger equation, or from folding model calculations using density-dependent effective interactions.

2.2.1. Woods-Saxon Parametrizations

Most analyses are performed using optical potentials fitted to proton elastic scattering data using simple Woods-Saxon (WS) shapes of the form

$$U^C(r) = V^C f(x_V) + iW^C f(x_W) + 4ia_S W^S g(x_S) \tag{5a}$$

$$U^{LS}(r) = \frac{2}{r}\left[V^{LS}g(x_{VLS}) + iW^{LS}g(x_{WLS})\right] \tag{5b}$$

where

$$
\begin{aligned}
f(x_i) &= [1 + e^{x_i}]^{-1} \\
g(x_i) &= -\partial f(x_i)/\partial r \\
x_i &= (r - R_i)/a_i \\
R_i &= r_i A^{1/3} \, .
\end{aligned}
$$

The factor $-4a_S$ is included to normalize the surface-absorption form factor to unity at its peak. For low energies, typically $T_p < 100$ MeV, surface absorption is parametrized by W_S, usually with $r_S = r_W$ and $a_S = a_W$. The real and imaginary spin-orbit potentials are usually assigned common geometrical parameters, $r_{WLS} = r_{VLS} = r_{LS}$ and $a_{WLS} = a_{VLS} = a_{LS}$. The Coulomb potential U^Z is usually obtained for a uniformly charged sphere of radius $R_Z = r_Z A^{1/3}$ with $r_Z \approx 1.25$ fm, but is sometimes obtained by folding the Coulomb interaction over the nuclear charge density.

The parameters may be obtained either from single-energy fits made to the data for each ejectile energy independently or from energy-dependent analyses which consider a broad range of proton energies. The former usually produce superior fits to the elastic scattering data, but the parameters may vary erratically with energy due to uncontrollable correlations among the parameters or to defects in the reaction mechanism. Energy-dependent optical models impose a smooth energy dependence upon the potentials, usually at the expense of local fit quality. Furthermore, global optical potentials also impose smooth functions upon the mass dependence of the geometrical paramters. However, one must be careful not to employ such potentials significantly beyond the ranges of either mass or energy originally fitted — they usually do not extrapolate well.

Several models which are used frequently have been coded directly, thus requiring minimal input. More detailed descriptions of these models are given in Sec. 8. Unfortunately, a global nonrelativistic optical potential for $A \geq 12$ and a broad range of energy does not appear to exist. For that we must appeal to Dirac phenomenology (DP).

2.2.2. Dirac Phenomenology

Suppose that a four-component Dirac spinor,

$$
\Psi(\mathbf{r}) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix}
$$

where ψ_+ and ψ_- are two-component Pauli spinors for positive and negative energy components, satisfies a Dirac equation of the form

$$
[\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta(m + S)] \, \Psi = (E - V - V^Z)\Psi \tag{6}
$$

with scalar and vector potentials S and V. Upon elimination of the lower components, an equivalent Schrödinger equation of the form

$$
\left[\nabla^2 + k^2 - 2\mu \left(U^Z + U^C + U^{LS} \boldsymbol{L} \cdot \boldsymbol{\sigma}\right)\right] \phi = 0 \tag{7}
$$

can be obtained, where ψ_+ is related to ϕ by the Darwin transformation

$$\psi_+ = B^{1/2}\phi \tag{8a}$$
$$B = 1 + \frac{S - V - V^Z}{E+m}\ . \tag{8b}$$

The equivalent Schrödinger potentials are then

$$U^Z = \frac{E}{\mu} V^Z \tag{9a}$$
$$U^C = \frac{E}{\mu}\left[V + \frac{m}{E} + \frac{S^2 - V^2}{2E} - \frac{V^Z(V^Z + 2V)}{2E}\right] + U^D \tag{9b}$$
$$U^D = \frac{1}{2\mu}\left[-\frac{1}{2r^2 B}\frac{d}{dr}(r^2 B') + \frac{3}{4}\left(\frac{B'}{B}\right)^2\right] \tag{9c}$$
$$U^{LS} = -\frac{1}{2\mu}\frac{B'}{rB} \tag{9d}$$

where U^D is the Darwin potential. The Schrödinger solutions are phase-equivalent to the Dirac solutions in the sense that the asymptotic phase shifts, and hence observables for elastic scattering, are the same. However, the Dirac wave function is modified in the interior by a nonlocality factor similar in form to the Perey-Buck nonlocality factor, except that it depends upon $S - V$, which is closely related to the spin-orbit potential, rather than upon the central potential. Hence, C_{rel} can also be deduced from the spin-orbit potential directly [1]. When used in nonrelativistic calculations, the positive energy spinor ψ_+, including the Darwin factor, is identified with the distorted wave χ.

Hama *et al.* [2] produced global Dirac optical potentials for $A \geq 40$ and $65 \leq T_p \leq 1040$ MeV. The scalar and vector potentials were parametrized by symmetrized Woods-Saxon functions, of the form

$$f(x) = \left[(1+e^{-x})(1+e^{x})\right]^{-1} \tag{10}$$

where $x = (r-R)/a$ for each component, as before. In addition, surface absorption proportional to $f'(x)$ was included. Two fits were made, here designated DP1 and DP2. The strengths and shape parameters for DP1 were expanded in the form

$$V_i = R_i \sum_{j=0}^{3} V_{ij} E^{-j}$$
$$R_i = A^{1/3}\left[\sum_{j=0}^{2} R_{ij} A^{-j} + \sum_{j=3}^{5} R_{ij} E^{2-j}\right]$$
$$a_i = \sum_{j=0}^{2} a_{ij} A^{-j} + \sum_{j=3}^{5} a_{ij} E^{2-j}$$

where the subscript i refers to real and imaginary parts of the scalar and vector potentials. A slightly different parametrization was employed for DP2. DP1 has 77 parameters, compared with 84 for DP2, but both give approximately the same reduced $\chi^2_\nu \approx 8.3$ for more than 4500 degrees of freedom.

The global Dirac optical potential was then extended to the ranges $A \geq 12$ and $20 \leq T_p \leq 1040$ MeV, including more than 8700 data points, by Cooper *et al* [3]. The parametrizations are more complicated and several essentially equivalent variations of the global potential were provided. In addition, best-fit energy-dependent potentials were produced for everyone's favorite targets: ^{12}C, ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb.

Although the scalar+vector (SV) model of Dirac phenomenolgy is not unique, and relatively simple but arbitrary shapes are employed for the potentials, this work represents the most extensive and systematic analyses of proton optical potentials available. The data are described very well by potentials whose properties vary smoothly with both mass and energy.

2.2.3. Folded Optical Potentials

In the simplest form of the folding model, the central and spin-orbit potentials become

$$U^C(r) = \frac{2}{\pi} \int dq\; q^2 j_0(qr) \eta t^C(q,\rho) \tilde{\rho}(q) \tag{11}$$

$$F^{LS}(r) = \frac{2}{\pi} \int dq\; q^2 j_0(qr) \eta t'^{LS}(q,\rho) \tilde{\rho}(q) \tag{12}$$

where

$$\tilde{\rho}(q) = \int dr r^2 j_0(qr) \rho(r) \tag{13}$$

is the Fourier transform of the ground-state density ρ. Note that a sum over nucleon or isospin indices has been left implicit. For simplicity, the density dependence of the effective interaction is evaluated at the site of the projectile, but we find that other prescriptions give very similar results.

In nonrelativistic models, η is interpreted as the Jacobian between NN and NA frames [4] and is often called the Moller factor. However, since the nonrelativistic reduction of the IA2 model is performed in the NA frame and gives a wave equation of slightly different form, the Jacobian must be replaced by $\eta = \frac{E}{\mu}$, where $E^2 = k^2 + m^2$ is the projectile energy in the NA center-of-mass frame, to cast both models in the same form. Furthermore, since the IA2 model is relativistically covariant, the transformation between NN and NA frames is more complicated than the simple Moller factor used by nonrelativistic models.

2.3. Scattering Potentials for Nucleon-Nucleus Scattering

In this section we present the pseudopotential formalism for nucleon-nucleus scattering potentials. Although the notation is different, the formulation is similar to that of Refs. [5–7].

2.3.1. Pseudopotential representation of the nucleon–nucleon interaction

A local pseudopotential representation of the nucleon-nucleon (NN) interaction [8,9] that is useful for the folding model of nucleon-nucleus scattering can be written in the form

$$V = \sum_{ST} V^C_{ST}(r) P^S P^T + \sum_T V^{LS}_T(r) \mathbf{L}\cdot\mathbf{S} P^T + \sum_T V^T_T(r) S_{12}(\hat{\mathbf{r}}) P^T \tag{14}$$

where

$$\mathbf{L} = \frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_2) \otimes (\mathbf{p}_1 - \mathbf{p}_2) \tag{15a}$$

$$\mathbf{S} = \frac{1}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \tag{15b}$$

$$S_{12}(\hat{\mathbf{r}}) = 3\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}}\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \tag{15c}$$

are the two-body orbital angular momentum, spin, and tensor operators and where P^S (P^T) are projection operators for spin (isospin). The Love and Franey exchange prescription [8] requires antisymmetrized matrix elements of the pseudopotential to fit the nucleon-nucleon t-matrix, such that

$$t_{NN}(\mathbf{k}_f, \mathbf{k}_i) = \langle \mathbf{k}_f | V(1-X) | \mathbf{k}_i \rangle \tag{16}$$

where X denotes the exchange operator. Hence, the t-matrix can be expressed in the form

$$\begin{aligned} t(\mathbf{k}_f, \mathbf{k}_i) = &\sum_{ST} t^C_{ST} P^S P^T + i \sum_T t^{LS}_T (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \hat{\mathbf{n}} P^T \\ &+ \sum_T t^{TD}_T(q) S_{12}(\hat{\mathbf{q}}) P^T + \sum_T t^{TX}_T(Q) S_{12}(\hat{\mathbf{Q}}) P^T \end{aligned} \tag{17}$$

where $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the direct momentum transfer, $\boldsymbol{Q} = \boldsymbol{k}_i + \boldsymbol{k}_f$ is the exchange momentum transfer, $\hat{\mathbf{n}} = \boldsymbol{q} \otimes \boldsymbol{Q} / \mid \boldsymbol{q} \otimes \boldsymbol{Q} \mid$ is the unit normal to the scattering plane, and $S_{12}(\hat{\mathbf{q}}) = 3\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{q}}\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{q}} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$ is the two-body tensor operator. The interaction form factors

$$t^C_{ST} = \tilde{V}^C_{ST}(q) - (-)^{S+T} \tilde{V}^C_{ST}(Q) \tag{18a}$$

$$t^{LS}_{ST} = \frac{1}{4} qQ [\tilde{V}^{LS}_T(q) + (-)^{1+T} \tilde{V}^{LS}_T(Q)] \tag{18b}$$

$$t^{TD}_T(q) = -\tilde{V}^T_T(q) \tag{18c}$$

$$t^{TX}_T(Q) = -(-)^T \tilde{V}^T_T(Q) \tag{18d}$$

are related to Fourier-Bessel transforms of the pseudopotentials by

$$\tilde{V}^C(q) = 4\pi \int dr\, r^2\, j_0(qr) V^C(r) \tag{19a}$$

$$\tilde{V}^{LS}(q) = 4\pi \int dr\, r^4\, \frac{j_1(qr)}{qr} V^{LS}(r) \tag{19b}$$

$$\tilde{V}^T(q) = 4\pi \int dr\, r^2\, j_2(qr) V^T(r)\ . \tag{19c}$$

Note that the direct and exchange contributions to the central (C) and spin-orbit (LS) interactions have the same operator structure, but that the tensor direct (TD) and exchange (TX) operators are different.

Therefore, the nucleon-nucleon t-matrix can be represented in the standard form

$$
\begin{aligned}
t_{NN} = t^{C} + t^{C}_{\tau}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + t^{C}_{\sigma}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + t^{C}_{\sigma\tau}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
+it^{LS}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\hat{\mathbf{n}} + it^{LS}_{\tau}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\hat{\mathbf{n}}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
+t^{TD}S_{12}(\hat{\mathbf{q}}) + t^{TD}_{\tau}S_{12}(\hat{\mathbf{q}})\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
+t^{TX}S_{12}(\hat{\mathbf{Q}}) + t^{TX}_{\tau}S_{12}(\hat{\mathbf{Q}})\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2
\end{aligned}
\tag{20}
$$

where

$$t^{C} = \frac{1}{16}(t^{C}_{00} + 3t^{C}_{01} + 3t^{C}_{10} + 9t^{C}_{11}) \tag{21a}$$

$$t^{C}_{\tau} = \frac{1}{16}(-t^{C}_{00} + t^{C}_{01} - 3t^{C}_{10} + 3t^{C}_{11}) \tag{21b}$$

$$t^{C}_{\sigma} = \frac{1}{16}(-t^{C}_{00} - 3t^{C}_{01} + t^{C}_{10} + 3t^{C}_{11}) \tag{21c}$$

$$t^{C}_{\sigma\tau} = \frac{1}{16}(t^{C}_{00} - t^{C}_{01} - t^{C}_{10} + t^{C}_{11}) \tag{21d}$$

are the central interactions and

$$t^{m} = \frac{1}{4}(t^{m}_{0} + 3t^{m}_{1}) \tag{22a}$$

$$t^{m}_{\tau} = \frac{1}{4}(-t^{m}_{0} + t^{m}_{1}) \tag{22b}$$

for $m = \{LS, TD, TX\}$ are the spin-orbit and tensor interactions.

2.3.2. Nucleon-nucleus scattering potentials

The nucleon-nucleon interaction in the nucleon-nucleus frame is expressed as

$$t_{NA}(q) = \eta t_{NN}(q, k_A) \tag{23}$$

where the Moller factor η represents the Jacobian between NN and NA frames [4] and where, for the zero-range exchange approximation, the exchange momentum transfer is evaluated in the static approximation $\mathbf{Q} \approx k_A\hat{\mathbf{Q}}$ where k_A is the nucleon momentum in the NA frame and $\hat{\mathbf{Q}}$ is the unit vector that bisects the scattering angle. Several variations of this approximation are available but are essentially equivalent for $T_p > 100$ MeV [10]. In this approach both direct and exchange interactions are reduced to local form and only spatially diagonal transition densities are required, some of which can be obtained directly from electron scattering data.

The nucleon-nucleus scattering operator can now be expanded in terms of multipole operators and scattering potentials

$$U^N = \sum_{\lambda J} \Theta^N_{\lambda J} \cdot \nu^N_{\lambda J} + \sum_J \Theta^{TX}_{JJ} \cdot \nu^{TX}_{JJ} \tag{24a}$$
$$U^A = \sum_{\lambda J} \Theta^A_{\lambda J} \cdot \nu^A_{\lambda J} + \sum_{J,L=J\pm 1} \Theta^{TX}_{LJ} \cdot \nu^{TX}_{LJ} \tag{24b}$$

where N denotes *normal* parity transfer $\Delta\pi = (-)^J$ to the target, A denotes *abnormal* parity transfer $\Delta\pi = (-)^{J+1}$, and TX denotes tensor exchange. The radial potentials $\nu_{\lambda J}$ may include derivative operators which act on the projectile wave function. The angular momentum operators are

$$\begin{aligned}
\Theta^N_{1J} &= Y_J \\
\Theta^N_{2J} &= [Y_J \otimes L]_J \\
\Theta^N_{3J} &= [Y_J \otimes \sigma]_J \\
\Theta^N_{4J} &= \gamma_i Y_J \\
\Theta^N_{5J} &= (\gamma_i - \gamma_f) Y_J \\
\Theta^N_{6J} &= (J(J+1) - (\gamma_f - \gamma_i)(\gamma_f - \gamma_i + 1)) Y_J \\
\Theta^A_{1J} &= [Y_{J-1} \otimes L]_J \\
\Theta^A_{2J} &= [Y_{J-1} \otimes \sigma]_J \\
\Theta^A_{3J} &= [Y_{J+1} \otimes \sigma]_J \\
\Theta^{TX}_{LJ} &= \sqrt{24\pi} \sum_K (-)^{J+K} \hat{K} \begin{Bmatrix} 2 & 1 & 1 \\ L & K & J \end{Bmatrix} [Y_2(\hat{\mathbf{Q}}) \otimes [Y_L \otimes \sigma]_K]_J
\end{aligned}$$

where

$$\sigma \cdot L | l_a j_a \rangle = \gamma_a | l_a j_a \rangle \tag{25}$$

and where the subscripts i(f) denote initial(final) states.

The scattering potentials, obtained by folding components of the nucleon-nucleon interaction with nuclear transition densities are listed below, where t^C refers to the spin-independent and t^C_σ to the spin-dependent central interactions and where isospin labels and summation are suppressed for brevity. To simplify the formulas, it is useful to introduce the auxiliary spin-orbit interaction

$$t'^{LS} = -\frac{2}{qQ} t^{LS} = -(k^2 \sin\theta)^{-1} t^{LS} \; . \tag{26}$$

The scattering potentials for normal parity transfer are

$$\nu^N_{1J} = \frac{2}{\pi} \int dq\, q^2 j_J(qr) \left[t^C(q,\rho) \tilde{\rho}_J(q) + t'^{LS}(q,\rho) \tilde{\Upsilon}_J(q) + \sqrt{J(J+1)} t'^{LS}(q,\rho) \tilde{\mathcal{S}}_{JJ}(q) \frac{1}{r}\frac{\partial}{\partial r} \right] \tag{27a}$$
$$\nu^N_{2J} = \frac{2}{\pi} \int dq\, q^2 t'^{LS}(q,\rho) \left[qr j_{J+1}(qr) - (J+1) j_J(qr) \right] \tilde{\mathcal{S}}_{JJ}(q) \frac{1}{r^2} \tag{27b}$$
$$\nu^N_{3J} = -\frac{2}{\pi} \int dq\, q^2 j_J(qr) \left[t'^{LS}(q,\rho) \tilde{\mathcal{P}}^E_J(q) + \left(t^C_\sigma(q,\rho) - t^{TD}(q,\rho) \right) \tilde{\mathcal{S}}_{JJ}(q) \right] \tag{27c}$$

$$\nu_{4J}^{N} = \frac{1}{r}\frac{\partial}{\partial r} F_J^{LS}(r) \tag{27d}$$

$$\nu_{5J}^{N} = F_J^{LS}(r)\frac{1}{r}\frac{\partial}{\partial r} \tag{27e}$$

$$\nu_{6J}^{N} = F_J^{LS}(r)\frac{1}{2r^2} \ . \tag{27f}$$

Several of these potentials arise from a common spin-orbit potential of the form

$$F_J^{LS}(r) = \frac{2}{\pi}\int dq\ q^2 j_J(qr) t'^{LS}(q,\rho)\tilde{\rho}_J(q) \tag{28}$$

Similarly, the abnormal parity potentials are

$$\nu_{1J}^{A} = \left[\frac{2J+1}{J+1}\right]^{1/2} \frac{1}{r}\frac{2}{\pi}\int dq\, q^3 j_J(qr) t'^{LS}(q,\rho)\tilde{\mathcal{S}}_J^B(q) \tag{29a}$$

$$\begin{aligned}\nu_{2J}^{A} = \frac{2}{\pi}\int dq\, q^2 j_{J-1}(qr)\Bigg[&\left(t_\sigma^C(q,\rho) + \frac{J-1}{2J+1} t^{TD}(q,\rho)\right)\tilde{\mathcal{S}}_{J-1,J}(q) \\ &+ \left[\frac{J+1}{2J+1}\right]^{1/2} t'^{LS}(q,\rho)\tilde{\mathcal{P}}_J^B(q) + 3\frac{[J(J+1)]^{1/2}}{2J+1} t^{TD}(q,\rho)\tilde{\mathcal{S}}_{J+1,J}(q)\Bigg]\end{aligned} \tag{29b}$$

$$\begin{aligned}\nu_{3J}^{A} = \frac{2}{\pi}\int dq\, q^2 j_{J+1}(qr)\Bigg[&\left(t_\sigma^C(q,\rho) + \frac{J+2}{2J+1} t^{TD}(q,\rho)\right)\tilde{\mathcal{S}}_{J+1,J}(q) \\ &- \left[\frac{J}{2J+1}\right]^{1/2} t'^{LS}(q,\rho)\tilde{\mathcal{P}^B}_J(q) + 3\frac{[J(J+1)]^{1/2}}{2J+1} t^{TD}(q,\rho)\tilde{\mathcal{S}}_{J-1,J}(q)\Bigg] \ .\end{aligned} \tag{29c}$$

Finally, the tensor exchange potentials are

$$\nu_{LJ}^{TX} = -\frac{2}{\pi}\int dq\, q^2 j_L(qr) t^{TX}(q,\rho)\tilde{\mathcal{S}}_{LJ}(q) \ , \tag{30}$$

where the potentials with $L = J$ contribute to normal-parity and $L = J \pm 1$ to abnormal-parity transfer.

Each interaction component is considered to be a function of both momentum transfer q and local density ρ. For simplicity, the density dependence of the effective interaction is evaluated at the site of the projectile, but we find that other prescriptions give very similar results. The density dependence can be taken from nuclear matter theory or can be fitted to nucleon scattering data.

The nuclear structure is described by a set of one-body matter, spin, and current transition densities, which in r-space take the form

$$\rho_J(r) = \langle f||Y_J(\hat{\mathbf{r}})||i\rangle \tag{31a}$$

$$\mathcal{S}_{LJ}(r) = \langle f||[Y_L(\hat{\mathbf{r}})\otimes\sigma]_J||i\rangle \tag{31b}$$

$$\mathcal{P}_{LJ}(r) = \langle f||[Y_L(\hat{\mathbf{r}})\otimes\frac{1}{i}\nabla]_J||i\rangle \tag{31c}$$

where each operators acts on a single nucleon and the sum over nucleons remains implicit. The q-space forms are then defined as

$$\tilde{\rho}_J(q) = \int dr\, r^2\, j_J(qr)\rho_J(r) \tag{32a}$$
$$\tilde{\mathcal{S}}_{LJ}(q) = \int dr\, r^2\, j_L(qr)\mathcal{S}_{LJ}(r) \tag{32b}$$
$$\tilde{\mathcal{P}}_{LJ}(q) = iq\int dr\, r^2\, j_L(qr)\mathcal{P}_{LJ}(r)\ . \tag{32c}$$

It is useful to define longitudinal and transverse linear combinations which obey Coulombic (C), electric (E), or magnetic (B) selection rules as follows.

$$\tilde{\mathcal{S}}_J^C = \sqrt{\frac{J+1}{2J+1}}\tilde{\mathcal{S}}_{J+1,J} + \sqrt{\frac{J}{2J+1}}\tilde{\mathcal{S}}_{J-1,J} \tag{33a}$$
$$\tilde{\mathcal{S}}_J^E = \tilde{\mathcal{S}}_{J,J} \tag{33b}$$
$$\tilde{\mathcal{S}}_J^B = \sqrt{\frac{J}{2J+1}}\tilde{\mathcal{S}}_{J+1,J} - \sqrt{\frac{J+1}{2J+1}}\tilde{\mathcal{S}}_{J-1,J} \tag{33c}$$
$$\tilde{\mathcal{P}}_J^C = \sqrt{\frac{J+1}{2J+1}}\tilde{\mathcal{P}}_{J+1,J} + \sqrt{\frac{J}{2J+1}}\tilde{\mathcal{P}}_{J-1,J} \tag{33d}$$
$$\tilde{\mathcal{P}}_J^E = \sqrt{\frac{J}{2J+1}}\tilde{\mathcal{P}}_{J+1,J} - \sqrt{\frac{J+1}{2J+1}}\tilde{\mathcal{P}}_{J-1,J} \tag{33e}$$
$$\tilde{\mathcal{P}}_J^B = \tilde{\mathcal{P}}_{J,J} \tag{33f}$$

Finally, the spin-orbit density that contributes to nucleon-nucleon scattering is defined as

$$\tilde{\Upsilon}_J = \langle f||\boldsymbol{\nabla} j_J(qr)Y_J(\hat{\mathbf{r}}) \otimes \frac{1}{i}\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}||i\rangle\ . \tag{34}$$

2.4. Models of the Effective Interaction

2.4.1. Empirical Effective Interaction

To compare various models of the effective interaction, it is often convenient to use the parametrization which was introduced in Refs. [10,7]:

$$\begin{aligned} t_i(q,\kappa_F) = {} & (S_i - d_i\kappa_F^{\alpha_i})\, t_i^{(f)}(q) \\ & + \kappa_F^{\gamma_i} q^{\delta_i}\sum_{n=1}^{N} a_{in} y^{\beta_i}(q/\mu_{in}). \end{aligned} \tag{35}$$

Here, $\kappa_F = k_F/1.33$ represents the local Fermi momentum relative to saturation, $t^{(f)}(q)$ is the free interaction at zero density, $y(x) = (1+x^2)^{-1}$ is a Yukawa function, and the μ_{in} are various mass parameters which are chosen to optimize the fit to component i. Theoretical interactions require the scale factors S_i to be unity, although the scale factors may be allowed to vary in empirical analyses of scattering data. If the individual components of the interaction are interpreted as Fourier transforms of Yukawa potentials [10], one finds that the natural exponents β are 1 for central, 2 for spin-orbit, and 3 for tensor interactions. Similarly, $\delta = 2$ for tensor interactions and $\delta = 0$ otherwise. For the spin-orbit components of the interaction, we apply this parametrization to t'^{LS}.

The parametrization given in Eq. (35) applies to the real and imaginary parts of each component of the effective interaction separately. The ranges and exponents are chosen such that good fits to theoretical effective interactions are obtained with a small number of strength or damping parameters, a or d, for each component. Although the representation given in Eq. (35) can be used to fit the density dependence of any component of the effective interaction to nucleon scattering data, so far only data for normal-parity isoscalar transitions dominated by the spin-independent central and spin-orbit interactions have been analyzed in detail. Hence it is often convenient to number the Ret^C_{00}, Imt^C_{00}, Ret'^{LS}_0, and Imt'^{LS}_0 components as $i = 1, 4$.

2.4.2. Relationship between inelastic and elastic interactions

The effective interactions for elastic and inelastic scattering are generally different. In nonrelativistic models, the effective interaction applicable to inelastic scattering is usually related to the effective interaction for elastic scattering in nuclear matter by means of the Cheon rearrangement relation [11,12]

$$t^{inelastic}(q,\rho) = (1 + \partial/\partial\rho) t^{elastic}(q,\rho). \tag{36}$$

This relationship, based primarily upon collective model arguments, is applied to each of the interaction components. However, the relativistic IA2 model provides a method for calculating the effective interaction for inelastic scattering directly without recourse to the Cheon prescription and finds some significant departures from that relationship [13]. On the other hand, the IA2 interaction does not accurately describe proton scattering data for $T_p \leq 200$ MeV where nucleon knockout experiments have been performed.

2.5. Collective Models

2.5.1. Deformation Procedures

A relatively general formulation of the collective model may be based upon the deformation procedure

$$r \longrightarrow r'(\Omega) = r \left[1 - \sum_{\ell} \left(\frac{r}{R} \right)^{K-1} \alpha_\ell \cdot Y_\ell(\Omega) \right] \; + \; \mathcal{O}(\alpha^2) \tag{37}$$

where R defines a characteristic radial scale and $\mathcal{O}(\alpha^2)$ indicates second–order corrections required for volume conservation but not immediately relevant to first–order transitions. The standard collective model is recovered by choosing $K = 0$. Other useful modles include uniform radial strain ($K = 1$) and the hydrodynamic or Tassie model ($K = \ell - 1$).

Deformed multipoles of the radial function $f(r)$ are then obtained from the deformation procedure

$$f(r) \longrightarrow f(\mathbf{r}) = f(r) + \sum_{\ell m} f_{\ell m}(r) Y^*_{\ell m}(\hat{\boldsymbol{r}}) \tag{38a}$$

where $\ell \geq 2$. For small deformation, the radial multipole densities become

$$\alpha \to 0 \Longrightarrow f_{\ell m}(r) = \alpha_{\ell m} R \left(\frac{r}{R}\right)^K \frac{\partial f}{\partial r}\,. \tag{39}$$

It is customary to define reduced matrix elements according to

$$\left\langle \begin{matrix} I_f \\ M_f \end{matrix} \middle| f_{\ell m} \middle| \begin{matrix} I_i \\ M_i \end{matrix} \right\rangle = \left\langle \begin{matrix} I_i & \ell \\ M_i & m \end{matrix} \middle| \begin{matrix} I_f \\ M_f \end{matrix} \right\rangle f_\ell \tag{40a}$$

$$\left\langle \begin{matrix} I_f \\ M_f \end{matrix} \middle| \alpha_{\ell m} \middle| \begin{matrix} I_i \\ M_i \end{matrix} \right\rangle = \left\langle \begin{matrix} I_i & \ell \\ M_i & m \end{matrix} \middle| \begin{matrix} I_f \\ M_f \end{matrix} \right\rangle \beta_\ell / \hat{\ell} \tag{40b}$$

whereby

$$\hat{\ell} f_\ell(r) = -\beta_\ell R \left(\frac{r}{R}\right)^K \frac{\partial f}{\partial r} = -\delta_\ell \left(\frac{r}{R}\right)^K \frac{\partial f}{\partial r} \tag{41}$$

and where $\delta_\ell = \beta_\ell R$ is known as the deformation length. The standard collective model is obtained by choosing $K = 0$ and assuming that $f(r) = g(r - R)$ is symmetric with respect to the surface radius R.

Application of this procedure to the charge density ρ produces Coulomb multipole potentials of the form

$$\hat{\ell} U^Z_\ell(r) = \delta_\ell \frac{Z' e^2}{2\ell + 1} \int dr'\, r'^2 \left(\frac{r'}{R}\right)^K \frac{\partial \rho(r')}{\partial r'} \frac{r^\ell_<}{r^{\ell+1}_>} \tag{42}$$

where Z' is the projectile charge and $r_<$ ($r_>$) is the lesser (greater) of r' and R. Asymptotically, this potential reduces to

$$r \to \infty \Longrightarrow U^Z_\ell(r) \to \frac{4\pi Z' e^2}{2\ell + 1} \frac{M_\ell}{r^{\ell+1}} \tag{43}$$

where

$$M_\ell = \int dr\, r^{\ell+2}\, \rho_\ell(r) = \frac{\delta_\ell}{\hat{\ell}} \frac{Z}{4\pi} (\ell + K + 2) \frac{\langle r^{\ell+K-1} \rangle}{R^K} \tag{44}$$

is the Coulomb matrix element, which is related by partial integration to a moment of the ground–state charge density by

$$\langle r^{\ell+K-1} \rangle = \frac{\int dr\, r^2 \rho(r)\, r^{\ell+K-1}}{\int dr\, r^2 \rho(r)}\,. \tag{45}$$

For a uniform charge density, the Coulomb matrix element reduces to

$$\rho(r) = \frac{3Z}{4\pi R^3}\Theta(R-r) \Longrightarrow M_\ell = \frac{\beta_\ell}{\hat{\ell}}\frac{3Z}{4\pi}R^\ell \tag{46}$$

for any choice of K.

The reduced transition density for a deformed charge density is

$$B(C\ell) = \frac{2I_f+1}{2I_i+1}\left[\frac{\delta_\ell}{\hat{\ell}}\frac{Z}{4\pi}\frac{\langle r^{\ell+K-1}\rangle}{R^K}\right]^2 \tag{47}$$

and reduces to

$$\text{uniform } \rho,\ I_i = 0 \Longrightarrow B(C\ell) = \left[\frac{3Z}{4\pi}\beta_\ell R^\ell\right]^2 \tag{48}$$

for the special case of a uniform charge density and $I_i = 0$.

This procedure may also be applied to optical potentials derived from folding models. For simplicity, consider a real potential based upon the local density–independent interaction $\nu(s)$, whereby

$$V(r) = \int d^3r'\ \rho(r')\nu(|\mathbf{r}-\mathbf{r}'|)\ .$$

Multipole potentials may be constructed by deformation of the optical potential itself or by deformation of the density ρ, in which case

$$V_\ell(r) = \frac{2}{\pi}\int dq\, q^2\, j_\ell(qr)\tilde{\rho}_\ell(q)\tilde{\nu}(q)\ .$$

To compare these methods, it is useful to define the moment functionals

$$M_\lambda[f] = \int dr\, r^{2+\lambda}\, f(r) \qquad \lambda > 0 \tag{49a}$$

$$M_0[f] = 4\pi\int dr\, r^{2+\lambda}\, f(r) \qquad \lambda = 0\ . \tag{49b}$$

If V_ℓ is obtained from folding ν against a deformed ρ_ℓ, we obtain

$$M_\ell[V_\ell] = \frac{\delta_\ell}{\hat{\ell}}\tilde{\nu}(0)\frac{A}{4\pi}(\ell+K+2)\frac{\langle r^{\ell+K-1}\rangle_\rho}{R_\rho^K}$$

where R_ρ is the radial scale parameter appropriate to the charge distribution. Alternatively, if V_ℓ is obtained by deformation of the spherical potential, we find

$$M_\ell[V_\ell] = \frac{\delta_\ell}{\hat{\ell}}M_0[V]\frac{\ell+K+2}{4\pi}\frac{\langle r^{\ell+K-1}\rangle_V}{R_V^K}$$

where R_V is the radial scale parameter appropriate to the poential V. Recognizing that the folding model predicts

$$M_\ell[V_\ell] = M_\ell[\rho_\ell] M_0[\nu]$$
$$M_0[V] = A M_0[\nu] = A\tilde{\nu}(0) \; ,$$

the transition moments can be estimated from the deformed potential according to

$$M_\ell[\rho_\ell] = M_\ell[V_\ell]/M_0[V] \tag{50a}$$
$$= \frac{\ell+K+2}{4\pi\hat{\ell}} \left[\delta_\ell \frac{\langle r^{\ell+K-1} \rangle}{R^K} \right]_\rho \tag{50b}$$
$$= \frac{\ell+K+2}{4\pi\hat{\ell}} \left[\delta_\ell \frac{\langle r^{\ell+K-1} \rangle}{R^K} \right]_V \; . \tag{50c}$$

For the special case of a uniform distribution,

$$V(r) = \frac{3}{4\pi R^3} M_0[V] \Theta(R-r) \Longrightarrow \langle r^{\ell+K-1} \rangle_V = \frac{3}{\ell+K+2} R_V^{\ell+K-1} \; , \tag{51}$$

we find

$$\hat{\ell} M_\ell[V_\ell] = \frac{3}{4\pi} \delta_\ell^V M_0[V] R_V^{\ell-1}$$
$$\hat{\ell} M_\ell[\rho_\ell] = \frac{3}{4\pi} \delta_\ell^\rho A R_\rho^{\ell-1} \; .$$

Equality between these expressions for $M_\ell[\rho_\ell]$ requires

$$\beta_\ell^V R_V^\ell = \beta_\ell^\rho R_\rho^\ell \; . \tag{52}$$

Unfortunately, unless ν has zero range, this condition cannot be satisfied with a ratio $\beta_\ell^\rho/\beta_\ell^V$ that is independent of ℓ. It is common practice to assume that the quantity βR is independent of probe, but it appears impossible to justify this assumption. Rather, it would appear necessary to apply the normalization factor

$$\beta_\ell^\rho = \beta_\ell^V \left(\frac{R_V}{R_\rho} \right)^\ell \tag{53}$$

to deduce $B(C\ell)$ from hadronic deformation parameters. Due to the finite range of ν, this factor is expected to be greater than unity and to increase rapidly with ℓ. This behavior is in fact observed.

More generally, calculation of $B(C\ell)$ from hadronic defomation lengths requires numerical computation of the normalization factors

$$\delta_\ell^\rho/\delta_\ell^V = \left[\frac{\langle r^{\ell+K-1} \rangle}{R^K} \right]_V \Big/ \left[\frac{\langle r^{\ell+K-1} \rangle}{R^K} \right]_\rho \; . \tag{54}$$

In the original deformation prescription, the surface radius R entered only as an arbitrary scale parameter. If we require the normalization factor to be unity for zero range interactions, we must choose $R_V = R_\rho$. Therefore, the normalization factor reduces to

$$\frac{\beta_\ell^\rho}{\beta_\ell^V} = \frac{\langle r^{\ell+K-1}\rangle_V}{\langle r^{\ell+K-1}\rangle_\rho} \tag{55}$$

under those conditions.

Finally, $B(C\ell) \propto R^{2\ell}$ remains highly sensitive to the choice of R. The best procedure is to choose the K which gives the best fit to either the data or a known transition density of the same ℓ in a nearby nucleus and then to select the R which reproduces a known $B(C\ell)$ and finally to scale R as $A^{1/3}$. The model is then fully calibrated and can be expected to give reliable results for similar transitions in nearby nuclei.

2.6. Channel Coupling in Nucleon–Nucleus Scattering

2.6.1. General Description

Channel coupling is included by expanding the wave function for each nucleon–nucleus channel in the form

$$\Psi_\alpha^{(+)} = \sum_\beta \chi_{\alpha\beta}^{(+)} \psi_\beta \tag{56}$$

where ψ_β represents the internal state of the nucleus and $\chi_{\alpha\beta}^{(+)}$ represents the relative wave function containing an incoming plane wave in channel α and outgoing spherical waves in each channel β. The relative wave functions satisfy coupled equations of the form

$$(E_\beta - K_\beta - U_\beta)\chi_{\alpha\beta} = \sum_\gamma U_{\beta\gamma}\chi_{\alpha\gamma} \tag{57}$$

where K_β is the kinetic energy operator, U_β is the optical potential, and

$$U_{\beta\gamma}(\mathbf{r}_\beta) = (\psi_\beta|U|\psi_\gamma) \tag{58}$$

is the scattering operator with couples channel γ to channel β. For simplicity, we include only the spherical optical potential on the left–hand side of Eq. (57) and classify nonspherical elastic potentials as coupling potentials which contribute to the right–hand side. Note that we often refer to nonspherical elastic potentials as reorientation potentials.

For each pair of channels (with suppressed labels), we assume that the scattering operator can be decomposed into a sum of products

$$U = \sum_{\kappa\lambda} \nu_{\kappa\lambda}(r)\mathcal{P}_{\kappa\lambda} \cdot \mathcal{T}_{\kappa\lambda} \tag{59}$$

in which $\nu_{\kappa\lambda}(r)$ contains the dependence upon relative separation and where the multipole operators $\mathcal{P}_{\kappa\lambda}$ and $\mathcal{T}_{\kappa\lambda}$ depend only on the angular momenta and internal variables of the projectile and target, respectively. The angular momentum transfer is designated λ, whereas κ is used to distinguish between different operators with the same multipolarity. Partial–wave potentials of the form

$$U_{\beta\gamma J} = \langle l_\beta s_\beta j_\beta I_\beta JM|U|l_\gamma s_\gamma j_\gamma I_\gamma JM\rangle \tag{60}$$

then become

$$U_{\beta\gamma J} = \sum_{\kappa\lambda} \Gamma_{\lambda J}(j_\beta I_\beta; j_\gamma I_\gamma) \nu_{\beta\gamma\kappa\lambda} \tag{61}$$

where the recoupling coefficient is

$$\Gamma_{\lambda J}(j_\beta I_\beta; j_\gamma I_\gamma) = (-)^{j_\gamma + I_\beta + J} \hat{j}_\beta \hat{I}_\beta \begin{Bmatrix} j_\beta & j_\gamma & \lambda \\ I_\gamma & I_\beta & J \end{Bmatrix} \tag{62}$$

and where

$$\nu_{\beta\gamma\kappa\lambda}(r) = \nu_{\kappa\lambda}(r) \langle l_\beta s_\beta j_\beta || \mathcal{P}_{\kappa\lambda} || l_\gamma s_\gamma j_\gamma \rangle \langle \beta I_\beta || \mathcal{T}_{\kappa\lambda} || \gamma I_\gamma \rangle \tag{63}$$

are the appropriate multipole potentials, including angular and target matrix elements.

The coupling potentials are obtained either from the folding model or from phenomenological models. Within the folding model, all transition potentials described in Sec. 2.3.2 are included except those originating in the tensor–exchange interaction.

2.6.2. Sequential Iteration of Coupled Equations

A standard partial wave analysis of the coupled equations is made and the equations for each channel spin are solved using a sequential iteration algorithm based upon the ECIS method of Raynal [14] in the subroutine `SICE`. Note that SICE stands for sequential iteration of coupled equations and is essentially the same acronym coined by Raynal except that in French the natural word order is inverted and hence SICE is ECIS spelled backwards.

Partial waves for the coupled–channels problem satisfy systems of coupled equations of the form

$$\mathcal{D}_{\beta J} \chi_{\alpha\beta J} = 2\mu_\beta \sum_\gamma V_{\beta\gamma J} \chi_{\alpha\gamma J} \tag{64}$$

where $\mathcal{D}_{\beta J}$ is a linear differential operator that is diagonal with respect to channel parameters $\beta J \equiv \{n_\beta \ell_\beta I_\beta j_\beta I_B J\}$. The entrance channel containing an incident plane (or Coulomb) wave is identified with the label α. The exit channels β (including α) are coupled to other channels γ via the coupling potential $V_{\beta\gamma J}$, which is diagonal with respect to total angular momentum and parity. The boundary conditions are specified by the asymptotic behavior

$$\chi_{\alpha\beta J} \sim \delta_{\alpha\beta} F_\beta + C_{\alpha\beta J} H_\beta \tag{65}$$

where the common label α may be suppressed when clarity permits. For simplicity, assume that $V_{\beta\gamma J}$ is local and that

$$\mathcal{D}_{\beta J} = \frac{d^2}{dr^2} - \frac{\ell_\beta(\ell_\beta + 1)}{r^2} + k_\beta^2 - 2\mu_\beta U_{\beta J}(r) \tag{66}$$

where $U_{\beta J}$ is also local and does not contain derivative operators. These assumptions for $\mathcal{D}$ and V are suitable for the Schrödinger equation with customary optical potentials.

For each channel βJ a Green function $\mathcal{G}_{\beta J}$ can be defined as the solution to

$$\mathcal{D}_{\beta J}\mathcal{G}_{\beta J}(r,r') = 2\mu_\beta \delta(r-r') \tag{67}$$

subject to the boundary conditions

$$\begin{aligned} r \to 0 &\Longrightarrow \mathcal{G}_{\beta J}(r,r') \propto f_{\beta J}(r) \\ r \to \infty &\Longrightarrow \mathcal{G}_{\beta J}(r,r') \propto h_{\beta J}(r) \end{aligned}$$

where f and h are regular and irregular solutions to the homogeneous equations

$$\mathcal{D}_{\beta J} f_{\beta J}(r) = 0 \qquad\qquad f_{\beta J}(r) \propto r^{\ell_\beta+1} \text{ as } r \to 0$$

$$\mathcal{D}_{\beta J} h_{\beta J}(r) = 0 \qquad\qquad h_{\beta J}(r) \propto r^{-\ell_\beta} \text{ as } r \to 0$$

with standard boundary conditions for the uncoupled equations. Thus, we obtain the usual

$$\mathcal{G}_{\beta J}(r,r') = -\frac{2\mu_\beta}{k_\beta} f_{\beta J}(r_<) h_{\beta J}(r_>) \tag{68}$$

where $r_<$ ($r_>$) is the lesser (greater) of r and r'.

The asymptotic behavior of the solutions to the homogeneous equations can be expressed as

$$\begin{aligned} f_{\beta J} &\sim \delta_{\alpha\beta} F_\beta + C^{(0)}_{\beta J} H_\beta \\ h_{\beta J} &\sim H_\beta \end{aligned}$$

so that f consists of an incoming plane wave and outgoing spherical waves whereas h is purely outgoing. Therefore, formal solutions to the coupled equations can be expressed as integral equations of the form

$$\chi_{\alpha\beta J} = \delta_{\alpha\beta} f_{\alpha J} + \sum_\gamma \int dr'\ \mathcal{G}_{\beta J}(r,r') V_{\beta\gamma J}(r') \chi_{\alpha\gamma J}(r')\ . \tag{69}$$

Asymptotically, such solutions approach

$$\chi_{\alpha\beta J} \sim \delta_{\alpha\beta}\left[F_\alpha + C^{(0)}_{\alpha J} H_\alpha\right] - \frac{2\mu_\beta}{k_\beta} h_{\beta J}(r) \sum_\gamma \int dr'\ f_{\beta J}(r') V_{\beta\gamma J}(r') \chi_{\alpha\gamma J}(r') \tag{70}$$

so that we can identify the C–matrix as

$$C_{\alpha\beta J} = \delta_{\alpha\beta} C^{(0)}_{\alpha J} - \frac{2\mu_\beta}{k_\beta} \sum_\gamma \int dr\ f_{\beta J}(r) V_{\beta\gamma J}(r) \chi_{\alpha\gamma J}(r)\ . \tag{71}$$

An iterative solution to a system of coupled equations can be developed with the aid of an order parameter λ introduced into the system as follows:

$$\mathcal{D}_{\beta J}\chi_{\alpha\beta J} = 2\mu_\beta \sum_\gamma \lambda V_{\beta\gamma J}\chi_{\alpha\gamma J}$$

The formal solution

$$\chi_{\alpha\beta J} = \delta_{\alpha\beta} f_{\alpha J} + \sum_{\gamma} \int dr' \; \mathcal{G}_{\beta J}(r,r') \lambda V_{\beta\gamma J}(r') \chi_{\alpha\gamma J}(r') \; .$$

involves χ on both sides. With the ansatz

$$\chi_{\alpha\beta J} = \sum_n \lambda^n \chi^{(n)}_{\alpha\beta J}$$

we find

$$\sum_n \lambda^n \chi^{(n)}_{\alpha\beta J} = \delta_{\alpha\beta} f_{\alpha J} + \sum_n \lambda^{n+1} \sum_{\gamma} \int dr' \; \mathcal{G}_{\beta J}(r,r') \lambda V_{\beta\gamma J}(r') \chi^{(n)}_{\alpha\gamma J}(r') \; .$$

Equating the coefficients of λ^n on both sides, we obtain

$$\chi^{(0)}_{\alpha\beta J} = \delta_{\alpha\beta} f_{\alpha J} \tag{72a}$$

$$\chi^{(n)}_{\alpha\beta J} = \sum_{\gamma} \int dr' \; \mathcal{G}_{\beta J}(r,r') V_{\beta\gamma J}(r') \chi^{(n-1)}_{\alpha\gamma J}(r') \; . \tag{72b}$$

Similarly,

$$C_{\alpha\beta J} = \sum_n \lambda^n C^{(n)}_{\alpha\beta J} \tag{73a}$$

$$C^{(0)}_{\alpha\beta J} = \delta_{\alpha\beta} C^{(0)}_{\alpha J} \tag{73b}$$

$$C^{(n)}_{\alpha\beta J} = -\frac{2\mu_\beta}{k_\beta} \sum_{\gamma} \int dr \; f_{\beta J}(r) V_{\beta\gamma J}(r) \chi^{(n-1)}_{\alpha\gamma J}(r) \tag{73c}$$

so that truncation at $n = 1$ yields the familiar DWBA for $C_{\alpha\beta J}$. Recall that $C^{(0)}_{\alpha J}$ contains the phase shifts for the solutions to the homogeneous equations for the entrance channel.

2.6.3. Symmetric Rotor Model

The optical potential for an axially symmetric nucleus can be expanded in multipoles

$$V(\mathbf{r},\mathbf{r}') = 4\pi \sum_{\lambda} V_\lambda(r) Y_\lambda(\hat{\boldsymbol{r}}) \cdot Y_\lambda(\hat{\boldsymbol{r}}') = \sum_{\lambda} (2\lambda+1) V_\lambda(r) P_\lambda(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}}') \tag{74}$$

where $\mathbf{r}$ is the projectile position and $\hat{\boldsymbol{r}}'$ is the orientation of the symmetry axis. The radial multipole densities may be obtained by Legendre projection, such that

$$V_\lambda(r) = \frac{1}{2} \int_{-1}^{1} dx \; P_\lambda(x) V(\mathbf{r}, x) \tag{75}$$

where $x = \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}}'$ is the cosine of the angle between $\boldsymbol{r}$ and $\hat{\boldsymbol{r}}'$.

For an even–even nucleus, the wave function has the form

$$|\alpha IMK\rangle = \psi^I_{MK}(\omega)|\alpha K\rangle \tag{76}$$

where (I, M) denote the total angular momentum, α the internal quantum numbers of the intrinsic state, and K the projection of the intrinsic angular momentum upon the symmetry axis. The rotational wave function is

$$\psi^I_{MK}(\omega) = (1+\delta_{K0})^{-1/2}\frac{\hat{I}}{4\pi}\left[\mathcal{D}^I_{MK}(\omega) + (-)^I\mathcal{D}^I_{M,-K}(\omega)\right] \tag{77}$$

where ω denotes the set of Euler angles which specify the nuclear orientation with respect to the laboratory system and where $\mathcal{D}$ is an element of the rotation operator. The second term is needed to symmetrize the wave function with respect to inversion of the symmetry axis.

Using standard relationships between spherical harmonics and rotation matrix elements, it can be shown that the coupling potentials within a rotational band for the symmetric rotor become

$$\langle I'M'K'|V|IMK\rangle = \delta_{K,K'}\sqrt{4\pi}\sum_{\lambda\mu}\frac{\hat{\lambda}\hat{I}}{\hat{I}'}\left\langle \begin{matrix} I & \lambda \\ M & \mu \end{matrix}\middle| \begin{matrix} I' \\ M' \end{matrix}\right\rangle \left\langle \begin{matrix} I & \lambda \\ K & 0 \end{matrix}\middle| \begin{matrix} I' \\ K' \end{matrix}\right\rangle V_\lambda(r)Y^*_{\lambda\mu}(\hat{\boldsymbol{r}})\ . \tag{78}$$

Comparing this result with Eq. (59), we identify the multipole potentials and the projectile and target transition operators as

$$\nu_\lambda(r) = V_\lambda(r) \tag{79}$$

$$\mathcal{P}_{\lambda\mu} = Y_{\lambda\mu}(\hat{\boldsymbol{r}}) \tag{80}$$

$$\mathcal{T}_{\lambda\mu} = \sqrt{4\pi}\frac{\hat{\lambda}\hat{I}}{\hat{I}'}\left\langle \begin{matrix} I & \lambda \\ M & \mu \end{matrix}\middle| \begin{matrix} I' \\ M' \end{matrix}\right\rangle \left\langle \begin{matrix} I & \lambda \\ K & 0 \end{matrix}\middle| \begin{matrix} I' \\ K' \end{matrix}\right\rangle \delta_{K,K'} \tag{81}$$

so that the target reduced matrix elements become

$$\langle I'K'||\mathcal{T}_\lambda||IK\rangle = \sqrt{4\pi}\frac{\hat{\lambda}\hat{I}}{\hat{I}'}\left\langle \begin{matrix} I & \lambda \\ K & 0 \end{matrix}\middle| \begin{matrix} I' \\ K' \end{matrix}\right\rangle \delta_{K,K'}\ . \tag{82}$$

2.6.4. Vibrational Model

If a spherical field $V(r)$ is deformed according to Eq. (37), then to first order in the deformation variables $\alpha_{\lambda\mu}$ the multipole potentials and projectile and target transition operators become

$$\nu_\lambda(r) = -R\left(\frac{r}{R}\right)^K \frac{\partial V(r)}{\partial r} \tag{83}$$

$$\mathcal{P}_{\lambda\mu} = Y_{\lambda\mu}(\hat{\boldsymbol{r}}) \tag{84}$$

$$\mathcal{T}_{\lambda\mu} = \alpha_{\lambda\mu}\ . \tag{85}$$

The phonon operators are quantized using standard methods and we limit consideration here to single–phonon transitions and, hence to 0, 1, and 2 phonon states.

Let $|0\rangle$ represent the zero–phonon ground–state,

$$|\lambda_1\mu_1; IM\rangle = \delta_{\lambda_1 I}\delta_{\mu_1 M} b^\dagger_{\lambda_1\mu_1}|0\rangle \tag{86}$$

represent a single–phonon state, and

$$|\lambda_1\lambda_2; IM\rangle = (1+\delta_{\lambda_1\lambda_2})^{-1/2}[b^\dagger_{\lambda_1}\otimes b^\dagger_{\lambda_2}]_{IM}|0\rangle \tag{87}$$

represent a two–phonon state with total angular momentum and magnetic quantum numbers I and M. The reduced matrix elements for single–phonon transitions are then

$$\langle\lambda; I||\alpha_\lambda||0\rangle = \delta_{\lambda I}\beta_\lambda/\hat{\lambda} \tag{88}$$

$$\langle 0||\alpha_\lambda||\lambda; I\rangle = \delta_{\lambda I}(-)^I\beta_\lambda \tag{89}$$

$$\langle\lambda_2; I'||\alpha_\lambda||\lambda_1; I\rangle = 0 \tag{90}$$

$$\langle\lambda_2\lambda_3; I'||\alpha_\lambda||\lambda_1; I\rangle = \delta_{\lambda_1 I}\frac{\beta_\lambda}{\hat{\lambda}}\left[(-)^{\lambda+I-I'}\delta_{\lambda\lambda_2}\delta_{\lambda_3 I} + \delta_{\lambda\lambda_3}\delta_{\lambda_2 I}\right]/(1+\delta_{\lambda_2\lambda_3})^{1/2} \tag{91}$$

$$\langle\lambda_1; I||\alpha_\lambda||\lambda_2\lambda_3; I'\rangle = \delta_{\lambda_1 I}\frac{\beta_\lambda}{\hat{\lambda}}(-)^\lambda\frac{\hat{I}'}{\hat{I}}\left[\delta_{\lambda\lambda_2}\delta_{\lambda_3 I} + (-)^{\lambda+I-I'}\delta_{\lambda\lambda_3}\delta_{\lambda_2 I}\right]/(1+\delta_{\lambda_2\lambda_3})^{1/2}\,. \tag{92}$$

3. LINEAR EXPANSION ANALYSIS

3.1. General Method

We represent the scattering amplitude T for the binary reaction $A(\vec{a},\vec{b})B$ as a linear expansion

$$T = \sum a_n T^n(\theta) \tag{93}$$

of coefficients a_n times basis amplitudes $T^n(\theta)$, where the four spin projections (m_A, m_a, m_b, m_B) have been suppressed for clarity. The quadratic forms

$$X^{nn'}_{\alpha\beta}(\theta) = Trace\left[T^n(\theta)\sigma_\alpha T^{n'}(\theta)^*\sigma_\beta\right] \tag{94}$$

are then constructed as traces over spin projections of products involving the basis amplitudes and the polarization vectors σ_α and σ_β. The polarization vectors are simply Pauli matrices for nucleons. The observables are then contractions of these quadratic forms:

$$\sigma_0(\theta) = \frac{\mu_a\mu_b}{(2\pi)^2}\frac{k_b}{k_a}\frac{I_0(\theta)}{2J_i+1} \tag{95}$$

$$I_0(\theta) = \frac{1}{2}\sum_{nn'} a_n X^{nn'}_{00}(\theta)a^*_{n'} \tag{96}$$

$$I_o D_{\alpha\beta} = \frac{1}{2}\sum_{nn'} a_n X^{nn'}_{\alpha\beta}(\theta)a^*_{n'} \tag{97}$$

where J_i is the ground-state target spin and where $\mu_a(\mu_b)$ is the reduced energy and $k_a(k_b)$ is the wave number in the incident (exit) channel. The analyzing power $A_y = D_{y0}$ and the induced polarization $P = D_{0y}$ are special cases of the depolarization matrix $D_{\alpha\beta}$ defined by Ohlsen.

To reduce storage requirements, we require the coefficients a_n to be real and exploit the fact that

$$X_{\alpha\beta}^{nn'^*} = X_{\alpha\beta}^{n'n}$$

to obtain

$$I_0 D_{\alpha\beta} = \sum_{n'=1}^{N} \sum_{n=1}^{n} a_n X_{\alpha\beta}^{nn'} a_{n'} \tag{98}$$

where $X_{\alpha\beta}^{nn'} = Re X_{\alpha\beta}^{nn'}$ is stored as a one-dimensional array.

These methods are applicable to any model of nuclear structure or of the nucleon-nucleon interaction for which the scattering amplitude can be reduced to a linear expansion in the parameters of the model. Although the program provides generic routines to perform these tasks, two particular models have been developed in considerable detail. These applications are discussed in the following sections. Other applications may be developed easily.

3.2. Empirical Effective Interaction

The nucleon-nucleon effective interaction is known to depend strongly upon the target density within the interaction region. Although the several theoretical calculations presently available agree as to the general characteristics of the medium modifications, their detailed predictions vary considerably. Therefore, it is important to develop a phenomenological description of the effective interaction suitable to the analysis of data.

We have found that the density dependence of all available theoretical interactions can be parametrized using the generic function

$$t_i(q, \kappa_F) = (S - d\kappa_F^{\alpha}) t_i(q, 0) + \kappa_F^{\gamma} q^{\delta} \sum a_n \left[1 + \left(\frac{q}{\mu_n} \right)^2 \right]^{-\beta} \tag{99}$$

where $\kappa_F = k_F/1.33$ represents the local Fermi momentum k_F relative to saturation. If we consider the various components of the t-matrix to be appropriate Fourier transforms of Yukawa expansions, we find that the natural exponents β are 1 for central, 2 for spin-orbit, and 3 for tensor interactions. Similarly, we use $\delta = 2$ for tensor interactions and $\delta = 0$ otherwise. The scale factors S are usually constrained to unity when reparametrizing theoretical interactions but may vary for phenomenological analyses. The damping parameters (d) represent Pauli blocking corrections and are used primarily for the imaginary part of the central interaction. The Yukawa parameters a_n and μ_n describe short-range modifications to the pair wave function. Good fits to theoretical interactions are obtained using $\alpha = \gamma = 2$ for imaginary parts and $\gamma = 3$ for real parts of both central and spin-orbit interactions. The free interaction $t(q, 0)$ is obtained by extrapolating the G-matrix to zero density.

For fixed choices of exponents $(\alpha, \beta, \gamma, \delta)$ and ranges (μ_n), the empirical effective interaction is linear in its strength parameters (S, d, a_n) and hence, amenable to the LEA method, provided that the nuclear structure is known with sufficient accuracy. In practice, this requirement upon structure amplitudes has limited applications to normal-parity isoscalar excitations of selfconjugate targets. Transitions of this type are described by a single transition density, the matter density $\rho(r)$. The transition charge density can be measured quite accurately using electron scattering and the proton transition density determined by unfolding the nucleon form factor. Charge symmetry then ensures that the neutron and proton transition densities for self-conjugate targets are very nearly equal. Therefore, electroexcitation measurements suffice to determine the relevant aspects of nuclear structure with sufficient accuracy that medium modifications of the isoscalar spin-independent central and isoscalar spin-orbit interactions can be fitted to proton scattering for normal-parity excitations of self-conjugate targets with little residual uncertainty due to nuclear structure.

However, the most general form of the empirical effective interaction carries more parameters than can be extracted from data. To reduce the correlations between parameters while retaining the essential physics of the model, a simplified version

$$\Re t^C(q,\kappa_F) = S_1 \Re t^C(q,0) + \kappa_F^{\gamma_1} b_1 \left[1+(q/\mu_1)^2\right]^{-1} \tag{100}$$

$$\Im t^C(q,\kappa_F) = \left[S_2 - d\kappa_F^{\gamma_2}\right] \Im t^C(q,0) \tag{101}$$

$$\Re \tau^{LS}(q,\kappa_F) = S_3 \Re \tau^{LS}(q,0) + \kappa_F^{\gamma_3} b_3 \left[1+(q/\mu_3)^2\right]^{-2} \tag{102}$$

has been used for all analyses of data reported to date.

If the local density approximation (LDA) is to be considered sound, the empirical effective interaction should satisfy three basic criteria. First, for a given target the interaction should be independent of state. Second, the interaction should also be independent of target. Third, the parameters should vary smoothly with energy and be roughly in accord with the theoretical predictions upon which the model is based. Therefore, the fitting procedure allows many states of a given target to be fitted simultaneously using a common set of parameters. Furthermore, data for several different targets at the same projectile energy may be fitted simultaneously. However, no provision has yet been made for simultaneous analysis of multiple energies.

It has also been established, at least for this class of excitation, that the density dependences for inelastic and elastic scattering are related by the rearrangement factor

$$t(inelastic) = \left[1 + \rho\frac{\partial}{\partial\rho}\right] t(elastic) \tag{103}$$

based upon the local ground-state density. It is the elastic interaction which emerges from nuclear matter theory and to which we usually compare the fitted interaction. Notice that the rearrangement factor enhances the coefficient of any term proportional to κ^γ by the factor $(3+\gamma)/3$. Hence, for inelastic scattering a term proportional to density ($\gamma = 3$) is enhanced by a factor of 2 relative to elastic scattering.

To maintain consistency between distortion and scattering, we embed the fit to inelastic scattering data within a self-consistency cycle. We begin by computing optical potentials based upon the best available theory of the G-matrix. These optical potentials are used to generate distorted waves. Overlap integrals are then computed for each state and each term of the expansion of the effective interaction. The coefficients are then fitted to all available data. The coefficients fitted to inelastic scattering data are then used to recalculate the optical potentials and distorted waves for the next iteration. New overlap integrals are computed and the fit repeated. This procedure is iterated until convergence is obtained for the parameters of the effective interaction.

3.3. Transition Densities

3.3.1. Radial Densities

A radial density $\rho_\ell(r)$ can be represented as a linear expansion

$$\rho_\ell(r) = \sum_\nu a_\nu f_{\nu\ell}(r) \tag{104}$$

where the radial basis functions $f_{\nu\ell}(r)$ are drawn from any convenient complete set. The expansion coefficients a_ν can be fitted by minimizing the composite χ^2 for all available data. The error envelope can then be deduced from the error matrix. This type of analysis is almost model independent in the sense that rather than fitting with a restrictive, and arbitrary, analytic form, the significant coefficients of an expansion in a complete basis of radial functions are fitted. The resulting density is then not biased by the choice of model. Virtually any radial function can be represented in this manner, with only minor restrictions being imposed by the inevitable truncation of the series.

For comparisons with electroexcitation data it is convenient to define the form factor for transitions between nuclear states with initial and final spins J_i and J_f as

$$F_\lambda(q) = \frac{\sqrt{4\pi}}{N_\lambda} \frac{\hat{J}_f}{\hat{J}_i} \rho_\ell(q) \tag{105}$$

where

$$\tilde{\rho}_\ell(q) = \int dr r^2 j_\ell(qr) \rho_\ell(r) = \sum_\nu a_\nu \tilde{f}_{\nu\ell}(q) \tag{106}$$

is the Fourier-Bessel transform of the transition density and where $\hat{x} = \sqrt{2x+1}$. The particle number N_λ is either N or Z according to whether $\lambda = n$ or p. In the plane-wave approximation, the cross section for nucleon scattering is proportional to the square of the form factor and to an elementary cross section.

Electron scattering data are most often analyzed using some variation of the Fourier-Bessel expansion (FBE)

$$f_{\nu\ell}(r) = \begin{cases} j_\ell(q_\nu r) & r \leq R \\ 0 & r \geq R. \end{cases} \tag{107}$$

The principal advantage of this expansion is that the dominant contribution each term ν makes to the form factor is localized near its characteristic momentum transfer q_ν, such that

$$\tilde{f}_{\nu\ell}(q) = \frac{q_\nu R^2}{q_\nu^2 - q^2} j_\ell(qR) j_{\ell+1}(q_\nu R) \quad (q \neq q_\nu) \tag{108}$$

$$\tilde{f}_{\mu\ell}(q_\nu) = \frac{R^3}{2} j_{\ell+1}^2(q_\nu R) \delta_{\mu\nu}. \tag{109}$$

Thus, only one term of the FBE contributes at each characteristic momentum q_ν. While other expansions are useful, none has a relationship between its expansion coefficients and the form factor that is so transparent. If the plane-wave approximation were accurate, the expansion coefficients could be determined directly from measurements performed at $q = q_\nu$ for each $\nu = 1, \ldots, N$ such that $(N + \ell/2) \lesssim \frac{q_m R}{pi}$, where q_m is the maximum momentum transfer accessible to measurement.

A variation of the FBE used by Heisenberg and his collaborators we call the HFBE, for which

$$j_{\ell-1}(q_\nu R) = 0. \tag{110}$$

When using roots of the Bessel function of order $(\ell - 1)$, we find

$$\tilde{f}_{\nu\ell}(q) = \frac{q_\nu R^2}{q^2 - q_\nu^2} [q j_{\ell+1}(qR) j_\ell(q_\nu R) - q_\nu j_\ell(qR) j_{\ell+1}(q_\nu R)], \qquad q \neq q_\nu \tag{111}$$

$$\tilde{f}_{\mu\ell}(q_\nu) = \frac{R^3}{2} j_\ell^2(q_\nu R) \delta_{\mu\nu}. \tag{112}$$

A significant defect of the FBE is that each basis function is oscillatory at large radius. Thus, unless sufficient data exist at small momentum transfer or unless the asymptotic radial behavior is suitably biased, undesirable oscillations will persist at unreasonably large radii.

The polynomial-Gaussian expansion (PGE),

$$f_{\nu\ell}(r) = \left[a^3 y^\ell e^{-y^2} \right] y^{2\nu} \tag{113}$$

where $y = \alpha r$, provides a useful alternative with a set of advantages and disadvantages complementary to that of the FBE. The PGE declines exponentially for both large radius and large momentum transfer. If α is chosen according to the harmonic oscillator model, a natural radial scale is introduced which minimizes the number of coefficients required to represent any plausible radial variation. However, the form factors for each basis function are not localized in momentum transfer. Moreover, the radial basis functions overlap strongly, causing the fitted coefficients to be highly correlated.

A third alternative can be found in the Laguerre-Gaussian expansion (LGE)

$$f_{\nu\ell}(r) = x^\ell e^{-x^2} L_\nu^{\ell+1/2}(2x^2) \tag{114}$$

where $x = r/b$ and where L_ν^a is a generalized Laguerre polynomial. This expansion also enjoys exponential decay at both large radius and large momentum transfer. The oscillator parameter b establishes a natural radial scale. However, as an orthogonal series, the correlation between adjacent coefficients is considerably less than that which plagues the PGE. We have found the LGE to be the parametrization most convenient for the analysis of proton scattering data.

3.3.2. Incompleteness Error

Experimental data, and theoretical models, always span a finite range of momentum transfer $q < q_m$. In the absence of physical constraints, spatial frequencies beyond the measured range of momentum transfer are completely undetermined. If uncontrolled, the uncertainty in high-frequency Fourier components causes the error band containing the radial density to diverge. Therefore, we must apply a physical bias upon $\tilde{\rho}_\ell(q)$ to limit the amplitude of unmeasurable frequencies and to estimate the uncertainties $\delta\rho_\ell(r)$ required by the permissible variability of $\tilde{\rho}_\ell(q)$ for $q > q_m$.

The range of $\rho(r)$ that is consistent with the postulated behavior of $\tilde{\rho}(q)$ beyond the maximum measured momentum transfer q_m can be ascertained by performing fits of the data supplemented by many random sets of permissible pseudodata beyond q_m. Dreher *et al.* have demonstrated that a more economical prescription produces equivalent results. The upper limit envelope can be attached at q_m using

$$\tilde{\rho}^{\mathrm{lim}}(q) = \tilde{\rho}(q_m)(q_m/q)^4. \tag{115}$$

The analysis is formulated most clearly using the FBE. A uniform distribution of permissible $\tilde{\rho}(q)$ points can be represented by a supplemental set of pseudodata selected at the characteristic momentum transfers q_n beyond q_m such that

$$\tilde{\rho}(q_\nu) = 0 \quad \text{for } q_\nu > q_m \tag{116}$$

with variances

$$\left[\delta\tilde{\rho}_\ell(q_\nu)\right]^2 = \frac{1}{3}\left[\tilde{\rho}^{\mathrm{lim}}(q_\nu)\right]^2. \tag{117}$$

The factor 1/3 occurs because a uniform, rather than normal, distribution is assumed.

The uncertainty $\delta\rho(r)$ in the fitted density can be decomposed into a statistical contribution $(\delta\rho)_{stat}$ due to the uncertainties δy_i in the measured data $\{y_i, i = 1, N_d\}$ and a model contribution $(\delta\rho)_{model}$ due to the uncertainties in the high-q pseudodata $\{y_i, i = N_d + 1, N\}$ by analyzing the propagation of errors formula

$$[\delta\rho(r)]^2 = \sum_{i=1}^{N}(\delta y_i)^2\left[\frac{\partial\rho(r)}{\partial y_i}\right]^2. \tag{118}$$

If we represent the density $\rho(r)$ using a set of fitting parameters $\{a_\nu\}$, we find that

$$\frac{\partial\rho}{\partial y_i} = \sum_\nu \frac{\partial\rho}{\partial a_\nu}\frac{\partial a_\nu}{\partial y_i}. \tag{119}$$

If we denote the fit to the i^{th} data point as $\bar{y}_i$, we find

$$\frac{\partial a_\nu}{\partial y_i} = \sum_\mu \frac{\epsilon_{\nu\mu}}{(\delta y_i)^2}\frac{\partial\bar{y}_i}{\partial a_\mu} \tag{120}$$

where $\epsilon = \alpha^{-1}$ is the error matrix.

The curvature matrix $\alpha_{\mu\nu}$ can be decomposed into two parts:

$$\alpha_{\mu\nu}^{stat} = \sum_{i=1}^{N_d} \frac{1}{(\delta y_i)^2} \frac{\partial \bar{y}_i}{\partial a_\mu} \frac{\partial \bar{y}_i}{\partial a_\nu} \tag{121}$$

$$\alpha_{\mu\nu}^{model} = \sum_{i=N_d+1}^{N} \frac{1}{(\delta y_i)^2} \frac{\partial \bar{y}_i}{\partial a_\mu} \frac{\partial \bar{y}_i}{\partial a_\nu} \tag{122}$$

by assigning the measured data to α^{stat} and the pseudodata to α^{model}. We can then decompose the error matrix

$$\epsilon_{\mu\nu} = \epsilon_{\mu\nu}^{stat} + \epsilon_{\mu\nu}^{model} \tag{123}$$

using

$$\epsilon_{\mu\nu}^{stat} = \sum_{\mu'\nu'} \epsilon_{\mu\mu'} \alpha_{\mu'\nu'}^{stat} \epsilon_{\nu'\nu} \tag{124}$$

$$\epsilon_{\mu\nu}^{model} = \sum_{\mu'\nu'} \epsilon_{\mu\mu'} \alpha_{\mu'\nu'}^{model} \epsilon_{\nu'\nu}. \tag{125}$$

Note that although ϵ is the inverse of α, ϵ^{stat} is not the inverse of α^{stat} when pseudodata have been included. Substituting all of this, we find

$$[\delta\rho]_{stat}^2 = \sum_{\mu\nu} \frac{\partial \rho}{\partial a_\mu} \epsilon_{\mu\nu}^{stat} \partial\rho\partial a_\nu \tag{126}$$

$$[\delta\rho]_{model}^2 = \sum_{\mu\nu} \frac{\partial \rho}{\partial a_\mu} \epsilon_{\mu\nu}^{model} \frac{\partial \rho}{\partial a_\nu}. \tag{127}$$

This analysis is not limited to the density, but applies to any function of the fitting parameters $\{a_\nu\}$.

The procedure of Dreher *et al.* consists of analyzing the error matrix for an extended data set extrapolated into the unmeasured region of momentum transfer. Therefore, we call this method of regularizing the expansion and estimating the associated incompleteness error the error matrix extrapolation method. A significant advantage of this method is that it provides a realistic error band with a single fit.

3.3.3. Tail Bias

Expansions with enough flexibility to estimate the incompleteness errors often produce undesirable oscillations in the fitted density at large radii. Unless good data exist at very low momentum transfer, these oscillations must be damped during the fitting procedure by means of a tail bias. This technique is necessary to the extraction of stable moments.

The tail bias is enforced by adding to χ^2 a penalty function

$$\chi_t^2 = \sum_{i=1}^{N_t} w_i \left[\rho(r_i) - t(r_i)\right]^2 \tag{128}$$

which inhibits deviation from a tail function

$$t(r) = t_0 \frac{e^{-dr}}{r^2} \tag{129}$$

where the parameters t_0 and d are matched to the fitted density at the match radius R_t. The density and the tail are compared on the radial mesh

$$r_i = R_t + (i-1)^* dr \qquad (i = 1, N_t) \tag{130}$$

and the weights are assigned according to

$$w_i = [wt(r_i)]^{-2} \tag{131}$$

where w is a normalization constant.

It is often useful to describe the strength and shape of the transition density using moments of the form

$$M_{KJ\lambda} = \int dr r^{2+K} \rho_{J\lambda}(r) \tag{132}$$

where $\lambda = p$ or n for proton or neutron densities or $\lambda = 0$ or 1 for isoscalar or isovector densities. For transitions allowed when $q \to 0$, the matrix element M_λ and transition radius R_λ are traditionally defined as

$$\text{allowed} \Longrightarrow M_\lambda = M_{JJ\lambda} \qquad R_\lambda^2 = \frac{M_{J+2,J\lambda}}{M_{JJ\lambda}}. \tag{133}$$

For forbidden or almost forbidden transitions, the moment M_{JJ} vanishes or is very small. It is then more useful to define

$$\text{forbidden} \Longrightarrow M_\lambda = M_{J+2,J\lambda} \qquad R_\lambda^2 = \frac{M_{J+4,J\lambda}}{M_{J+2,J\lambda}} \tag{134}$$

for $\Delta J^\pi = 0^+$ inelastic transitions or for isoscalar $\Delta J^\pi = 1^-$ transitions. The sign of M_λ cannot be determined from cross section data and is thus arbitrarily taken as positive. Occasionally we find that densities with more than one major lobe have negative values of R_λ^2. Therefore, we customarily assign the sign of R_λ^2 to R_λ.

These definitions of the multipole moments are most appropriate in the long-wavelength limit or to strongly absorbed probes. Thus, these parameters are useful for γ-decay, low-energy (e, e'), or for alpha scattering. However, the emphasis upon very small densities at very large radii is not appropriate for more penetrating probes, such as intermediate-energy electrons or protons, which are more sensitive to the bulk density. Therefore, it can be difficult to extract stable model-independent moments unless extraordinarily good data are available at unusually low momentum transfers. Extraction of reliable moments usually requires application of a tail bias.

The tail bias should be applied using a match radius R_t sufficiently large that the bulk density is unaffected but small enough to suppress oscillations. This choice can be made by examining the quantity $r^{J+2}\rho_J(r)$, which is listed in the density file. A fit is made using a relatively small number of terms, such as 4 terms of the LGE, and a plot of $r^{J+2}\rho_J$ is made. If R_t is chosen near the radius at which this quantity approaches zero but before the onset of oscillatory behavior, then stable moments may be extracted from the data using an arbitrary number of free parameters. Choosing the spacing as $dr = 0.2$ fm and the weight parameter as $w = 1.0$ generally serves to stabilize the tail at an expense to χ^2 of less than 10%.

4. PROGRAMMING STRATEGY

4.1. Organization of the Program

The program is designed to meet two basic criteria. First, standard options should be easy to use and the input should be as nearly self-explanatory as possible. Second, new options should be easy to add with minimal changes to standard routines. Several design decisions were made to satisfy these requirements. First, options are selected by character variables whose meaning should be obvious to the user while preparing input files with a text editor. Second, routines performing related tasks are organized into several libraries. Third, parameter statements and common blocks are collected in several files which are included where needed using compiler directives. Fourth, options are chosen within `IF-THEN-ELSE` loops which permit new options to be added easily.

At present, five libraries are available. General tasks related to establishing nuclear structure quantities, initializing variables, and performing basic I/O functions are collected in the library `LEA_LIB`. Routines used primarily for nucleon scattering, or for final-state interactions with nucleon–knockout, are collected in the library `NUCLEON_LIB`. Routine used for electron scattering are collected in the library `ELECTRON_LIB`. Routines which handle fitting tasks are collected within `NAFIT_LIB`. The subprograms in these libraries can receive input from common blocks within the `INCLUDE` files or from calling arguments. Although several other programs also access these libraries, new programs must be designed to be compatible with the `INCLUDE` files. In addition, routines performing general numerical analysis or common functions are collected in the library `JJKLIB`. These subprograms do not use the `INCLUDE` files and are used by many other programs besides `LEA`. A handful of machine-dependent routines are also provided.

Four `INCLUDE` files are used to specify parameters and pass information. The file `GENERAL.INC` is used by most of the subprograms contained within `LEA_LIB` and `NUCLEON_LIB` to specify array dimensions and to store reaction information, control variables, and mesh parameters. The file `DENSITY.INC` is used for ground-state and transition densities in both r-space and q-space. The file `NUCLEON.INC` is used for control variables and interaction parameters specific to nucleon scattering. It also specifies arrays of scattering potentials and observables. The file `ELECTRON.INC` is used for variables specific to by electron scattering, including nucleon–knockout. Finally, `NAFIT.INC` is used to store fitting parameters and results.

The order of calculation can be described as a series of steps. For some of these steps, many options are available. These options are selected by character variables with suggestive values that are intended to be easy to remember. An `IF-THEN-ELSE` loop is then used to select the proper administrative subroutine for that option. Thus new options can easily be added to those described by this report.

The input required to run `LEA` depends strongly upon the options chosen, but much of it is obtained by a relatively small number of subroutines with specific requirements described in the later sections. For example, most routines need input to describe the transition density and to specify the interaction. This information is usually obtained from the subroutines `TRDEN` and `INITF`, respectively. Therefore, to minimize redundancy, the input descriptions below often refer to subroutine descriptions that may be found scattered throughout the report. A brief description of the most important subroutines follows.

`LEA`	executive main program selects mode of operation
`CALC`	basic DWA calculation
`SICE`	Sequential Iteration of Coupled Equations (coupled channels)
`SPECTD`	$(e, e'N)$ calculations
`NAFIT`	fits generic model to data
`PSEUDO`	analyzes pseudodata
`PWEE`	plane-wave electron scattering
`FITD`	fits generic transition density
`FITG`	fits empirical effective interaction
`FITN`	fits neutron transition density
`GRID`	compares calculations and data when a parameter varies on $1d$ grid
`GSDEN`	computes ground state density
`TRDEN`	computes transition densities
`READST`	obtains description of initial and final states
`RDDATA`	obtains data
`INITF`	initializes theoretical effective interactions
`INITG`	initializes empirical effective interaction

4.2. General Rules for Input

Numeric input is generally entered in free format, indicated by the format code `(*)`. According to standard Fortran rules for free format input, data is read until all variables are satisfied or until a slash terminator (`/`) is encountered. Therefore, when a list is read using `(*)` format, it is not necessary to confine the input to a single record. These items can be spread over several lines with any spacing that enhances visual clarity for screen editing. Another property of free format input is that variables that would have been read had a slash terminator not been encountered are not altered.

Long file names are usually entered in format (`A80`). Exceptions occur when it is desirable to specify additional variables on the same line. The file name is then entered in free format `(*)` and must be enclosed with single quotes (`' '`). Character variables used for selecting options are entered in `(*)` format using uppercase characters. For many options, it is possible to specify `'SAME'` if the option has already been chosen in similar context at an earlier stage. It is also often possible to specify `'NONE'` if the quantities in question are to be zeroed out.

Logical variables are often entered in character form and then converted internally to logical variables. For example, to request a detailed print-out of quantities related to the nucleon-nucleon force, the value `'PRINT F'` should be entered for the variable `CPRNTF`. The code then assigns a logical variable

```
PRINTF = CPRNTF .EQ. 'PRINT F'
```

so that any other value inhibits this option. Although this style of input is particularly well suited to the use of screen editors to prepare new input files from existing prototypes, true values are achieved only if the character variable is precisely correct. For example, lower-case input will not produce the desired effect. We recommend that options like these be inhibited by adding `NO` to the appropriate character variable. For this example, the output is inhibited by the choice `'NO PRINT F'`.

The initial and final states are assigned character labels. These labels are used for two purposes. First, if `ISTATE` and `FSTATE` are identical, elastic scattering is assumed and the calculation terminates after elastic scattering for the initial channel has been completed. Second, these labels are used in the construction of files that contain results in a form suitable for plotting. Within these files, various quantities are distinguished by labels of the form

```
FIT--QUANTITY--STATE
```

where `QUANTITY` may be `SIGMA` or `AY` or one of many other observables. The `STATE` label is either `ISTATE` for an elastic quantity or `FSTATE` for an inelastic quantity. Data files are stored in similar format, except that `FIT` is replaced by `DATA`. The plotting programs used by the author decode labels of this type and create screen or hard-copy plots with formats appropriate to `QUANTITY` and names based upon `STATE`. For `VMS` systems, convenient file names are created by `STATE` labels of the form `9BE.3P2` for the second $\frac{3}{2}^{+}$ state of ^{9}Be or `16O.1M1` for first 1^{-} state of ^{16}O. States of unknown multipolarity can be identified by labels of the form `18O9.36` for a state in ^{18}O at 9.36 MeV of excitation. File names can then be formed by concatenating part of the `QUANTITY` label with the `STATE` label.

It is convenient to enter angular momenta in integer form as twice the actual spin. Energies are entered in MeV, angles in degrees, radii in fm, and momenta in fm^{-1}. Projectile masses are entered in pmu (938.28 MeV) and target masses are entered in amu (931.5 MeV).

4.3. Calculation Parameters

To reduce redundancy throughout the description of the input, we describe many of the variables in this section.

4.3.1. File Handling

Logical unit numbers are assigned variables of the form `LUN`x where x is some integer presently in the range 1-18. When the program is loaded these variables are initialized so that that `LUN`x=x. (Note that the initialization can be changed by editing a `DATA` statement.)

LUNx	name	purpose
LUN1		primary input
LUN2		primary output
LUN3	DATFIL	data files
LUN4	OPTIONS	interaction parameters
LUN5	INFILE	secondary input file
LUN6	OUFILE	secondary output file
LUN7		incoming distorted waves (scratch)
LUN8		outgoing distorted waves (scratch)
LUN9	PLTFIL	plot file for observables
LUN10	POTFIL	plot file for potentials
LUN11		unused
LUN12	IFILE	overlap integrals
LUN13	DENFIL	plot file for fitted density
LUN14	PLTFIL	plot file for fitted quantities
LUN15		tracks random number seed
LUN16		plot file for multiple-trial analysis
LUN17	B1FILE	plot file for BORN1 results
LUN18	B2FILE	plot file for BORN2 results
20+IS	XFILE	X–amplitudes for state number IS

Depending upon the mode of calculation, some of the unit numbers may be reassigned. For example, because it is not necessary to distinguish between primary and secondary I/O files in the 'CALC' mode, we reassign LUN5=LUN1 and LUN6=LUN2. However, when multiple data sets are analyzed, we need different files for each state and hence retain LUN5 and LUN6 for each. The file names INFILE and OUFILE are stored in arrays. If OPTIONS is left blank or given the value NONE, the input normally supplied there is expected in the secondary input file INFILE instead.

The status of the amplitude and integral files, XFILE and IFILE, are governed by the variables STATUSX and STATUSI, respectively. If a status variable has the value 'NEW', a new file is created and calculated values are written into it. If the value 'SCRATCH' is used, a scratch file is opened and it disappears upon completion of the calculation. This is usually most appropriate for IFILE, which we rarely wish to preserve. If the value 'OLD' is used, the program assumes that the file already exists and will read the information it needs instead of recalculating it. This is most convenient for density fits for which it may be desirable to study the effect of various constraints without recalculating the scattering amplitudes each time. Finally, if the value 'UNKNOWN' is used, the program will use an old file if it exists or will produce a new file if it does not.

4.3.2. Mesh Parameters

Several variables are defined on uniform meshes of the form

```
X(i) = X0 + (i-1)*DX for i=1,NX
```

where X is either radius, momentum transfer, or angle as appropriate. The radial mesh is established by specifying the maximum radius RMAX and the increment DR. The momentum transfer mesh for folding-model calculations is specifying by LQ, such that

$$\text{DQF} = \pi/\text{RMAX}/\text{LQ}.$$

NR,DR,RO	radial mesh parameters
NTH,DTH,THO	angles for distorted wave calculations
NQB,DQB,QOB	momentum transfer for Born approximation
NQF,DQF,QOF	momentum transfer for folding calculations
NQX,DQX,QOX	momentum transfer for X-amplitudes in addition to data

To facilitate comparison between calculations using the Born approximation and similar results using the distorted-wave formalism, the same mesh is used for both when DTH=0.0 is specified in the input file.

4.3.3. Partial Wave Limits

The maximum orbital angular momentum, ℓ_{max}, used for partial wave expansion is determined from the variable LMAX. If LMAX > 0, then $\ell_{max} =$ LMAX. If LMAX < 0, then ℓ_{max} is chosen such that $|C_{\ell j}| < 10^{\text{LMAX}}$ for the first distorted wave that is calculated. In either case, ℓ_{max} may not exceed the parameter MNL set in the include file GENERAL.INC.

4.3.4. State Description using READST

This section describes the input required to specify the reaction and its kinematics, select mesh parameters, and choose I/O options. This input is read from the secondary input file LUN5, which for some applications is the same as the primary input file LUN1.

LEA comes with a table for atomic mass excess which can be used to obtain accurate values for masses and reaction Q–values without Precise input. Target masses, TMI and TME, are read in amu, but if the input values are close to integral the mass table is used instead. Similarly, if projectile mass input is integral, tabulated nucleon masses are used.

line	quantity	variable
Line 1 (*):	character label for initial state	ISTATE
Line 2 (*):	Description of initial channel	
	projectile charge	PZI
	projectile mass in pmu	PMI
	twice projectile spin	IPI
	target charge	TZI
	target mass in amu	TMI
	twice target spin	ITI
	target parity	IPARI
Line 3 (*):	character label for final state	FSTATE
Line 4 (*):	Description of final channel	
	ejectile charge	PZE
	ejectile mass in amu	PME
	twice ejectile spin	IPE
	target charge	TZE
	target mass in amu	TME
	twice target spin	ITE
	target parity	IPARE
	excitation energy in MeV	EXC
Line 5 (*):	Kinematics	
	laboratory kinetic energy in MeV	TLAB
	maximum L for partial waves	LMAX

Note that Line 5 is not needed when `MODE='ESCAT'`.

4.4. Initial Input

The initial input is handled by the `LEA` executive program. The first line is a title for the calculation that will be reproduced on the output file. Next, `MODE` is read and the subsequent input depends upon the mode selected. The following values of `MODE` will be recognized.

'CALC'	one-shot calculation without fit
'TWOPOT'	elastic scattering with nonspherical contributions using "two–potential" formula
'SICE'	Sequential Iteration of Coupled Equations (coupled channels)
'NNOBS'	nucleon-nucleon elastic scattering
'SPECTD'	$(e, e'N)$ calculations
'TRANSP'	nuclear transparency in $A(e, e'N)B$
'ENSCAT'	$N(e, e')$
'ESCAT'	PWIA for elastic or inelastic electron scattering to discrete states
'FIT'	fit data
'GRID'	compare data with calculations with a parameter varying along a grid. Finds optimum value assuming parabolic chisquare profile.
'GRIDO'	compare data with calculations with a parameter varying along a grid
'SCANO'	produces table of elastic cross sections versus energy
'PSEUDO'	analyze pseudodata
'TEST'	some test options

If MODE='FIT', 'GRID', 'GRIDO', or 'PSEUDO', then FITMOD should be chosen from the list below.

FITMOD	subroutine	purpose
'TEFF'	FITG	empirical effective interaction
'NEUTRON'	FITN	neutron transition density
'GS NEUTRON'	FITNGS	ground–state neutron density
'DENSITY'	FITD	generic transition density
'COLLECTIVE'	FITC	deformation lengths for collective model
'PEREY'	FITP	Perey factor
'TWOPOT'	FIT2	coefficients for potentials in 'TWOPOT' mode
'OTHER'	NAFIT	generic models

The subroutines of the type FITx are specialized to particular models and provide much useful output. Others choices result in a call to the generic fitting routine NAFIT.

Line 1 (A): title

Line 2 (*): MODE

Line 3 (*): FITMOD for MODE = 'FIT', 'GRID', 'GRIDO' or 'PSEUDO'

Following this initial input, the next block of input depends upon the choice of MODE, as detailed below.

4.4.1. MODE = 'CALC'

The subroutine CALC governs most one–shot calculations of nucleon elastic or inelastic scattering, including charge exchange. Its primary tasks are outlined below.

Step 1) Initial specification of reaction parameters and control options.

Step 2) Description of ground-state densities.

Step 3a) Calculation of incoming waves and elastic scattering for initial channel.

Step 3b) Calculation of outgoing waves and elastic scattering for final channel.

Step 4) Compute scattering potentials and overlap integrals.

Step 5) Compute scattering amplitudes and observables.

Many options are available at each step and the input depends upon the options that are selected. However, considerable effort has been given to making the input required for each option as independent from other choices and as selfcontained as possible. Although some redundancy may be encountered, the net result is still simpler than using independent input streams for each application. Thus several of the input lines listed below actually refer to blocks of input obtained from other subroutines which are employed by many of the options and which are described in separate sections of this report.

line	LUN	description	subroutine	section
1 (A)	LUN1	OPTIONS file name		
2	LUN1	description of reaction	READST	Sec. 4.3.4
3	LUN5	initialization of DWA calculation	INITDW	Sec. 6.1
4	LUN5	ground–state densities	GSDEN	Sec. 7.2
5	LUN5	self–consistent wave number	SCWK	Sec. 6.6
6	LUN5	incident optical potential	OPTN	Sec. 8
7	LUN5	exit optical potential	OPTN	Sec. 8
8 (*)	LUN5	OPTION for inelastic scattering		
9	LUN5	input for OPTION selection		Sec. 10

Upon completion of the initialization phase, the program calls upon subroutine GSDEN to produce the ground state density for the initial channel. The input to GSDEN is described in Sec. 7.2. If a self–consistent wave number was requested using ISC = 'SCWN' among the kinematics options, it is then necessary to supply optical potential information to the subroutine SCWK, described in Sec. 6.6. The next step is calculation of the incoming optical potential and distorted waves. Note that some input is needed here even when the optical potential was used by SCWK, but if the optical model options are chosen to be 'SAME', this input is minimal. The input needed for OPTN is described in Sec. 8. For elastic scattering, which is specified by FSTATE = ISTATE, the calculation terminates and no further input is needed. Otherwise, the next step for inelastic scattering or charge exchange would be to produce outgoing distorted waves using a second call to OPTN; only minimal input is needed if the optical potential does not change. For single-charge exchange, it may be necessary to recalculate the ground-state density if only to renormalize the charge density. This input is specified in the description of OPTN.

Finally, the type inelastic scattering calculation is decided by the character variable OPTION. The program then branches to the appropriate subroutine. The options that are presently available are listed below and the input required to use these options is described in subsequent sections.

OPTION	description	section
'FOLD'	general folding model	Sec. 10.2
'COLLECTIVE'	collective model	Sec. 10.3
'TEST'	tests various options	Sec. ??

4.4.2. MODE = 'TWOPOT'

The subroutine TWOPOT governs elastic scattering calculations in which contributions due to nonspherical scattering potentials, or to perturbative corrections to the spherical optical potential, are evaluated in first–order using the two–potential formula. The input stream is quite similar to that of CALC, except that only the 'FOLD' and 'COLLECTIVE' options are recognized. There are small differences at this stage that are identified in the appropriate sections.

4.4.3. MODE = 'FIT'

Line 1 (*): MODE
Line 2 (*): FITMOD
Line 3 (A): PLTFIL

Following these initial entries, the program branches to the fitting routine selected by the value of FITMOD. These are described in Sec. IV.

4.4.4. MODE = 'GRID'

Line 1 (*): MODE
Line 2 (*): FITMOD
Line 3 (A): PLTFIL

Following these initial entries, the program branches to the grid routine selected by the value of FITMOD. These are described in Sec. IV.G-H.

4.4.5. MODE = 'PSEUDO'

Line 1 (*): MODE
Line 2 (*):

This option has not been used since the codes NEUT and NAFIT were merged together into LEA and should not be used until further notice.

5. FITTING ROUTINES

5.1. General Description

The steps required to fit a model to data are the following.

Step 1) select model
Step 2) initialize model and its constraints
Step 3) specify data sets
Step 4) construct amplitudes for each set of data
Step 5) initialize fitting parameters
Step 6) perform fit
Step 7) analyze results

Since many of the models may analyze data for several states of several targets, or for the same state at several beam energies, it is useful to separate the input that governs the model and the fitting procedure from the input which governs the distorted wave calculations. Therefore, we distinguish between two type of input files. The primary input file, assigned logical unit number `LUN1`, governs the fitting procedure and its associated output is written to `LUN2`. Each distorted wave calculation is governed by a secondary input file, sequentially assigned to `LUN5`, and writes output to `LUN6`. Although the primary input files for each model are quite similar in structure, some variations are unavoidable. Therefore, the input for each choice of `FITMOD` is described separately in the subsequent subsections despite a certain level of redundancy. The common features of the primary input files for the various models are described in Sec. 5.2, whereas the model–specific variations are described in subsequent subsections. Similarly, the input for the secondary input files in described in Sec. 12, after the common features have been established.

5.2. Input to `NAFIT`: fitting to generic models

Generic expansions may be fitted to data using the subroutine `NAFIT`, which is the prototype for the more specialized routines described in succeeding sections. The first line of the input specifies a mesh of momentum transfer on which amplitudes are calculated in addition to the angles for which data exist. This may be used to produce smoother plots or `NQX` may be made zero to save computation time. The number of terms in the fitting model is given by `NAMP` and the number of data sets which are to be analyzed is `NSTATE`. Lines 3-12 are repeated for each of the `NSTATE` data sets. The input for lines 11 and 12 is described in the sections describing the subroutine `READST` and `RDDATA`. Line 15 is repeated for each of the `NAMP` amplitudes. Lines 16-17 are repeated for each of the `NOVCS-1` additional sets of vary codes.

Line	variables	description
1 (*)	`NQX, DQX, QX0`	mesh for additional amplitudes
2 (*)	`NAMP, NSTATE`	number of amplitudes and states
3 (*)	`STATE`	state label
4 (A)	`TITLE`	descriptive title
5 (A)	`OPTIONS`	input file for interaction options `LUN4`
6 (A)	`INFILE`	secondary input file for current `STATE`
7 (A)	`OUFILE`	secondary output file for current `STATE`
8 (*)	`STATUSX, STATUSI`	status variables for `XFILE` and `IFILE`
9 (A)	`XFILE`	file of X–amplitudes for current `STATE`
10 (A)	`IFILE`	file of overlap integrals for current `STATE`
11	specification of transition using subroutine `READST`, Sec. 4.3.4	
12	specification of data set using subroutine `RDDATA`, Sec. 5.9	
13 (*)	`NOVCS`	number of sets of vary codes
14 (*)	`MNFIT, CONV, CHIMIN`	convergence criteria
15 (*)	`AI(i), IVC(i), ACON(i)`	initial parameters and constraints
16 (*)	`MNFIT, CONV, CHIMIN`	convergence criteria for second or later vary codes
17 (*)	`IVC` array	second or later set of vary codes

The character variable STATE is a label that will be used in the print output and to differentiate between entries within the plot file PLTFIL. The output will also reproduce the TITLE provided to help describe the calculation.

The OPTIONS file provides the interaction input for subroutine INITF and is described in Sec. 9.3. For models which can include data sets for several beam energies simultaneously, it is necessary to read the OPTIONS file name for each STATE in case different energies are employed. For models which are restricted to a single energy, the common OPTIONS file may be read before the state–dependent input. Hence the placement of Line 5 varies with FITMOD as detailed below.

For each state, the names of the secondary input and output files for the distorted wave calculations are read as INFILE and OUFILE, respectively. Each distorted wave calculation will produce a file of overlap integrals, named IFILE, and a file of X–amplitudes, named XFILE. These files may be assigned 'NEW', 'OLD', 'SCRATCH' or 'UNKNOWN' status.

The initial parameters are specified by an array AI containing NAMP entries, where NAMP is the number of amplitudes in the model. These parameters may be free to vary or may be constrained. Several types of constraints may be used. The array IVC contains a set of vary codes which has the value IVC(i)=0 if parameter i is to be held fixed to its initial value or IVC(i)=90 if it is free to vary. Intermediate values are reserved for future developments.

In addition, a parameter may be allowed to vary but be biased so that it remains near its initial value. This is accomplished by adding a penalty function

$$\chi_p^2 = \sum \left[\frac{\mathtt{C(i)} - \mathtt{AI(i)}}{\mathtt{ACON(i)}} \right]^2 \tag{135}$$

to chi-square which inhibits large changes in the parameters C(i) from their initial values AI(i). If the tolerance ACON(i) is entered as zero, no contribution to the penalty function is made.

The fit proceeds until any of three criteria are fulfilled. First, the maximum number of iterations is specified by MNFIT. Second, if the relative change in χ^2 drops below CONV, the fit is judged to have convergence. Third, if the reduced χ^2 drops below CHIMIN, the fit is judged satisfactory.

By choosing NOVCS greater than one, it is possible to use several sets of vary codes. It is often useful to first perform a fit with a minimal number of free parameters and then to use a second set to vary a larger set of parameters. The first fit gets close to the final result and the second refines the result.

5.3. Input to FITG: empirical effective interaction

The empirical effective interaction may be fitted to data for several states, possibly within several different targets, using the subroutine FITG. The scattering amplitudes are produced by subroutine AMPG based upon secondary input files whose structure is described in Sec. 12.2.

The fitting procedure includes a self-consistency cycle in which the distorted wave are based upon the preceding iteration or iterations and are updated as the cycle progresses. The maximum number of passes made through the fitting procedure is specified by NPASS, but if the relative change in χ^2 between passes drops below `CHANGE` we judge the fit to have converged upon a self-consistent interaction. Three options for estimating the distorting potentials from the fitted interaction are available. First, if `AMPMOD='AVERAGE'` is selected, the average of the parameters emerging from the previous two passess is used to compute optical potentials for the next pass. (The average between the initial guess and the first pass is used for the second pass.) This is the recommended procedure and is the default. Second, if `AMPMOD='LAST'` is selected, the parameters from the previous pass are used. Third, if `AMPMOD='BEST'`, the set of parameters produced by an earlier pass with the lowest χ^2 is used. However, this method tends to abort the procedure prematurely if χ^2 begins to increase between passes.

The fitting model is initialized using an early call to `INITF` and the description of the empirical interaction read from the file specified by `OPTIONS`. This file is common to all states used by the analysis; hence, it is not necessary to specify `NAMP` because that variable can be obtained from the `OPTIONS` file.

Line 1 `(A) OPTIONS`
Line 2 `(*) NQX, DQX, QXO`
Line 3 `(*) NSTATE, NPASS, CHANGE, AMPMOD`
Line 4 `(*) STATE`
Line 5 `(A) TITLE`
Line 6 `(A) INFILE`
Line 7 `(A) OUFILE`
Line 8 `(*) STATUSX, STATUSI`
Line 9 `(A) XFILE`
Line 10 `(A) IFILE`
Line 11 specification of transition using subroutine `READST`, Sec. 4.3.4
Line 12 specification of data set using subroutine `RDDATA`, Sec. 5.9
Line 13 `(*) NOVCS`
Line 14 `(*) MNFIT, CONV, CHIMIN`
Line 15 `(*) AI(i), IVC(i), ACON(i)`
Line 16 `(*) MNFIT, CONV, CHIMIN`
Line 17 `(*) IVC` array

Lines 4-12 are repeated for each of the `NSTATE` data sets. Line 15 is repeated for each of the `NAMP` amplitudes. Lines 16-17 are repeated for each of the `NOVCS-1` additional sets of vary codes.

Scattering amplitudes for variable component of the nucleon-nucleon interaction are then constructed from the description of the empirical effective interaction already obtained from an `OPTIONS` file near the beginning of the input.

Each component, t_i, of the effective interaction for which expansion parameters are supplied is assumed to be variable, whereas those that are not expanded are assumed to remain the same as in the interaction, $t_i^{(0)}$, upon which the expansion is based. The first fitting parameter, `A(1)`, is a scale factor S_0 which multiplies all terms $t_i^{(0)}$ not represented as an expansion. Hence, we ordinarily fix $S_0 = 1$ by entering `AI(1)=1.0` and `IVC(1) = 0`. Each variable component t_i of the effective interaction will produce two sets of several amplitudes, a set for the real part followed by a set for the imaginary part. Within each set, there may be several Yukawa terms if $N > 0$ is read from the `OPTIONS` file, or none if

$N \leq 0$. Thus the parameter array will have the following structure, where Lines 1 − 6 are repeated for each interaction component { i=1,NCOMP } described in the OPTIONS file and where N_i is the total number of parameters needed for component i.

Line	parameter numbers	description
0	1	Scale factor (S_0) applied to fixed terms in $t^{(0)}$
1	$2 + N_{i-1}$	Scale factor (S) applied to $Ret_i(q,0)$
2	$3 + N_{i-1}$	Damping factor (d) applied to $Ret_i(q,0)$
3	$4 + N_{i-1} : 4{+}N_{i-1} + N_i^R - 1$	Yukawa strengths ({ $a_{in}, n = 1, N_i^R$ }) for Ret_i (if $N_i^R > 0$
4	$5 + N_{i-1} + N_i^R - 1$	Scale factor (S) applied to $Imt_i(q,0)$
5	$6 + N_{i-1} + N_i^R - 1$	Damping factor (d) applied to $Imt_i(q,0)$
6	$7 + N_{i-1} + N_i^R - 1 : 7{+}N_{i-1} + N_i^R + N_i^I - 2$	Yukawa strengths ({ $a_{in}, n = 1, N_i^I$ }) for Imt_i (if $N_i^I > 0$

5.4. Input to FITN: fit neutron transition density

The neutron transition density for a single state can be fitted to data for a single energy or for several energies simultaneously, provided that the corresponding proton transition density is already available from electroexcitation measurements. The fitting procedure is governed by subroutine FITN based upon scattering amplitudes produced by subroutine AMPN using secondary input files described in Sec. 12.3. These routines are restricted to normal-parity transitions for which the absence of a significant transverse form factor indicates that spin and current densities may be neglected.

It is instructive to compare fits with a general expansion of the transition density to scale-factor fits made under the assumption

$$\rho_n(r) = S\rho_p(r). \tag{136}$$

This simple model will be most successful near the peak of the form factor and hence scale-factor fits should be restricted to relatively small momentum transfer. Deviations between scale-factor and more sophisticated LEA fits reveal the sensitivity of the data to differences between neutron and proton densities.

FITN begins with a call to INITDEN and then obtains the following information from LUN1. Note that it is not necessary to specity NAMP on Line 2 because that parameter is initialized by INITDEN. The code produces NTERMS+2 sets of scattering amplitudes. The first set represents the effect of the proton transition density ρ_p alone (with $\rho_n = 0$). Therefore, most fits are performed with the first parameter AI(1)=1.0 held fixed to unity via the constraint IVC(1)=0. The second set represents the effect of a neutron transition density alone, assuming that ρ_n now has the same form as the ρ_p already used for the preceding amplitude. Therefore, a scale-factor analysis corresponds to varying only the second parameter using

```
scale-factor fit ⇒ AI(1) = 1.0 IVC(1) = 0
                   AI(2) = 1.0 IVC(2) = 90
                   AI(n) = 0.0 IVC(n) = 0  for n>2.
```

The next NTERMS amplitudes correspond to basis functions, with unit amplitude, for the relevant expansion of ρ_n. Therefore, LEA fits to ρ_n generally use AI(1)=1.0 and AI(2)=0.0 held fixed, while up to NTERMS coefficients AI(n) with n>2 are allowed to vary.

If multiple sets of vary codes are employed, it is possible to enable different sets of biases during the course of the analysis. If good initial values are not available for the expansion coefficients, it is often useful to allow only the first few parameters to vary during the search using the first set of vary codes. This approach is most applicable to the LGE or PGE representations, for which only a few terms usually suffice to provide a good representation of the density. It is then convenient to begin with null coefficients. However, the tail bias procedure will not work unless the magnitude of the density is decreasing at the match radius. Therefore, the tail bias can be disabled during the initial phase of the search. A more complete set of parameters is then varied using a second set of vary codes. The larger set of free parameters is required to estimate the incompleteness error. However, unless very good data are available for rather small momentum transfers, it will be necessary to impose the tail bias upon the second phase of the procedure.

The character variable `CBIASR` and `CBIASQ` are used to control biases. The tail bias is enabled if `CBIASR='RBIAS'` and is disabled otherwise. Similarly, the high-q bias is enabled if `CBIASQ='QBIAS'` and is disabled otherwise. However, it is generally best to keep the high$-q$ bias enabled throughout the procedure.

Line 1 (*) `NQX, DQX, QXO`
Line 2 (*) `NSTATE`
Line 3 (*) `STATE`
Line 4 (A) `TITLE`
Line 5 (A) `OPTIONS`
Line 6 (A) `INFILE`
Line 7 (A) `OUFILE`
Line 8 (*) `STATUSX, STATUSI`
Line 9 (A) `XFILE`
Line 10 (A) `IFILE`
Line 11 specification of transition using subroutine `READST`, Sec. 4.3.4
Line 12 specification of data set using subroutine `RDDATA`, Sec. 5.9
Line 13 (*) `NOVCS`
Line 14 (*) `MNFIT, CONV, CHIMIN, CBIASR, CBIASQ`
Line 15 (*) `AI(i), IVC(i), ACON(i)`
Line 16 (*) `MNFIT, CONV, CHIMIN, CBIASR, CBIASQ`
Line 17 (*) `IVC` array

Lines 3-12 are repeated for each of the `NSTATE` data sets. Line 15 is repeated for each of the `NAMP` amplitudes. Lines 16-17 are repeated for each of the `NOVCS-1` additional sets of vary codes.

5.5. Input to `INITDEN`: initialization of density models

The subroutine `INITDEN` initializes the parameters required to describe a transition density as a linear expansion and establishes the constraints to be placed upon fits of the density to data. The type of expansion used to describe the transition density is specified by the character variable `EXPDEN='LGE'`, `'FBE'`, or `'PGE'`. The orbital angular momentum is given by `LD`.

Line	format	variables	interpretation or restrictions
1	(A)	DENFIL	name of density file
2	(*)	EXPDEN, LD, NTERMS	(FITMOD='NEUTRON')
2	(*)	EXPDEN, LD, ND1, ND2, NAMP	(FITMOD='DENSITY')
3	(*)	RMAXD, DRD, NQD, DQD	r- and q-mesh for density
4	(*)	RMATCH, RWEIGHT, NTAILR, DTAILR	tail bias
5	(*)	QMATCH, RHOQMX	high$-q$ bias
6	(*)	APGE	α for PGE only
6	(*)	RMAX, FBVER	R_m for FBE only
6	(*)	BLGE	b for LGE only
7	(*)	NTAILQ, DTAILQ	PGE or LGE
8	(*)	NFBE, RFBE, QM	only if QMATCH=0

5.6. Input to FITP: fit Perey factor

A simple model of medium modifications to the effective interaction resembles the traditional Perey factor. Suppose that the scattering potentials are multiplied by the function

$$P(r) = \sum a_n \left(\rho(r)/\rho_0\right)^n \tag{137}$$

where $\rho_0 = 0.16 fm^{-3}$ represents saturation density and $\rho(r)$ is the local ground-state matter density. This modification can be interpreted as either a zero-range modification of the G-matrix or as the square of the Perey damping factor normally applied to the amplitude of the wave function that results from an equivalent local potential. The net effect upon the overlap integral is the same for either interpretation. Note that for the Perey-factor interpretation we expect $a_0 = 1$ and $a_1 \approx -0.4$.

The Perey parameters can be fitted to data for many states simultaneously. Any of the available models can be used to calculate scattering potentials, including the G-matrix models, but the same OPTIONS file is used for all states in the analysis.

Line 1 (A) OPTIONS
Line 2 (*) NQX, DQX, QXO
Line 3 (*) NAMP, NSTATE
Line 4 (*) STATE
Line 5 (A) TITLE
Line 6 (A) INFILE
Line 7 (A) OUFILE
Line 8 (*) STATUSX, STATUSI
Line 9 (A) XFILE
Line 10 (A) IFILE
Line 11 specification of transition using subroutine READST, Sec. 4.3.4
Line 12 specification of data set using subroutine RDDATA, Sec. 5.9
Line 13 (*) NOVCS
Line 14 (*) MNFIT, CONV, CHIMIN
Line 15 (*) AI(i), IVC(i), ACON(i)
Line 16 (*) MNFIT, CONV, CHIMIN
Line 17 (*) IVC array

Lines 4-12 are repeated for each of the NSTATE data sets. Line 15 is repeated for each of the NAMP amplitudes. Lines 16-17 are repeated for each of the NOVCS-1 additional sets of vary codes.

5.7. Input to GRIDO: grid calculations without fit

The subroutine GRIDO is used to compare calculations with data when some parameter is varied along a uniform grid. Although fits are not performed by this routine, the input is similar to that required for fitting routines because χ^2 is computed for each value of the gridded parameter. Although a series of one-shot calculations provides much of the same information, this is the most convenient method for assessing the sensitivity of the data to a given parameter. GRIDO provides an informative summary of the grid and analyzes the shape of the χ^2 curve.

Although only a single type of grid has been implemented to date, the subroutine is designed for ease of modification by the user who wishes to insert additional options. The application that presently exists performs a notch test by comparing calculations for which the scattering potential is artificially set to zero within some radius (or notch):

$$U(r) \rightarrow 0 \text{ for } r<\mathtt{RNOTCH}.$$

The notch itself is gridded according to

```
RNOTCH(i) = RNOTCHO + (i-1)*DNOTCH, i=1,MGRID.
```

This test can be interpreted as a coarse measure of the sensitivity of nucleon scattering to the transition density in the nuclear interior. However, it is not as accurate as the pseudodata analysis because the range of the interaction is not considered when taking a notch out of the scattering potential.

Line 1 (A) OPTIONS
Line 2 (*) NQX, DQX, QXO
Line 3 (*) NSTATE, MGRID, DNOTCH, RNOTCHO
Line 4 (*) STATE
Line 5 (A) TITLE
Line 6 (A) INFILE
Line 7 (A) OUFILE
Line 8 (*) STATUSX, STATUSI
Line 9 (A) XFILE
Line 10 (A) IFILE
Line 11 specification of transition using subroutine READST, Sec. 4.3.4
Line 12 specification of data set using subroutine RDDATA, Sec. 5.9

Lines 4-12 are repeated for each of the NSTATE data sets. Line 3 should be modified for alternative applications.

5.8. Input to GRID: fit with gridded parameter

The GRID subroutine fits a model to data for each point along a 1-dimensional grid of a particular parameter. Two applications have been implemented to date. If FITMOD='TEFF', the empirical effective interaction is fitted to data using FITG. At each point in the grid, one of the parameters, such as a scale factor, is held fixed while several others are varied to obtain the best fit possible given a fixed parameter. Each of these grid points may represent a self-consistency cycle. This procedure can be used to investigate the range of variation available to the parameter of interest, perhaps to determine whether the parameter is actually expendable. Alternatively, if FITMOD='PEREY', FITP will be called with one of its parameters gridded.

It should be possible to add other applications relatively easily. For the applications described above, the input consists of the single line

Line 1 (*): IFIX = index for parameter to grid
AFIXO = initial value of gridded parameter
DAFIX = grid increment
MGRID = number of grid points

followed by the input for either FITG or FITP as appropriate.

5.9. Input to RDDATA: read data

The data used by fitting routines is read by the subroutine RDDATA. For the present purposes each set of data, which may include several observables, is considered a STATE. All of the data for a given STATE must share a common projectile energy and must actually correspond to the same state of the target. If data for several energies are analyzed simultaneously, the program treats each energy as a different STATE for the purpose of counting data sets. It is permissible to treat several sets of data at the same energy as different STATES, but all of the data for a particular STATE must be found within a single data file.

A single data file may include several observables for each of many states. The program finds the data it needs by searching for internal labels. Thus, data files must have the following structure.

```
LABEL
N
X(1), Y(1), DY(1)
X(2), Y(2), DY(2)
...
X(N), Y(N), DY(N)
LABEL
N
X, Y, DY
...
```

The subroutine scans the file until it finds a LABEL which matches an input DATLAB precisely, including case and spacing. It then reads N data points for which X is either center-of-mass angle or momentum transfer, Y is the observable, and DY is its uncertainty (absolute rather than relative).

The kinematic variable is chosen by the character variable QFLAG with the self-explanatory values 'Q' or 'ANGLE' (both upper and lower case are acceptable). Units of fm^{-1} are used for momentum transfer or degrees for angles. It is often desirable to analyze only those data points which fall within the interval of momentum transfer

$$\mathtt{QMIN} \leq \mathrm{q} \leq \mathtt{QMAX}.$$

For example, a scale factor may be fitted to the peak of the angular distribution or a transition density may be fitted to momentum transfers $q \leq 2k_F$. Note that the limits are ignored if valid input is not supplied.

Observables are identified by the character variable EXP, which must be chosen from the following list.

variable	quantity
'SIGMA'	$d\sigma/d\Omega$
'AY'	A_y
'POL'	P
'SFP'	$S_{NN} = (1 - D_{NN})/2$
'DNNP'	D_{NN}
'DLLP'	$D_{LL'}$
'DSSP'	$D_{SS'}$
'DLSP'	$D_{LS'}$
'DSLP'	$D_{SL'}$

Several modifications of the experimental data are available. For the differential cross section EXP='SIGMA', a normalization factor SNORM and its uncertainty ENORM are read. If ENORM>0 the code will estimate the uncertainty of the fitted parameters to uncertainties in cross section normalization by evaluating numerical derivatives of the fitted parameters with respect to each cross section normalization independently and adding appropriate uncertainties in quadrature. For other observables, additional random errors can be added in quadrature to the experimental error bars read from the data file. This option allows the user to regulate the relative weights of various data sets or to include an estimate of uncertainties in the reaction model. For cross sections, the additional uncertainty is entered in percent. For other observables, absolute errors are supplied.

The data sets are specified in the LEA input file using the following lines.

Line 1	(A)	`DATFIL`	name of data file.
Line 2	(*)	`QFLAG, QMIN, QMAX`	
Line 3	(*)	`NEXP`	number of data sets to be selected from `DATFIL`
Line 4	(*)	`EXP`	character label of observable.
Line 5	(A)	`DATLAB`	label of data set within `DATFIL`
Line 6a	(*)	`SNORM, ENORM, SYSERR`	for cross section **OR**
Line 6b	(*)	`SYSERR`	for other observables

When analyzing pseudodata (`MODE='PSEUDO'`), the pseudodata for each observable and data set are produced on a uniform mesh of either angle or momentum transfer. This mesh, and the fluctuations to be applied to the data, are specified by replacing Line 6 with the following input.

Line 6′ (*)	`NPTS`	number of pseudodata
	`X0`	first angle or momentum transfer according to `QFLAG`
	`DX`	increment
	`ERRBAR`	percent uncertainty of $d\sigma/d\Omega$ absolute uncertainty for spin observables.

6. OPTIONS FOR DISTORTED WAVES

6.1. Initialization using `INITDW`

The `MODE` and `FITMOD` have already been selected before `INITDW` is called. Also, the parameters which describe the quantum numbers of the reaction have also been read for a particular transition. Note that if data for several states are to be analyzed, `INITDW` will be called for each.

Although most of the input is read from `LUN5`, other files may be used for particular applications. At this stage, one must be careful about the placement of Line 7. If an `OPTIONS` file is used, then Line 7 is read from that file, defined as `LUN4`. If not, then `LUN4` is reassigned to `LUN5` and Line 7 is read from here. Also, `LEA` may choose to reassign some of the unit numbers internally, but these changes should be transparent to the user.

unit	line	format	description
LUN5	1	(*)	Radial mesh parameters.
			RMAX = maximum radius (fm)
			DR = radial increment
			RZMAX = radius containing target charge
LUN5	2	(*)	Mesh parameters for q-space folding.
			NQF = number of mesh points.
			LQ: determines mesh size, such that DQF= π/RMAX/LQ
LUN5	3	(*)	Mesh parameters for Born calculations.
			NQB = number of q-points.
			DQB = q-spacing for Born calculations.
LUN5	4	(*)	Mesh parameters for angular distributions.
			NTH = number of angles
			DTH = angular spacing
			TH0 = smallest angle
LUN5	5	(*)	Parameters for acceptance averaging.
			NXTRA = number of angular divisions
			DTHETA0 = $\Delta\theta$
			DPHI0 = $\Delta\phi$
LUN5	6	(*)	Parameters governing shell-model calculations.
			KCOM='NO-CM' $\rightarrow$ no center-of-mass correction
			KCOM='C-O-M' $\rightarrow$ apply c.m. correction
			KTM: determines normalization of form factors
			DEFALPHA = default alpha ($1/b$) for c.m. correction
LUN4	7	(*)	Kinematics options (see Sec. 6.2).
			KINTYP, ISC, IDW79, DLAB, WIGNER, MOLLER
LUN5	8	(*)	CPRNTF, CPRNTR, CPRNTQ, CPRNTP, CPRNTO
			Print options are entered as
			CPRNTX = 'PRINT X' to print X
			CPRNTX = 'NO PRINT X' to not print X,
			where X is F, R, Q, P, or O.
			= F: forces
			= R: radial densities
			= Q: momentum densities
			= P: potentials
			= O: overlap integrals (large output).

LUN5 9 (*) CBORN1, CFOLD, CBORN2, CDWBA, CPARTIAL
Control options are entered as
CXXXX = 'XXXX' to perform step XXXX
CXXXX = 'NO XXXX' to omit step XXXX,
where XXXX has the values
BORN1: analytic Born approximation, excluding density dependence. Also covers (e, e').
FOLD: compute scattering potentials
BORN2: Born approximation computed from folded potentials. Includes density dependence.
DWBA: distorted wave approximation
PARTIAL: plot partial cross sections for each JT.

LUN5 10 (*) CPLTEL, CPLTB1, CPLTB2, CPLTU, CPLTDW
Plot options are entered as
CPLTX = 'PLOT X' to enter X into plot file
CPLOTC = 'NO PLOT X' to omit X from plot file,
where X is EL, B1, B2, U, or DW.
EL: elastic scattering quantities
B1: Born quantities from q-space
B2: Born quantities from folded potentials
U: scattering potentials
DW: DWA quantities.

LUN5 11 (A) PLTFIL = name of plot file for observables from DWBA.
This line is omitted if neither 'PLOT U' nor 'PLOT DW' were selected.

LUN5 12 (A) POTFIL = name of file for scattering potential.
This line is omitted if CPLTU .NE. 'PLOT U'.

LUN5 13 (A) B1FILE = name of plot file for BORN1 results.
This line is omitted if CPLTB1 .NE. 'PLOT B1'.

LUN5 14 (A) B2FILE = name of plot file for BORN2 results.
This line is omitted if CPLTB2 .NE. 'PLOT B2'.

6.2. Kinematics Options

The kinematics options, read and interpreted by the subroutine KINOPT, are summarized below.

variable	value	interpretation
KINTYP	'REL'	relativistic kinematics (default)
	'NN'	relativistic kinematics for NN scattering
	'IA2'	special kinematics for IA2 interaction
	'N-R'	nonrelativistic kinematics (discouraged)
	'BORN'	incoming and outgoing kinematics set to Born values for comparison with PWBA.
ISC	'A-WN'	asymptotic wave number (default)
	'SCWN'	local self-consistent wave number
IDW79	'DW79'	omit spin-orbit recoil factor
DLAB	'DLAB'	transform $D_{\alpha\beta}$ from c.m. to lab frames (default)
	'NO DLAB'	leave $D_{\alpha\beta}$ in c.m. frame
WIGNER	'WIGNER'	include Wigner rotation in transformation of $D_{\alpha\beta}$ (default)
	'NO WIGNER'	omit Wigner rotation
MOLLER	'MOLLER'	include Moller factor (default)
	'NO MOLLER'	omit Moller factor

For most applications, standard relativistic kinematics are selected by `KINTYP = 'REL'`. For nucleon–nucleon scattering with `MODE='NNOBS'`, use of `KINTYP = 'NN'` ensures that the exchange momentum transfer is handled correctly rather than using the approximate methods for nucleon–nucleus scattering. When testing the internal consistency of various options using plane–wave calculations, it is sometimes useful to choose `KINTYP = 'BORN'` to ensure that incoming and outgoing wave numbers are identical. Finally, nonrelativistic kinematics can be chosen with `KINTYP = 'N-R'`; this option is generally discouraged, but it is provided so that comparisons with other calculations employing nonrelativistic kinematics can be made.

The short–range exchange approximations for nucleon–nucleus scattering are based upon the approximation $Q \approx k_A$ where Q is the exchange momentum transfer and k is the wave number in the nucleon–nucleus center–of–mass frame. When `ISC = 'A-WN'`, this wave number is set equal to its asymptotic value, $k = k_A$. When `ISC 'SCWN'`, the exchange approximation uses the local wave number

$$k(r) = \frac{A}{A+1}\sqrt{\frac{E(r)(E(r)+2m_N)}{1+\frac{2A}{(A+1)^2}\frac{E(r)}{m_N}}} \tag{138}$$

where

$$E(r) = T_{cm} - U^Z(r) - ReU^C(r) \tag{139}$$

is the local and T_{cm} the asymptotic kinetic energy.[1]

---

[1]Note that for nonrelativitic kinematics, we use

$$k(r) = \sqrt{2\mu E(r)}$$

where μ is the reduced mass.

The transformation of ejectile polarization observables from center of mass to laboratory frames is governed by the parameters `DLAB` and `WIGNER`. If `DLAB = 'DLAB'` the longitudinal and sideways components of the depolarization matrix $D_{\alpha\beta}$ are transformed. If `WIGNER = 'WIGNER'`, the Wigner rotation is included also.

The t–matrices in the nucleon–nucleon (NN) and nucleon–nucleus (NA) frames are related by the Moller factor, η, such that

$$t_{NA} = \eta t_{NN} \tag{140a}$$

$$\eta = \frac{\varepsilon_1 \varepsilon_2}{E_1 E_2} \tag{140b}$$

where the projectile and struck nucleon energies are ε_1 and ε_2 in the NN frame and E_1 and E_2 in the NA frame. Thus, if the interaction is specified in the NN frame, choose `MOLLER = 'MOLLER'` to include the Moller factor in the definition of t_{NA}, but if the interaction is specified in the NA frame choose `'NO MOLLER'` to omit that factor ($\eta \to 1$).

The IA2 interaction is based upon a somewhat different version of the wave equation. Thus, the special option `KINTYP = 'IA2'` is provided for that case.

6.3. Use of BORN Approximations

Two independent plane-wave calculations are available for testing the program and for investigating the relative importance of various effects. The `BORN1` calculation uses analytic formulae to evaluate the $t\rho$ approximation before any folding is done. This approximation neglects density dependence. Alternatively, the `BORN2` calculation evaluates Fourier transforms of the folded potential and thus includes density dependence if it is present in the interaction. Finally, if the optical potentials are null, the distorted wave routines will also produce a plane-wave result. All three calculations are independent. Therefore, the accuaracy with which agreement between them is attained constitutes an important test of the internal consistency of the code and of the numerical accuracy of the procedures.

To make optimal use of this facility, a calculation should be performed for a typical transition and kinematic conditions in which all three Born approximations are compared. To ensure that the three calculations match as closely as possible, a density-independentinteraction should be used with Born kinematics and null optical potentials. The following parameters should be used.

```
QVAL = 0.0
KINTYP = 'BORN'
OPTMOD = 'NONE'
OPTZ = 'NONE'
IDW79 = 'DW79'
CDD = 'NO DD'
```

6.4. Nonlocality Corrections

Since the nuclear mean field is inherently nonlocal, use of a local Schrödinger equation implicitly involves an equivalent local potential and a transformation of the wave function. This transformation is usually approximated as a Perey factor. If χ_L is the solution of a Schrödinger equation based upon a local optical potential that is supposed to be phase equivalent to a more fundamental nonlocal potential, the phase-equivalent solution to the original nonlocal Schrödinger equation is then supposed to be $\chi_{NL}(r) \approx P(r)\chi_L(r)$ where $P(r)$ is a complex function known as the Perey factor. Many models are available for $P(r)$, which are selected by the character variable `CPEREY`. The Perey factor is omitted (set equal to unity) by choosing `CPEREY = 'NO PEREY'`. If $P(r)$ has been determined at an earlier stage, then choosing `CPEREY = 'SAME'` maintains that function without needing further input.

The original Perey–Buck parametrization takes the form

$$P(r) = \left[1 - \frac{m\beta^2}{2\hbar^2} V(r)\right]^{-1/2} \tag{141}$$

where $V(r)$ is the real part of the central optical potential and β is the nonlocality range [15,16]. Typically one assumes that $\beta \approx 0.85$ fm based upon the Perey and Buck analysis for low-energy neutron scattering data, $E_n < 20$ MeV. Thus, if `CPEREY = 'PEREY'` we need to read the nonlocality parameter `BETANL`$= \beta$.

Alternatively, to the extent that the energy dependence of the optical potential is dominated by the exchange contribution to a Brueckner-Hartree-Fock potential, the nonlocality correction can be associated with the quasiparticle effective mass (k–mass) via

$$P(r) = \sqrt{m_k/m} \approx \sqrt{m^*/m} \; . \tag{142}$$

where

$$\frac{m^*(E)}{m} = 1 - \frac{dV}{dE} = \frac{m_k}{m}\frac{m_E}{m} \tag{143a}$$

$$\frac{m_k}{m} = \left[1 + \frac{m}{k}\frac{\partial \mathcal{V}}{\partial k}\right]^{-1} \tag{143b}$$

$$\frac{m_E}{m} = 1 - \frac{\partial \mathcal{V}(k,E)}{\partial E} \tag{143c}$$

are the the effective mass, the k–mass, and the E–mass. Thus, the original Perey-Buck parametrization is equivalent to the ansatz

$$\mathcal{V}(k,E) = \mathcal{V}_0(E) e^{-(\beta k/2)^2} \; , \tag{144}$$

In folding models we can related the k–mass to the momentum dependence of the effective interaction using

$$\frac{m_k}{m} = \left[1 + \frac{m}{k}\rho \frac{\partial t(q,k,k_F)}{\partial k}\right]^{-1} \; . \tag{145}$$

Therefore, selecting CKMASS = 'KMASS' produces a k–mass from Eq. 145 and selecting CPEREY = 'KMASS' produces $P(r)$ from Eq. 142.

A more phenomenological parametrization is provided by the expansion

$$P(r) = \sum_{n=0}^{N-1} a_n \left(\frac{\rho(r)}{\rho_0} \right)^n \tag{146}$$

where $\rho(r)$ is the ground–state density and $\rho_0 = 0.16$ fm^{-3} represents saturation density. Thus, if CPEREY = 'EXPANSION' read must read

$$N, \{a_n n = 1, N\}$$

at the appropriate location in the secondary input file (LUN5).

The relative importance of contributions originating in the nuclear interior can be assessed using the CPEREY = 'NOTCH' option, where

$$\begin{aligned} P(r) &= 0 \text{ for } r < \texttt{RNOTCH} \\ &= 1 \text{ for } r > \texttt{RNOTCH}. \end{aligned} \tag{147}$$

Obviously, RNOTCH is read from LUN5 when Perey input is requested.

Finally, reduction of a Dirac equation to an equivalent Schrödinger equation involves a Darwin factor that relates the relativistic and nonrelativistic wave functions in a manner analogous to the Perey factor. A Dirac equation of the form

$$\left[\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta(m + S) \right] \Psi = (E - V_0)\Psi \tag{148}$$

with scalar and vector potentials S and V_0 can, upon elimination of the lower components, be transformed into an equivalent Schrödinger equation of the form

$$\left[\nabla^2 + k^2 - 2\mu \left(U^C + U^{LS} \boldsymbol{L} \cdot \boldsymbol{\sigma} \right) \right] \phi = 0 \tag{149}$$

where the central and spin-orbit optical potentials U^C and U^{LS} are related by well-known formulae [17] to S and V_0 and where the positive-energy Dirac spinor ψ_+ is related to the Schrödinger wave function by $\psi_+ = P\phi$ with

$$P(r) = \left[1 + \frac{S - V_0}{E + m} \right]^{1/2} . \tag{150}$$

The Darwin factor is used when CPEREY = 'DP' is chosen in conjunction with an optical potential from Dirac phenomenology. Alternatively, since U^{LS} depends upon $(S - V_0)$, the Darwin factor can also be deduced from the spin-orbit potential directly [1] even when a nonrelativistic model of the optical potential is employed. Thus, choosing CPEREY = 'REL' produces

$$P(r) = \exp \left[- \int_r^\infty dr'\, r'\, U^{LS}(r') \right] . \tag{151}$$

This option is provided primarily for diagnostic purposes, such as checking the Darwin factor or nonrelativistic reduction.

6.5. Effective Mass Options

Closely related to the Perey factor is the nonlocality correction of the absorptive potential,

$$ImU^C(r) \longrightarrow \sqrt{\frac{m_k(r)}{m}} ImU^C(r) \; . \tag{152}$$

Several models of the effective mass $m_k(r)$ are available, as selected by the character variable `CKMASS`. This factor is omitted when `CKMASS = 'NO KMASS'`, which is the default.

If `CKMASS = 'PEREY'`, the effective mass is determined from the Perey factor according to

$$\frac{m_k(r)}{m} = \left[1 - \frac{m\beta^2}{2\hbar^2} V(r)\right]^{-1} \tag{153}$$

where $V(r)$ is the real part of the central optical potential. The nonlocality range `BETANL` $= \beta$ is read from the same place that it would be for `CPEREY = 'PEREY'`. Therefore, to use the same β for both $m_k(r)$ and $P(r)$ while avoiding redundant input, use `CPEREY = 'KMASS'` in conjunction with `CKMASS = 'PEREY'`.

Alternatively, if `CKMASS = 'KMASS'` we use Eq. 145 for all models of the effective interaction except `NFORCE = 'JLM'` for which the explicit parametrization provided by the JLM model is used.

6.6. Self-Consistent Wave Number

Calculation of the local wave number requires additional optical model input to subroutine `SCWK` to be supplied in the appropriate position; for example, Line 5 in Sec. 4.4.1 calls for input to `SCWK`. At that point if `ISC='SCWN'` a call to `OPTN` requests a subset of the input described in Sec. 8. This subset is indicated below. Note `CPEREY` is read but is not used and Lines 2, 5, 6 from Sec. 8 are omitted.

line	variable	description	section
Line 1 (*)	`OPTMOD`	optical potential option	
	`ZMODE`	Coulomb potential option	
	`CPEREY`	Perey factor option	
Line 3		input needed for `ZMODE` selection	Sec. 8.2
Line 4		input needed for `OPTMOD` selection	Sec. 8.1

For most `OPTMOD` choices, the code will compute the chosen optical model and use it in Eq. (138) to compute the local wave number. However, if `OPTMOD='FOLD'` it is assumed that the effective interaction used in the folding model depends upon the local wave number so that it becomes necessary to perform a self–consistency iteration. First, the folding model potential is calculated using the asymptotic wave number. The local wave number is then calculated and is used to recompute the optical potential. The new optical potential is used to calculate new local wave number. The current wave number is compared to the previous local wave number at the origin and the calculation is iterated until the difference is less than 0.01 fm^{-1} or until 5 iterations have been made. Note that the iterations do not require input.

After the self–consistent wave number has converged, most modes call for construction of a new optical potential for the initial state. This new potential need not use the same model as used by SCWK. Thus, one could use a standard phenomenological optical potential to produce a good approximation to the local wave number without iteration, saving some time, and then compute a folding model potential with that approximate local, but not self–consistent, wave number. Note that OPTMOD='SAME' should not be used at this point — even if the same model is used, it is assumed that the potential depends upon $k(r)$ and hence it needs to be recomputed once more.

7. MODELS FOR GROUND-STATE OR TRANSITION DENSITIES

7.1. General Description

Ground-state or transition densities can be specified in many ways depending upon the value of a character variable read from LUN5 with (*) format as the first line of input to subroutine GSDEN for the ground-state or TRDEN for transition densities. This variable is called GSMODE for ground-state densities or TRMODE for transition densities. The input streams for both GSDEN and TRDEN are sufficiently similar that the bulk of the description can be handled in this general section. A brief list of the available options is given below.

'NONE'	: ground-state densities vanish
'READ'	: densities read from a file
'SAME	: present density same as previous density
'SHELL'	: shell model
'CONSTANT'	: use constant Fermi momentum (for ground-state only)
'ISO'	: parametrized isoscalar/isovector densities
'P-N'	: parametrized proton/neutron densities

If the xxMODE variable is 'NONE' the relevant densities are assumed to vanish. If xxMODE is 'SAME' and the relevant density has already been evaluated, then it is not necessary to supply any further input for that density. If xxMODE is 'READ', the densities are read from an external file. If xxMODE is 'SHELL', spectroscopic amplitudes for the shell model are obtained using the subroutine INSPEC; either harmonic oscillator or Woods-Saxon radial wave functions are available.

If xxMODE is either 'P-N' or 'ISO', then the density is evaluated using an analytic parametrization. In these cases, two sets of input are required. For 'P-N', the proton density is described first and is followed by the neutron density. For 'ISO', the isoscalar density is followed by the isovector density. Note that the two densities may be described with different parametrizations. These parameterizations are evaluated using the subroutine GSMODEL for the ground-state or TRPAR for transition densities. Only a single type of density may be parametrized at a time, with other densities assumed to vanish. For the ground state, the matter density RJ is evaluated but the spin-convection density is assumed to vanish. For transitions it is possible to choose the array that is evaluated from the list of all transition densities.

Although the scattering calculations require point–nucleon densities, it is often useful to employ densities obtained from electron scattering measurements which usually include nucleon finite–size form factors. Thus, many of the density models allow the nucleon form factor to be unfolded from a parametrized or input density. This option is governed by the character variable `FORMFF`. If `FORMFF='NO FOLD'` is entered, we assume that the input to follow describes point densities. The proton charge form factor will be automatically folded into the Coulomb potential and into form factors for electron scattering. If `FORMFF='UNFOLD'` is entered, we assume that the input describes densities that include the nucleon finite–size. The proton form factor remains in the charge transition density and will be divided out of all other transition densities in q-space. Finally, `FORMFF='FOLD'` causes the form factor to be folded into the point density. This option is used by other programs that employ the same libraries but is only useful to `LEA` for limited diagnostic purposes.

7.2. Input to GSDEN: ground-state densities

In this section we describe the specific input required to produce ground-state densites. Input for `GSDEN` is obtained from `LUN5`. The first line, with `(*)` format, supplies `GSMODE`. Subsequent input depends upon that selection as described below. Some options are described below and the others are described in the sections cited.

<u>GSMODE</u>	<u>description</u>
`'NONE'`	densities vanish. No further input required.
`'SHELL'`	shell model. See Sec. 7.6
`'P-N'`	use parametrizations of ρ_p and ρ_n selected from Sec. 7.5.1 or 7.5.2.
`'ISO'`	use parametrizations of ρ_0 and ρ_1 selected from Sec. 7.5.1 or 7.5.2.
`'READ'`	read densities from a file.
`'CONSTANT'`	constant density for diagnostic purposes.

7.2.1. GSMODE = 'ISO' *or* 'P-N'

If either of these options is selected, two densities will be described separately by analytic parametrizations. For `'ISO'`, we assume that the isoscalar density is followed by the isovector density. For `'P-N'`, we assume that the proton density is followed by the neutron density. Thus, two blocks of input are required with the following pattern.

Line 2	(*)	`DENMOD`	selects parametrization for first density
		`FORMFF`	governs deconvolution of nucleon form factor
Line 3			input for first density
Line 4	(*)	`DENMOD`	selects parametrization for second density
		`FORMFF`	governs deconvolution of nucleon form factor
Line 5			input for second density

If `DENMOD = 'NONE'` the densities of the current type (proton, neutron, isoscalar, or isovector) are set to zero. Alternatively, once the first set of densities has been established, the second set of densities can be made proportional to the first choosing `DENMOD = 'SAME'`, such that $\rho_n = \frac{N}{Z}\rho_p$ for `'P-N'` or $\rho_1 = \frac{N-Z}{N+Z}\rho_0$ for `'ISO'`. Otherwise, one of the analytic parametrizations must be chosen and the subsequent input within that block depends upon the choice made for DENMOD. The available models are described in Sections 7.5.1 and 7.5.2.

If FORMFF='NO FOLD' is specified, the parametrization is assumed to describe a point-nucleon form factor. If FORMFF='UNFOLD', the parametrization is assumed to describe a charge or matter density from which the nucleon form factor must be unfolded numerically.

7.2.2. GSMODE = 'READ'

If the densities are to be read from a file, the file name is read with (A) format on the next line. The remaining input, lines (2b-2f), is obtained from the specified file.

Line 3a (A): FILNAM

Line 3b (*): N = number of radial points in each density.
The mesh size is assumed to agree with DR.

Line 3c (*): Isoscalar matter density, N points.

Line 3d (*): Isovector matter density.

Line 3e (*): Isoscalar LS density.

Line 3f (*): Isovector LS density.

Each density array is read with a single free-format statement. Therefore, although each density must begin on a new record, the subsequent spacing is arbitrary. A density array can be omitted simply by placing a slash (/) where the input should have occurred.

7.2.3. GSMODE = 'CONSTANT'

This option is occasionally useful in testing folding-model routines using density-dependent effective interactions. If this option is chosen, the next line must supply the Fermi momentum in (*) format. The local Fermi momentum will then be assumed everywhere uniform. The units are fm^{-1}.

7.3. Input to NEWGS: new ground–state densities for charge exchange reactions

Since charge exchange changes the matter densities, folding model optical potentials for the final state require a new set of ground state densities for the exit channel. The new densities are produced by the subroutine NEWGS, which requires the following input from LUN5.

Line 1 (*) SCALE

Line 2 input to GSDEN if SCALE$\neq$'SCALE'

It is usually sufficient to scale the densities to the proper proton and neutron numbers, but it is also possible to employ any of the models available to GSDEN. Thus, if the character variable SCALE is given the value 'SCALE, no further input is needed. Otherwise, a call to GSDEN is made.

7.4. Input to TRDEN: transition densities

In this section we describe the specific input required to produce transition densites. Input for TRDEN is obtained from LUN5. The first line, with (*) format, supplies TRMODE. Subsequent input depends upon that selection as described below.

TRMODE	description
'NONE'	densities vanish. No further input required.
'SHELL'	shell model. See Sec. 7.6
'P-N'	use parametrizations of ρ_p and ρ_n selected from Sec. 7.5.1.
'ISO'	use parametrizations of ρ_0 and ρ_1 selected from Sec. 7.5.1.
'READ'	read densities from a file.

This option permits preparation of the transition density using structure codes outside LEA. The file name is read in (A) format from the LEA input file. The remaining lines for this section are read from that external file. Each J-transfer must have its own file. The radial mesh parameters must match those supplied in the LEA input. Later revisions will relax these restrictions. As always, densities can be omitted simply by using the slash (/) terminator in their place.

Line 2 (A): name of the file containing the density arrays

Line 3 (*): number of points in each array

Line 4 (*): isoscalar densities.

For normal parity, the arrays are read in the order

{ RJ, RSJ, RJD, RLJ, RLSJ1, RLSJ2, RLSJ3}.

The order for abnormal parity is {RSJLL, RSJLU, RLJLL, RLJLU}.

Line 5 (*): isovector densities in same order as above.

7.4.1. TRMODE = 'ISO' *or* 'P-N'

If either of these options is selected, two densities will be described separately by analytic parametrizations. For 'ISO', we assume that the isoscalar density is followed by the isovector density. For 'P-N', we assume that the proton density is followed by the neutron density. Although LEA recognizes many types of transition density, this option is presently restricted to a single pair of densities of the same type. (This restriction may be relaxed in later versions of LEA). The density type is chosen on the next line: For normal-parity transitions with $\Delta\pi = (-)^{\Delta J}$, the choices for DENNAM are 'RJ', 'RSJ', 'RJD', 'RLJ', 'RLSJ1', 'RLSJ2', and 'RLSJ3'. For abnormal-parity transitions with $\Delta L = \Delta J \pm 1$, the choices for DENNAM are 'RSJLL', 'RSJLU', 'RLJLL', and 'RLJLU'. This option is most commonly used when electroexcitation measurements are available for ρ_p, hence DENNAM='RJ', with other densities presumed negligible.

Different models can be used for each of the two densities in the pair. Subsequent input for each density depends upon these choices. Detailed descriptions may be found in Sec. 7.5. Therefore, the input has the following pattern.

Line 2 (*) `DENNAM` selects type of density
Line 3 (*) `DENMOD` selects parametrization for first density
`FORMFF` governs deconvolution of nucleon form factor
Line 4 input for first density
Line 5 (*) `DENMOD` selects parametrization for second density
`FORMFF` governs deconvolution of nucleon form factor
Line 6 input for second density

7.5. Parametrized Densities

7.5.1. Linear Expansions

Linear expansions of a radial density can be expressed in the form

$$\rho_\ell(r) = \sum_{n=1}^{N} a_n f_{n\ell}(r)\Theta(R-r). \tag{154}$$

where the a_n are the expansion coefficients, $f_{n\ell}(r)$ are radial basis functions for multipolarity ℓ, and $\Theta(x)$ is the unit step function equal to unity for $x > 0$ and to zero otherwise. The expansions are linear in the coefficients a_n, which may be fitted to data using the LEA methods. The basis functions $f_{n\ell}(r)$ generally contain additional parameters governing the radial scale, but these nonlinear parameters must be preset and are not available as fitting parameters. Note that for most models $R \to \infty$, but for the FBE models the cut–off radius is the parameter which sets the radial scale.

The properties and relative merits of the most important linear expansion models were discussed in Sec. 3.3.1. These include the polynomial-Gaussion expansion (PGE), the Laguerre-Gaussian expansion (LGE), and the Fourier-Bessel expansion (FBE). Many variations of the FBE have been employed, which here are designated HFBE, MFBE, and MHFBE. Note that HFBE and MHFBE are not available for $\ell = 0$, for obvious reasons. We include also a variation of the PGE proposed by Kamimura; in that case we prefer to read R_N instead of A. The sum of Gaussians model (SOG) is applicable only to ground–state densities. The set of basis functions presently available is described in Table I. The input required to use these expansions is described in the final column and is read from `LUN5` in (*) format.

Ground–state densities from electron scattering measurements are usually presented in the form of charge densities from which we must unfold the proton form factor. For FBE models it is possible to exploit the deconvolution theorem to perform this unfolding efficiently. If the input parameters a_n describe a charge density, the point-nucleon density can be obtained using modified parameters a'_n, where

$$a'_n = a_n / F_p(q_n) \tag{155}$$

and where F_p is the proton form factor. This transformation is faster and more accurate than the numerical deconvolution procedure used for other models. To use this technique, append `'-CH'` to the label and, since we do not want to unfold the density twice, choose

TABLE I. Definitions and input for expansions available for both ground–state and transition densities.

label	$f_{n\ell}(r)$	conditions	input
'LGE'	$x^L e^{-x^2} L_n^{\ell+\frac{1}{2}}(2x^2)$	$x = r/b$	N, b $\{ a_n, n = 1, N \}$
'PGE'	$[\alpha^3 y^\ell e^{-y^2}] y^{2n}$	$y = \alpha r$	N, α $\{ a_n, n = 1, N \}$
'KAMIMURA'	$x_n^\ell e^{-x_n^2}$	$x_n = r/R_n, \quad R_{n+1} = AR_n$	N, R_1, R_N $\{ a_n, n = 1, N \}$
'FBE'	$j_\ell(q_n r)$	$j_\ell(q_n R) = 0$	N, R $\{ a_n, n = 1, N \}$
'MFBE'	$q_n j_\ell(q_n r)$	$j_\ell(q_n R) = 0$	N, R $\{ a_n, n = 1, N \}$
'MERLE'	$(-)^{n+1} \frac{q_n^2}{\pi} j_\ell(q_n r)$	$j_\ell(q_n R) = 0$	N, R $\{ a_n, n = 1, N \}$
'HFBE'	$j_\ell(q_n r)$	$j_{\ell-1}(q_n R) = 0$	N, R $\{ a_n, n = 1, N \}$
'MHFBE'	$q_n j_\ell(q_n r)$	$j_{\ell-1}(q_n R) = 0$	N, R
			$\{ a_n, n = 1, N \}$
'SOG'	$\left\{ e^{-(r-R_n)^2/\gamma^2} + e^{-(r+R_n)^2/\gamma^2} \right\}$	$a_n = \frac{Q_n}{2\pi^{3/2}\gamma^3[1+2(R_n/\gamma)^2]}$	N, γ $\{ R_n, Q_n, n = 1, N \}$

`FORMFF = 'NO FOLD'`. Thus, `'FBE'` becomes `'FBE-CH'`, `'MFBE'` becomes `'MFBE-CH'`, etc. The functional form and input are otherwise identical to the FBE versions described in Table I.

Most expansions are available for both ground–state and transition densities. The SOG model is an exception that is available only for the ground state. Also note that at the present time, the the `xFBE-CH` options have been implemented only for ground-state densities.

7.5.2. Specialized Parametrizations for Ground-State Matter Densities

Several additional parametrizations specialized to the ground-state matter density appear in the literature and are available to `GSDEN`. The commonly used three-parameter Fermi and Gaussian densities are designated 3pF and 3pG, respectively. In addition, the harmonic oscillar model for *sd*–shell nuclei is designated HO. Note that the charge and mass numbers are read as integers. A variation of the HO model, designated MHO for modified HO, is also provided and allows the polynomial portion to be adjusted independently. Finally, the `'SQUARE'` density is constant for $r < R$ and is sometimes useful for diagnostic purposes.

A composite model, designated either `GSMODE='3pF+FBE'` or `GSMODE='Miska'`, is useful for parametrizing differences between charge densities for an isotopic series. This model is represented by

TABLE II. Parametrizations of the ground–state density.

label	definition	input
`'3pF'`	$\rho(r) \propto \frac{1+w(r/c)^2}{1+e^{(r-c)/z}}$	c, z, w
`'3pG'`	$\rho(r) \propto \frac{1+w(r/c)^2}{1+e^{(r^2-c^2)/z^2}}$	c, z, w
`'HO'`	$\rho(r) \propto [1+a(r/b)^2]e^{-(r/b)^2}$ $a = a_0 b_0^2 / \left[b^2 + \frac{3}{2}a_0(b^2 - a_0^2)\right]$ $a_0 = (Z-2)/3$ $b_0^2 = \frac{A}{A-1}(b^2 - a_p^2)$ $a_p^2 = \frac{2}{3} < r_p^2 >, < r_p^2 >= 0.64 \text{ fm}^2$	b, Z, A
`'MHO'`	$\rho(r) = [1+a(r/b)^2]e^{-(r/b)^2}$	b, a
`'SQUARE'`	$\rho(r) \propto \Theta(R-r)$	R

$$
\left.\begin{array}{l}
\rho(r) = f_0(r) + \sum_{n=1}^{N} f_n(r) \\
f_0(r) \propto \frac{1+w(r/c)^2}{1+e^{(r-c)/z}} \\
f_n(r) = \sum_{m=1}^{N_n} \frac{a_{nm} q_{nm}}{4\pi} j_0(q_{nm} r)\Theta(R_n - r)
\end{array}\right|
\begin{array}{l}
\\
4\pi \int dr\, r^2\, f_0(r) = Z_0 \\
q_{nm} = \frac{m\pi}{R_n}
\end{array}
$$

where $f_0(r)$ is a 3pF density normalized to Z_0 and each $f_n(r)$ is an FBE density. The FBE components need not have common cut-off radii R_n. For a charge density, we ordinarily would normalize the 3pF component to the total charge, such that $Z_0 = Z$, and the FBE components to zero. However, although Z_0 must be positive it need not be equal to Z. Nor must the FBE components be chargeless. The normalization of the FBE components is determined by the user and is not checked. On the other hand, the normalization of the total density ρ is routinely readjusted if necessary. The input needed for this model is summarized below. Lines 3c and 3d are repeated N times.

Line 3a: c, z, w, Z_0
Line 3b: N
Line 3c: N_n, R_n
Lind 3d: $\{ a_{nm}, m = 1, N_n \}$

7.6. Shell Model Densities

Consider a one–body operator in a many–body system, such that

$$\mathcal{A} = \sum_{\alpha\beta} c_\alpha^\dagger \langle \alpha | A | \beta \rangle c_\beta \tag{156}$$

where α, β represent complete sets of single–particle quantum numbers and $c_\alpha^\dagger$ and c_β represent creation and annihilation operators, respectively. If $\mathcal{A}_J$ is a spherical tensor of rank–J, its reduced matrix elements[2] can be expressed in the form

$$\langle f || \mathcal{A}_J || i \rangle = \sum_{\alpha\beta} S_J^{fi}(\alpha, \beta) \langle \alpha || A_J || \beta \rangle \tag{158}$$

[2]Note that we use Brink and Satchler conventions in which

where

$$S_J^{fi}(\alpha,\beta) = \frac{\hat{j}_\alpha}{\hat{J}} \langle f||[c_\alpha^\dagger \otimes c_\beta]_J||i\rangle \tag{159}$$

is proportional to a one–body density matrix element (OBDME) relating the structure of the initial and final nuclear states i and f, and where $\langle\alpha||A_J||\beta\rangle$ is a reduced matrix element for a single–particle transition between orbitals β and α. Note that since a hole in orbital β is associated with magnetic quantum number $-m_\beta$, the coupling of creation and annihilation operators is defined as

$$[c_\alpha^\dagger \otimes c_\beta]_{JM} = \sum_{m_\alpha m_\beta} (-)^{\frac{1}{2}-m_\beta} \left\langle \begin{array}{cc} j_\alpha & j_\beta \\ m_\alpha & -m_\beta \end{array} \middle| \begin{array}{c} J \\ M \end{array} \right\rangle c_\alpha^\dagger c_\beta \ . \tag{160}$$

The isospin structure of the one-body density matrix is described analogously. For any angular momentum, the isospin matrix elements of a one–body operator can be expressed as

$$\langle f|\mathcal{A}_{TM_T}||i\rangle = \hat{T}^{-1} \sum_{\alpha\beta} S_{TM_T}^{fi}(\alpha,\beta)\langle\alpha|A_{TM_T}|\beta\rangle \tag{161}$$

where angular momentum labels have been omitted for brevity and where

$$S_{TM_T}^{fi}(\alpha,\beta) = \sqrt{2}\langle f||[c_\alpha^\dagger \otimes c_\beta]_{TM_T}|i\rangle \ . \tag{162}$$

Although we might prefer to maintain parallel definitions for S_T and S_J, the placement of the factors of $\sqrt{2}$ and $\hat{T}$ conform to prevalent conventions. Furthermore, since nucleon beams are prepared and detected with definite charges, it is usually more convenient to consider unreduced matrix elements. Upon analysis of the recoupling coefficients, we find

$$\begin{array}{l|l} S_{00} = S_{nn} + S_{pp} & S_{nn} = \frac{1}{2}(S_{00} + S_{10}) \\ S_{10} = S_{nn} - S_{pp} & S_{pp} = \frac{1}{2}(S_{00} - S_{10}) \\ S_{11} = -\sqrt{2}S_{np} & S_{np} = -\sqrt{\frac{1}{2}}S_{11} \\ S_{1-1} = \sqrt{2}S_{pn} & S_{pn} = \sqrt{\frac{1}{2}}S_{1-1} \end{array}$$

where we assign $t_3 = +\frac{1}{2}$ to the neutron.

Construction of shell model densities for either the ground state or for a transition requires both OBDME input and a model of the singe–particle wave functions. OBDME input and output for shell model densities is performed by the subroutine **INSPEC**, which is described in Sec. 7.6.1. At present, the single–particle wave functions can be represented in either the harmonic oscillator model or using Woods-Saxon potentials. For the harmonic oscillator model it is possible to enter a different oscillator parameter for each orbital, thus simulating changes to the radial wave functions for orbitals near the top of a finite well. For

---

$$\langle j_f m_f|A_{JM}|j_i m_i\rangle = \left\langle \begin{array}{cc} j_i & J \\ m_i & M \end{array} \middle| \begin{array}{c} j_f \\ m_f \end{array} \right\rangle \langle j_f||A_J||j_i\rangle \ . \tag{157}$$

the Woods-Saxon model it is possible to use different potentials for each orbital with either fixed depths or depths adjusted to produce a specified separation energy. In addition, center of mass and core polarization corrections can be applied.

The first few lines of input needed to specify shell model densities are the same for both harmonic oscillator, RTYPE='HO', and Woods-Saxon, RTYPE='WS', shell models. For the 'HO' model, the OBDME input follows immediately, as described in Sec. 7.6.1. For the 'WS' model it is necessary to initialize the radial wave functions, using input described in Sec. 7.6.3, before proceeding to the OBDME input. The center of mass correction for shell model densities is described in Sec. 7.6.4 and the Tassie model of core polarization is described in Sec. 7.6.5.

line	variable	type	description
Line 1 (*)	STYPE	character	governs OBDME input
	RTYPE	character	governs radial wave functions.
Line 2 (*)	ISOI	integer	twice initial isospin
	ISOF	integer	twice final isospin
Line 3 (*)	KCOM	character	governs c.m. corrections
	DEFALPHA	real	default α for c.m. corrections
	CTASSIE	character	governs core polarization (omitted for ground state)

7.6.1. OBDME Input using INSPEC

Configurations are specified by character variables ORBITP and ORBITH for particle and hole, respectively. The smallest principal quantum is 1. The orbital angular momentum is identified by its spectroscopic letter (capitalized). The total angular momentum j is specified by an integer equal to twice j. For example, the $1d_{5/2}$ orbit is identified as '1D5 '. Note that because the labels are defined with 4-character variables, many machines will require a trailing blank to be used after 3-character labels for proper matching against an internal list of acceptable labels. A special value ORBITP='END' is used to terminate the list of spectroscopic amplitudes.

Various authors present OBDME with many different normalization and phase conventions. For ease in preparing and checking input files, we prefer to enter the matrix element in the original form provided by the author, designated Z, and to convert to the LEA convention, designated S, using a conversion factor defined by

$$S_J^{fi}(\alpha,\beta) = \xi_J^{fi}(\alpha,\beta) Z_J^{fi}(\alpha,\beta) \tag{163}$$

where isospin labels are omitted here for brevity. Radial wave functions are assumed to be positive at the origin and in LEA do not include the i^ℓ factors preferred by some authors. The appropriate conversion factors are distinguished by the character variable STYPE and the available choices are listed in Table III, including phase adjustments where necessary. The total angular momentum, parity, and isospin are denoted J_i, Π_i, and T_i for the initial state and J_f, Π_f, and T_f for the final state. Single–particle orbital and total angular momenta are denote ℓ_α and j_α for the particle or ℓ_β and j_β for the hole.

TABLE III. Conversion factors for OBDME conventions.

STYPE	$\xi_J^{fi}(\alpha,\beta)$	description
'S'	1	standard LEA convention
'Z'	$\frac{\hat{J}_i\hat{j}_\alpha}{\hat{j}_f}$	Raynal for DWBA70
'SBAR'	$\frac{\hat{j}_\alpha}{\hat{J}}$	
'AMOS'	$\frac{\hat{j}_\alpha}{\hat{J}\hat{J}_f}$	
'BS'	$\frac{\hat{j}_\alpha}{\hat{J}} i^{\ell_\beta-\ell_\alpha}\sqrt{\Pi_i\Pi_f}$	Brink and Satchler convention
tt 'BROWN'	$\frac{\hat{j}_\alpha}{\hat{J}_f}\frac{\hat{T}}{\hat{T}_f}$	A. Brown convention requires KTC='RED'

For charge exchange only a single OBDME is needed for each transition, designated as Z1 $= Z_{11}$ for (p,n) reactions or Z1 $= Z_{1-1}$ for (n,p) reactions. For inelastic scattering it is necessary to supply two OBDME for each transition, either in isospin or nucleon representations according to the character variable KTC. If KTC='P-N', the matrix elements ZP $= Z_{pp}$ and ZN $= Z_{nn}$ are interpreted in the nucleon representation. If KTC='ISO', these matrix elements are interpreted as unreduced isospin matrix elements designated as Z0 $= Z_{00}$ and Z1 $= Z_{10}$. If KTC='RED', these matrix elements are interpreted as reduced with respect to isospin, such that Z0 $= Z_0$ and Z1 $= Z_1$, and are multiplied by appropriate Clebsch–Gordon coeffients. Note that the isospin Clebsch–Gordon factors are applied before the OBDME are written to the output file (LUN2 or LUN6), but the factors $\xi_J^{fi}(\alpha,\beta)$ are applied after.

Therefore, the following input is repeated until ORBIT='END' is encountered. The J-transfer must be legal and must match the current stage of calculation. Any value of ALPHA input as zero will be reassigned to DEFALPHA. Note that ALPHA is read but is irrelevant for RTYPE='WS' and may be omitted by terminating the line with slash.

elastic or inelastic scattering $\Longrightarrow$ ORBITP, ORBITH, J, ZP, ZN, KTC, ALPHA for KTC='P-N'
ORBITP, ORBITH, J, Z0, Z1, KTC, ALPHA otherwise
charge exchange $\Longrightarrow$ ORBITP, ORBITH, J, Z1, KTC, ALPHA

7.6.2. STYPE='MILLENER' *format*

A subroutine which handles several OBDME files the author received from D. J. Millener can be used with the input below. A specialized format is used to decode the structure of the n^{th} state with the multipolarity under consideration. For the ground-state density it is necessary to supplement the active model space with a description of the inert core. This is done using Line 3 of the general format with TYPE→TYPE2.

Line 3 (A): name of file carrying OBDME information
Line 4 (*): ISOSPN = 2*isospin for desired level
NUMBER = state number (n) for this multipolarity
TYPE2 = TYPE used for core configurations
Line 5 (*): return to Line 3 of previous section

7.6.3. Initialization of Woods-Saxon wave functions

When Woods-Saxon radial wave functions are used to construct transition densities, it is necessary to first initialize all of the orbitals for which OBDME's will be supplied. Thus, cumbersome input and recalculation of wave functions for orbitals involved in several OBDME's is avoided. The task is performed by the subroutine `INITWSWF`, whose input is outlined below. Line 5 is repeated until `ORBIT='END'` is encountered; the remainder of that line can be truncated using slash termination.

line	variable	type	description
Line 4 (*)	`CMTYPE`	character	
	`LSTYPE`	character	
Line 5 (*)	`ORBIT`	character	orbital code
	`IZP`	integer	particle charge
	`BE`	real	binding energy
	`V`	real	central depth
	`RRV`	real	central reduced radius
	`AV`	real	central diffuseness
	`VSO`	real	spin–orbit depth
	`RRVSO`	real	spin–orbit reduced radius
	`AVSO`	real	spin–orbit diffuseness
	`RRZ`	real	Coulomb reduced radius
	`BETA`	real	Perey nonlocality range

The well depths and binding energies are entered as positive values in units of MeV. If the central depth is zero upon input, it is adjusted to reproduce the input binding energy (which must be greater than 0.2 MeV). Otherwise the central depth is held fixed to its input value and the binding energy is computed, ignoring its input value. If `LSTYPE='FIXED'`, the spin–orbit depth is entered as a fixed value in MeV and is not adjusted even if the central depth is varied. If `LSTYPE='SCALED'`, the spin–orbit depth is scaled to the central depth, in which case the input parameter is interpreted as a factor multiplying the Thomas spin–orbit potential, such that $\lambda =$`VSO` where

$$V^{LS} = \left(\frac{m_\pi}{2m_p}\right)^2 \lambda V = 0.00554\lambda V \ . \tag{164}$$

Radius and diffuseness parameters are entered in units of fm. The well radii are entered in reduced form; for example, the central radius is `RRV` $\times (A-1)^{1/3}$ fm. The radial scale is determined by the character variable `CMTYPE`. Let $f(r)$ be the normalized solution for the specified well. If `CMTYPE='A-1'`, the radial variable is referred to the center of the $A-1$ residual system, such that the single–particle wave function, $\phi(r)$, becomes

$$\texttt{CMTYPE} =' \texttt{A}-\texttt{1}' \Longrightarrow \phi(r) = \left(\frac{A}{A-1}\right)^{1/3} f\left(\frac{A}{A-1} r\right) \tag{165}$$

Otherwise, the radial variable is referred to the center of mass of the nucleus, such that $\phi(r) = f(r)$.

7.6.4. Center of Mass Corrections

The center-of-mass form factor

$$f_{c.m.} = \exp(b^2/A) \tag{166}$$

is applied to the q-space densities when KCOM = 'C-O-M' and is omitted otherwise. The oscillator parameter is entered as $\alpha = b^{-1}$ for historical reasons. The value of DEFALPHA read in the initial input stage is used for this purpose.

The default α read by INSPEC is used for any configuration for which $\alpha = 0$ is read.

7.6.5. Core Polarization

8. OPTICAL MODELS

The conventions used to describe the optical model were presented in some detail in Sec. 2. In this section we describe the input needed to use the available options. The optical potential and related quantities are established by the subroutine OPTN and the routines it calls. A schematic outline of the input to OPTN is presented below. Depending upon the options selected, some lines may not be needed or may represent several lines of input as described in the indicated sections. The optical and Coulomb potential options are chosen by the character variables OPTMOD and ZMODE, respectively. Note that it is not necessary to read ZMODE for neutral projectiles. The model for possible nonlocality corrections is chosen by the character variable CPEREY. Note that for folding models this parameter is closely related to the effective mass option CKMASS determined by subroutine FORCEP; either or both may require input here.

line	variable	description	section
Line 1 (*)	OPTMOD	optical potential option	
	ZMODE	Coulomb potential option	
	CPEREY	Perey factor option	
Line 2		input to NEWGS (if needed)	Sec. 7.3
Line 3		input needed for ZMODE selection	Sec. 8.2
Line 4		input needed for OPTMOD selection	Sec. 8.1
Line 5		input needed for CKMASS option	Sec. 6.5
Line 6		input needed for CPEREY option	Sec. 6.4

For inelastic scattering, the optical potential must be described for both initial and final channels, so that the input file should contain two similar blocks of input as described in this section. The defaults for the final channel are 'SAME' for both nuclear and Coulomb potentials, so that the second block can be quite minimal. These defaults are invoked if slash terminators are encountered. The defaults for the initial channel are 'SCHWANDT' and 'FOLD', which require no input. Alternatively, for plane–wave calculations the optical potential is set to zero by choosing 'NONE' for both OPTMODE and ZMODE='NONE'. Otherwise, the input depends upon the model chosen.

The initial and final nuclei are different for charge exchange reactions and hence it may be necessary to readjust the ground state density arrays and Coulomb potential for the final channel. Hence for charge exchange the optical model input for the final state must include input to the subroutine NEWGS whenever either OPTMOD='FOLD' or ZMODE='FOLD' is selected. The simplest option is to merely rescale old arrays to new values of Z and N. However, for the folding model it may be desirable to evaluate an entirely new set of densities. Therefore, these reactions need an additional line of input

Line 2 (*) : SCALE

immediately preceding the specification of the optical potential for the outgoing channel. On this line, a character variable SCALE is read. If SCALE='SCALE', the ground-state densities are rescaled appropriately. Otherwise, GSDEN is called upon to provide a new set of densities using input described in Sec. 7.2. Following these new densities, the parameters of the outgoing optical potential are read in the manner above.

8.1. Optical Potential Choices

8.1.1. OPTMOD = 'WSAX'

The standard Woods-Saxon optical potential, described in Sec. 8.1.1, requires 5 lines of input containing 3 parameters each in (*) format. Each potential requires a strength V, reduced radius R, and diffuseness a.

Line 4a: V, R, a for real central
Line 4b: V, R, a for volume absorption
Line 4c: V, R, a for surface absorption
Line 4d: V, R, a for real spin-orbit
Line 4e: V, R, a for imaginary spin-orbit

8.1.2. Energy–Dependent Parametrizations

Several commonly used energy–dependent Woods-Saxon parametrizations from published work have been provided and require little or no input to use. These parametrizations are described in Table IV, including their applicable ranges of mass and energy. Adequate results should be obtained for nearby masses or energies, but none of these models bears extrapolation particularly well.

- Abdul-Jalil and Jackson model. Abdul-Jalil and Jackson [18,19] produced a potential for $A \approx 12$ and $50 \leq T_p \leq 160$, but in our opinion its description of proton scattering data is unsatisfactory. The absorptive potential becomes creative at the lower end of its energy range.

- Comfort and Karp model. Alternatively, the $p+{}^{12}$C potential of Comfort and Karp [20] for $T_p \leq 185$ MeV is preferred over the Abdul-Jalil and Jackson model. Fits were made at eight energies between 12 and 183 MeV; LEA performs linear interpolation of parameters between tabulated energies. Note that extrapolation is possible but not recommended.

- IUCF potentials. Several optical potentials have been produced by the IUCF group for proton energies between about 80 – 180 MeV. These potentials use a slightly different prescription for relativizing the kinematics of the Schrödinger equation. Thus, we must multiply their potential by the factor

$$\eta_{IUCF} = \left[1 + \frac{T_c}{T_c + 2m_p}\right] \frac{k^2}{2T_c\mu} \tag{167}$$

where T_c is the center of mass kinetic energy, k is the exact relativistic wave number, and μ is the reduced energy used in our version of the wave equation.

  – Schwandt model. The potential fitted by Schwandt *et al.* [21] to cross section and analyzing power for proton elastic scattering for $A \geq 40$ and $80 \leq T_p \leq 180$ MeV is probably used most often. It may be used for either proton or neutron scattering since it contains a parametrization of the symmetry potential. However, the Schwandt potential does not bear extrapolation in either mass or energy well. The energy dependence of the spin–orbit potential is much stronger in this model than in most others and the energy dependence of the absorptive potential also becomes quite steep near the upper end of the energy range.

  – Nadasen model. An earlier version of the IUCF optical potential fitted to cross section data alone. Two versions are implemented: the geometrical parameters for `'NADASEN0'` are A–indendent, whereas `'NADASEN'` uses A–dependent geometries.

- Raben potential. The NIKHEF group sometimes uses a potential due to Raben [22] in its analyses of $(e,e'p)$. This potential was developed as an incremental improvement of the Schwandt model, with a modest extension of the energy range.

- Dirac phenomenology. The Ohio State University group has produced global optical potentials using Dirac phenomenology (DP). These models are implemented in `LEA` as Schrödinger–equivalent potentials and provide the greatest ranges in mass and energy that are available.

  – Versions `'DP1'` and `'DP2'`, corresponding to fits 1 and 2 of Ref. [2], are implemented directly and require no input to use.

  – Versions `'EDADn'` where `n=1-3` correspond to the energy dependent A–dependent fits 1–3 of Ref. [3] and require a parameter file designated `DPDAT`. The file name is read on Line 4 of the optical model input in `(A)` format. The parameter file is provided with `LEA`.

  – Versions `'EDAIx'` where `x` is `C`, `O`, `CA`, `ZR`, or `PB` correspond to the energy dependent A–independent potentials for ^{12}C, ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb from Ref. [3]. These potentials also require the parameter file designated `DPDAT`.

TABLE IV. Energy–dependent optical model parametrizations.

OPTMOD	type	A	T_p (MeV)	input	Ref.
'CK'	Schrödinger	12	12 – 185	none	[20]
'ABDUL-JALIL'	Schrödinger	12	50 – 160	none	[18,19]
'SCHWANDT'	IUCF	40 – 208	80 – 180	none	[21]
'NADASEN'	IUCF	40 – 208	80 – 180	none	[23]
'NADASEN0'	fixed geometry			none	
'RABEN'	Schrödinger	40 – 208	65 – 200	none	[22]
'DP1', 'DP2'	Dirac	40 – 208	65 – 1040	none	[2]
'EDAD1', 'EDAD2', 'EDAD3'	Dirac	12 – 208	20 – 1040	DPDAT	[3]
'EDAIC'	Dirac	12	20 – 1040	DPDAT	[3]
'EDAIO'		16			
'EDAICA'		40			
'EDAIZR'		90			
'EDAIPB'		208			

8.1.3. Folding Model Calculation

The optical potential can also be calculated in the folding model using a variety of effective interactions in the local density approximation (LDA). The interaction is specified by input to the subroutine FORCEP, whose input is described in Sec. 9.2. The author recommends this model for consistent calculations of inelastic scattering, provided that a suitable density-dependent effective interaction is available. For test purposes it is sometimes useful to apply scale factors to the various terms of the potential. These scale factors are read on Line 4b and default to unity when a slash terminator (/) is encountered on that line.

Line 4a: input to FORCEP, described in Sec. 9.2

Line 4b: (*) scale factors to be applied to ReU^C, ImU^C, ReU^{LS}, and ImU^{LS}, respectively.

8.2. Coulomb Potential Choices

The Coulomb potential can be obtained either by folding the Coulomb interaction with the charge density or it can be parametrized. The only analytic models presently available are the point charge, ZMODE='POINT', and the uniformly charged sphere, ZMODE = 'UNIFORM', for which

$$U^Z(r) = \frac{Ze^2}{R_z}\left[\frac{3}{2} - \frac{1}{2}\left(\frac{r}{R_z}\right)^2\right] \tag{168}$$

when $r \leq R_z$. For ZMODE='UNIFORM', the reduced Coulomb radius, RC, is read on Line 3 of the optical model input such that $R_z = \mathrm{RC} \times A^{1/3}$ fm.

Line 3 (*) RC reduced Coulomb radius
(needed only for ZMODE='UNIFORM')

The Coulomb potential is omitted if ZMODE='NONE'. For the final state, the Coulomb potential remains the same as for the initial state if ZMODE='SAME'; do not choose that option for charge exchange.

9. MODELS OF THE EFFECTIVE INTERACTION

Several models are available for the two–nucleon effective interaction. Perhaps the simplest model is the Yukawa expansion of the free t-matrix using the pseudopotential representation, as parametrized by W. G. Love and M. A. Franey [8,9]. This option can be used simply by specifying NFORCE='LF' for the earlier version [8] or NFORCE='FL' for the later version [9] and the desired energy. A file tabulating all of the parameters from Ref. [9] is then scanned for the nearest tabulated energy. These files are supplied with the LEA program and require no user modifications. Alternatively, several G-matrix calculations have been reduced to pseudopotential form and tabulated as Yukawa expansions for several densities and many energies. Parameter files have been constructed for easy use in LEA, requiring only the file name and desired energy as input.

The tabulated interactions that are presently available are summarized in Table V. The character variable NFORCE identifies the interaction, wherever possible using the acronyms as the author's publications.[3] Density–independent interactions are identified by an entry of $k_F = 0$. Interactions whose density–dependence is parametrized as a continuous function are identified by ranges $k_F \geq 0$, whereas interactions tabulated for several discrete densities are indicated by more limited ranges of k_F. Some of the density–dependent interactions have been constructed only for the central component only, indicated by C in the second column, and are supplemented by density–independent spin–orbit and tensor components as described later in this section. Interactions available for a small number of discrete energies are identified by listing those energies, whereas those for which the tabulated energies are numerous or for which the energy dependence has been parametrized are distinguished by energy ranges in the third column. Note that interpolation with respect to energy has not been implemented. If the desired energy is not among those tabulated, a warning message is issued and the tabulated energy nearest the desired energy is used. This energy should be near the projectile energy but need not match it precisely because a large part of the energy dependence is adequately described by the energy dependence of the exchange approximation.

Alternatively, the user may construct independent parameter sets for either density–independent of density–dependent effective interactions using one of the generic formats described in Sec. 9.5. Finally, empirical medium modifications can be applied to the $k_F = 0$ part of any of the interactions introduced above. Empirical effective interactions (EEI) can be used either for complete calculations or for expansion purposes. In order to distinguish among the various interaction components, several of the input routines employ the character array CNAME, which carries the following set of labels.

---

[3] Note that for historical reasons, 'PARIS' is synonymous with 'PH' and 'BONN' with 'NL'.

TABLE V. Summary of available effective interaction models.

NFORCE	components	$T_p(MeV)$	k_F (fm^{-1})	Ref.
'JLM'	C	0 – 160	≥ 0	[24]
'YNM'	C	65 – 200	≥ 0	[25]
'CEG'	C	5 – 50	≥ 0	[26]
'M3Y'	C, LS, T			[27]
'BRG'	C	2 – 190	0.6 – 1.4	[28]
'NL'	C, LS, T	100, 140, 175, 210, 325	0 – 1.4	[29]
'PH'	C, LS, T	100 – 400	0.5 – 1.4	[30,31]
'LF'	C, LS, T	100 – 800	0	[8]
'FL'	C, LS, T	50 – 1000	0	[8]
'LR'	C, LS, T	200, 320, 400, 500, 650, 800	0.6 – 1.4	[32,33]
'IA2'	C, LS, T	200, 318, 500, 650, 800	0 – 1.4	[13]

'TC00'	$\rightarrow$	t^c_{00}	'TLS0'	$\rightarrow$	t'^{LS}_0	'TND0'	$\rightarrow$	V^{TD}_0
'TC01'	$\rightarrow$	t^c_τ	'TLS1'	$\rightarrow$	t'^{LS}_τ	'TND1'	$\rightarrow$	V^{TD}_τ
'TC10'	$\rightarrow$	t^c_σ				'TNX0'	$\rightarrow$	V^{TX}_0
'TC11'	$\rightarrow$	$t^c_{\sigma\tau}$				'TNX1'	$\rightarrow$	V^{TX}_τ

The subroutine INITF initializes the effective interaction. It begins by reading the force option NFORCE. It then calls the subroutine FORCEP, which obtains the interaction parameters from either the main input file or from an external file. It then obtains additional information that applies specifically to inelastic scattering. The various options available to folding model calculations and to the use of density-dependent interactions in the local density approximation are described in Sec. 9.1. Detailed input is then listed in Secs. 9.2–9.5.

9.1. Folding Model Options

Several variations of the folding model can be used. These variations primarily affect central potentials which are most sensitive to density dependence and to the exchange approximation. The spin-orbit and tensor potentials are evaluated with q-folding and SREA.

9.1.1. LDA Options

The simplest calculation evaluates the density dependence of the effective interaction at the site of the projectile. It is then possible to use q-space folding. For example, the central and spin-orbit potentials for normal-parity isoscalar transitions assume the form

$$U^C_J(r_1) = \frac{2}{\pi}\int dq q^2 \jmath_J(qr_1)\tilde{t}^C(q)\tilde{\rho}_J(q) \tag{169}$$

$$U^{LS}_J(r_1) = \frac{2}{\pi}\int dq q^2 \jmath_J(qr_1)\tilde{t}'^{LS}(q)\tilde{\rho}_J(q). \tag{170}$$

where

$$\tilde{t}(q) \longrightarrow \tilde{t}(q, \rho_g(r_1)) \tag{171}$$

uses the ground-state density at the projectile position r_1.

Alternatively, r-space folding can be used to evaluate the density dependence at the position of the struck nucleon r_2 or at the midpoint $c = |\frac{\vec{r}_1+\vec{r}_2}{2}|$. These calculations require double integrals that are far more time-consuming. For this reason, double-integral calculations are presently limited to central potentials for which these variations are most significant. The direct part of the integral has the form

$$U_\ell(r_1) = 2\pi \int d\cos\alpha \int ds s^2\, \rho_\ell(r_2) P_\ell(\cos\gamma) t(s, \rho_G) \tag{172}$$

where

$$r_2 = \left[r_1^2 + s^2 + 2r_1 s\cos\alpha\right]^{1/2} \tag{173}$$

$$c = \left[r_1^2 + (\frac{s}{2})^2 + r_1 s\cos\alpha\right]^{1/2} \tag{174}$$

$$\cos\gamma = (r_1 + s\cos\alpha)/r_2 \tag{175}$$

and where P_ℓ is a Legendre polynomial. The ground-state density ρ_G can be evaluated at one of the three positions

`IPOS = 0` $\Longrightarrow \rho_G = \rho_G(c)$
`IPOS = 1` $\Longrightarrow \rho_G = \rho_G(r_1)$
`IPOS = 2` $\Longrightarrow \rho_G = \rho_G(r_2)$.

The radial integral is expressed in terms of the separation $s = |\vec{r}_2 - \vec{r}_1|$ so that the Yukawa singularities can be handled gracefully. The radial mesh requires two parameters `NS` and `DS` specifying the number of points and the increment. This mesh need not match the `(NR,DR)` mesh for transition densities because interpolation will be required anyway.

The angular integral is performed by Gauss-Legendre quadrature. It is possible to subdivide the angular range into smaller intervals. It is also possible to test for convergence by halving these intervals several times and comparing the modulus of the (complex) integral with the previous result. The parameters governing the angular integral are:

`MPTS` = number of base points in each interval (2,3,4,5,6,10, or 15)
`NSTART` = initial number of intervals
`NMAX` = maximum number of halvings
`DELTA` = convergence criterion.

If `DELTA>0`, the intervals are halved repeatedly until the percent change in the total integral becomes less than `DELTA`. If `DELTA<0`, halving is repeated until the change in the integral is smaller than | `DELTA` | in magnitude. The maximum number of halving operations is `NMAX`.

The potential $U(r_i)$ is calculated on a radial mesh `DB`. Intermediate values are obtained by divided-difference interpolation of degree `MINT`. For E = 100-200 MeV, we have found that the following set of parameters gives good accuracy for moderate computing times:

```
NS=100 DS=0.1 MPTS=10 NSTART=1 NMAX=0 DB=0.5 MINT=4.
```

The accuracy of these results can be judged by comparing q-folding calculations for a density-independent interaction against r-folding. For a density-dependent calculation, q-folding can be compared with `IPOS=1`. The `TEST` option is useful in this respect.

9.1.2. Exchange Options

Several variations of the local-exchange approximation are available. These options are most readily described for the central potential, which can be expressed in the form

$$U^C(\vec{r}_1) = \int d^3r_2 \left[t^D(s,\rho_g)\rho(\vec{r}_2) + \jmath_0(ks)t^X(s,\rho_g)\rho(\vec{r}_1,\vec{r}_2) \right] \tag{176}$$

where D indicates the direct and X the exchange contribution and where k is the local wave number. The mixed transition density is assumed to be adequately represented by

$$\rho(\vec{r}_1,\vec{r}_2) = \rho(\vec{r}_2)C(k_F s) \tag{177}$$

where C is a correlation function describing the exchange nonlocality.

Three common approximations are available. When `KEA='ZREA'` is chosen, the zero-range exchange approximation replaces both $\jmath_0(ks)$ and $C(k_F s)$ by unity. When `KEA='FREA'` is selected, the finite-range exchange approximation retains $\jmath_0(ks)$ but still replaces the correlation function by unity. Finally, the Slater exchange approximation `KEA='SEA'` retains both factors, using a correlation function

$$C_{SEA}(x) = \begin{cases} 3\frac{\jmath_1(x)}{x} & \text{elastic} \\ \jmath_0(x) & \text{inelastic} \end{cases} \tag{178}$$

appropriate for excitations near the Fermi surface.

The direct and exchange contributions can be examined separately using the control variable `KXCHNG`. Normally, `KXCHNG='D+E'` is used to add both contributions coherently. However, `KXCHNG='DIR'` will give just the direct and `KXCHNG='ECH'` will give just the exchange contribution separately.

The exchange approximation is also affected by the control variable `ISC` which governs the local wave number k. When `ISC='A-WN'` is selected, the asymptotic wave number is employed. When `ISC='SCWN'`, the self-consistent wave number based upon the real part of the central optical potential is used.

9.1.3. Rearrangement Factor

According to Cheon *et al.*, the density dependence of the G-matrix for inelastic scattering is enhanced with respect to the elastic G-matrix G_0 by the factor

$$G(\rho) = (1 + \rho\frac{\partial}{\partial\rho})G_0(\rho). \tag{179}$$

This relationship is obtained by choosing the character variable `CHEON` as `'CHEON'` or is inhibited by `'NO CHEON'`.

9.2. Input to FORCEP

The subroutine FORCEP obtains and interprets input describing the effective interaction. Parameters governing folding model calculations are also read. Note that lines 3-6 are read only if required by the options selected in lines 1 and 2.

Line 1 (*)	NFORCE	interaction option
Line 2 (*)	CDBL	= 'DBLINT' $\rightarrow$ r-folding
		= 'Q-FOLD' $\rightarrow$ q-folding
	KXCHNG	= direct/exchange option
	KEA	= local exchange option
	ISC	= local wavenumber option
	CDD	= 'DD' $\rightarrow$ include density dependence
		= 'NO DD' $\rightarrow$ drop density dependence
	CPRINT	= 'PRINT' $\rightarrow$ detailed output
		= 'NO PRINT' $\rightarrow$ brief output
	CKMASS	= effective mass option (see Sec. 6.5)
	TNXTYPE	= tensor exchange option
Line 3 (*)	IPOS, NS, DS, MPTS, NSTART, NMAX, DELTA, DB, MINT	
	Parameters for r-folding read only if CDBL='DBLINT'.	
Line 4		option–dependent input, if needed
Line 5 (A)		Name of parameter file, if needed
Line 6 (*)		Interaction energy, if needed.

9.3. Input to INITF

The subroutine INITF initializes the effective interaction for inelastic scattering. It begins by calling the subroutine FORCEP, which is also used for elastic scattering routines and which was described in the preceding section. Note that this input can be curtailed simply by using NFORCE='SAME' to obtain consistency between elastic and inelastic scattering, provided that the folding model was used for the optical potential. INITF then obtains options that apply specifically to inelastic scattering. Any of these options can be disabled by adding NO.

Line 8 (*) KCOUL = 'COULX' $\Longrightarrow$ include Coulomb excitation
CHEON = 'CHEON' $\Longrightarrow$ include Cheon rearrangement factor

9.4. NFORCE Options

The type of interaction is determined by the character variable NFORCE. If NFORCE='SAME', it is assumed that the necessary information has already been obtained in an earlier stage of the calculation and the remainder of the FORCEP input is skipped. The available choices are described in the following subsections.

9.4.1. `NFORCE='LF'` *or* `NFORCE='FL'`

This option uses a file containing the t-matrix parameters of Love and Franey. There are two versions designated LF [8] and FL [9] with parameter files `LF81.dat` and `FL85.dat` that are supplied with the program. `FORCEP` input lines 5 and 6, containing the file name and interaction energy, are required.

9.4.2. `NFORCE='PH'` *or* `NFORCE='PARIS'`

This option uses the Paris-Hamburg G-matrix calculated by von Geramb. The file `PARIS.G` supplies the parameters for the complete density–dependent interaction, whereas the file `PARIS.T` describes an interaction that includes Fermi averaging but not Pauli blocking or the mean field. `FORCEP` input lines 5 and 6, containing the file name and interaction energy, are required.

9.4.3. `NFORCE='NL'` *or* `NFORCE='BONN'`

This option uses the G-matrix constructed by Nakayama and Love [29] using the Bonn potential. The file `NL88.G` supplies the parameters of the density–dependent interaction for several strategic energies between 100 and 325 MeV. `FORCEP` input lines 5 and 6, containing the file name and interaction energy, are required.

9.4.4. `NFORCE='M3Y'`

The M3Y interaction [27] is often used for low energies. The central, spin–orbit, and tensor components of G–matrices obtained from realistic interactions are fitted by three Yukawa contributions. Table 1 of Ref. [27] presents the parametrizations for each component. These are converted to `LEA` form by the subroutine `READM3Y`, whose input from `LUN4` consists of the line numbers from that table in following order.

Line 4a: line numbers for central interactions in the order:
singlet–even, triplet–even, singlet–odd, and triplet–odd

Line 4b: line numbers for even and odd tensor interactions

Line 4c: line numbers for even and odd spin–orbit interactions

Null entries cause the relevant component to be omitted. We recommend using the Elliot matrix elements, which obtained from the following input.

```
 3  6  7  8
13 14
16 18
```

9.4.5. NFORCE='CEG'

The interaction produced by Yamaguchi, Nagata, and Matsuda [26] for $5 \leq T_p \leq 50$ MeV was paramatrized in Gaussian form. The parameters are supplied in the file CEG.DAT and read using subroutine READCEG. The central components are complex and energy dependent, but noncentral components are real and energy independent. FORCEP input lines 5 and 6, containing the file name and interaction energy, are required.

9.4.6. NFORCE='YNM'

The YNM interaction is an extension of the CEG interaction to higher energies, $65 \leq T_p \leq 200$ MeV. The spin-orbit component is now complex but remains energy independent; no tensor component is provided. Both the energy and density dependence are parametrized. No option–dependent input is needed.

9.4.7. NFORCE='JLM'

The JLM interaction is based upon a calculation of the self–energy for a nucleon propagating in infinite nuclear matter [24]. Suppose that the optical potential for nuclear matter is expressed in the form

$$U(\rho, E) = \rho_0 \left(V_0(\rho, E) + iW_0(\rho, E)\right) + \rho_1 \left(V_1(\rho, E) + iW_1(\rho, E)\right) \tag{180}$$

where $\rho_0 = \rho_n + \rho_p$ is the isoscalar density and $\rho_1 = \rho_n - \rho_p$ is the isovector density. Isoscalar and isovector spin–independent central interactions can then be constructed as

$$t^C_{00}(q, \rho, E) = S_1 V_0(\rho, E) f(\mu_1 q) + iS_2 W_0(\rho, E) f(\mu_2 q) \tag{181}$$

$$t^C_{\tau}(q, \rho, E) = S_3 V_1(\rho, E) f(\mu_3 q) + iS_4 W_1(\rho, E) f(\mu_4 q) \tag{182}$$

where the S_i are scale (fudge) factors which can be used to improve the fit to data and where $f(x)$ with $x = \mu q$ is a shape function with range parameter μ. Gaussian or Yukawa shape functions can be selected with the character variable JLMSHAPE, such that

JLMSHAPE='GAUSSIAN' $\Longrightarrow f(x) = e^{-(x/2)^2}$

JLMSHAPE='YUKAWA' $\Longrightarrow f(x) = \left[1 + x^2\right]^{-1}$

Since the JLM interaction contains only central spin–independent components, the noncentral and spin–dependent interactions must be supplied from other sources. A simple density–independent parametrization of the spin–orbit interaction is available in the form

$$t'^{LS}_0(q) = V^{LS}_0 f(\mu_{LS} q) \tag{183}$$

$$t'^{LS}_\tau(q) = V^{LS}_\tau f(\mu_{LS} q)\,, \tag{184}$$

where the coefficients, V^{LS}_i, are complex. Components not produced by either the JLM model or the aforementioned spin–orbit parametrization can then be obtained from a supplementary NFORCE model. Hence, at the end of the JLM input we read another NFORCE option and its associated input.

The input needed for NFORCE='JLM' is outlined below. The variables are read in (*) format. Note that since the spin–orbit strengths are complex, (*) format requires the real and imaginary parts to be enclosed by parentheses and to be separated by a comma.

Line 4a:	JLMSHAPE	selects shape function
Line 4b:	$\{ \mu_i,\ i = 1,4 \}$	= central range parameters
	μ_{LS}	= spin–orbit range parameter
Line 4c	$\{ S_i,\ i = 1,4 \}$	= central scale factors
Line 4d	V_0^{LS}, V_τ^{LS}	= complex spin–orbit strength parameters
Line 4e	NFORCE	= interaction option for missing components
Line 4f		input needed for supplementary NFORCE selection

9.4.8. NFORCE='IA2'

The IA2 interaction is read from an external file by the subroutine READW. We assume that the file contains interactions for NKFIN densities uniformly distributed between 0 and 0.16 fm^{-3}. Each interaction is read for momentum transfers

$$\text{QIN(I) = I*DQIN, I=1,NQIN.}$$

Interpolation with respect to both q and ρ is performed within the input arrays. Note that the IA2 interaction is defined for particular targets, with mass number A_0, and laboratory kinetic energy, T_{lab}. These parameters are used to convert normalization conventions to LEA form.

The structure of the input file is outlined below. Lines 3-5 are repeated for each available interaction component. The interaction component is selected by the character variable LABEL, which must match one of the names in the CNAME array listed in Sec. 9. The real part is then read with one line for each q containing NKFIN densities. The imaginary part of that component then follows.

Line 1 A_0, T_{lab}
Line 2 NQIN, DQIN, NKFIN
Line 3 LABEL
Line 4 ($Ret(q_i, \rho_j)$, $j = 1$,NKFIN), i=1,NQIN)
Line 5 ($Imt(q_i, \rho_j)$, $j = 1$,NKFIN), i=1,NQIN)

9.5. Generic Interaction Files

The effective interaction can be supplied in several generic formats. These formats are described briefly below and in more detail separate sections.

- NFORCE='T' is used to paramatrize a density–independent interaction in Yukawa form.
- NFORCE='G' is used to parametrize a density–dependent interaction in Yukawa form. Parametrizations are supplied for several values of the Fermi momentum and interpolation is performed with respect to density.

- `NFORCE='TEFF'` represents a density–dependent interaction in EEI form. The medium modifications are parametrized and the interaction at zero–density is obtained using a second call to `FORCEP` with another `NFORCE` option.

- `NFORCE='KMT'` reads nucleon–nucleon scattering amplitudes $\mathcal{M}$ in KMT form as arrays in q. Sets for several Fermi momenta can be read. Interpolation is performed with respect to q and k_F.

9.5.1. `NFORCE = 'T'`

This option uses t-matrix parameters from a file with generic format. Two lines of input are required.

Line 6 `(A)` :	Name of file containing input parameters
Line 7 `(*)` :	Desired energy.

If the desired energy is not among those tabulated, a warning message is issued and the tabulated energy nearest is used.

The Yukawa expansions for the `'T'` option have the form

$$\tilde{V}(q) = \sum_{n=1}^{N} V_n \frac{e^{-r/b_n}}{r} \tag{185}$$

where b_n is the Yukawa range. The radial function has dimensions of $(\text{length})^{-1}$. Similar expression are used for spin-orbit and tensor interactions. The parameters are converted internally to `'G'` form.

Line 1r: `NCR, NLSR, NTNR`
Line 2r: `NCR` repetitions of $\{b, V_{SE}, V_{TE}, V_{SO}, V_{TO}\}$ for Ret^C
Line 3r: `NLSR` repetitions of $\{b, V_E, V_O\}$ for Ret^{LS}
Line 4r: `NTNR` repetitions of $\{b, V_E, V_O\}$ for Ret^T
Line 1i: `NCI, NLSI, NTNI`
Line 2i: `NCI` repetitions of $\{b, V_{SE}, V_{TE}, V_{SO}, V_{TO}\}$ for Imt^C
Line 3i: `NLSI` repetitions of $\{b, V_E, V_O\}$ for Imt^{LS}
Line 4i: `NTNI` repetitions of $\{b, V_E, V_O\}$ for Imt^T

9.5.2. `NFORCE ='G'`

This option uses G-matrix parameters from a file with a generic format. Two lines of input are required.

Line 6 `(A)` :	Name of file containing input parameters
Line 7 `(*)` :	Desired energy.

If the desired energy is not among those tabulated, a warning message is issued and the tabulated energy nearest is used.

The Yukawa expansions for the `'G'` option have the form

$$\tilde{V}(q) = \sum_{n=1}^{N} V_n \frac{e^{-m_n r}}{m_n r} \tag{186}$$

where m_n is a "mass" parameter equal to the inverse of the Yukawa range. The radial function is expressed in dimensionless form. Similar expression are used for spin-orbit and tensor interactions.

G-matrix files should be prepared with the following format. The first line is an 80 character title identifying the interaction in the `LEA` printed output. The next two lines must be present, but are skipped by the program, and may contain additional descriptive information. Each tabulated energy needs a block of input, separated from other blocks by two blank lines. The first line within each block carries the laboratory projectile energy in MeV. The next line specifies the number of densities tabulated for the central interaction. Next, we read {k_F, `NCR`, `NCI`} where k_F is the Fermi momentum, `NCR` is the numbers of terms in the expansion of the real part, and `NCI` is the number of terms for the imaginary part. The next `NCR` lines contain the mass parameter and the strength parameters for Ret^C in the order {SO, SE, TE, TO}. A similar pattern is used for Imt^C and for spin-orbit and tensor components. The format within each block is summarized below.

Line 0	Lab energy	
Line 1a	Number of densities for central interaction	
Line 2a	k_F, `NCR, NCI`	
Line 3a	`NCR` repetitions of $\{m, V_{SO}, V_{SE}, V_{TE}, V_{TO}\}$	for Ret^C
Line 4a	`NCI` repetitions of $\{m, V_{SO}, V_{SE}, V_{TE}, V_{TO}\}$	for Imt^C
Line 1b	Number of densities for spin-orbit interaction	
Line 2b	k_F, `NLSR, NLSI`	
Line 3b	`NLSR` repetitions of $\{m, V_E, V_O\}$	for Ret^{LS}
Line 4b	`NLSI` repetitions of $\{m, V_E, V_O\}$	for Imt^{LS}
Line 1c	Number of densities for tensor interaction	
Line 2c	k_F, `NTNR, NTNI`	
Line 3c	`NTNR` repetitions of $\{m, V_E, V_O\}$	for Ret^T
Line 4c	`NTNI` repetitions of $\{m, V_E, V_O\}$	for Imt^T

9.5.3. `NFORCE = 'KMT'`

The scattering matrix can be expressed in the KMT form

$$\mathcal{M} = A + B\vec{\sigma}_1 \cdot \hat{n}\vec{\sigma}_2 \cdot \hat{n} + C(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \hat{n} + E\vec{\sigma}_1 \cdot \hat{q}\vec{\sigma}_2 \cdot \hat{q} + F\vec{\sigma}_1 \cdot \hat{Q}\vec{\sigma}_2 \cdot \hat{Q} \tag{187}$$

where each amplitude has the form $A = A_0 + A_1\tau_1 \cdot \tau_2$. Amplitude arrays are read from an external file. The program will normalize the amplitudes and form appropriate linear combinations to convert $\mathcal{M}$ to pseudopotential form. Density dependence can be included by reading sets of amplitudes for several values of the Fermi momentum. Interpolation with respect to both q and k_F is performed within the input arrays, but no provision has been made for extrapolation.

The external file supplies amplitudes on the q-mesh

```
QIN(I) = Q0IN + (I-1)*DQIN
```

for I=1, NQIN. For each of NKFIN Fermi momenta, a set of isoscalar amplitudes is read first, followed by a set of isovector amplitudes. Each term is read as a single free-format record so that unneeded amplitudes can be omitted by use of the slash terminator. Note that complex variables are read in the form (real, imaginary). The structure of the external file is described below. Lines 2-12 are repeated NKFIN times.

Line 1 (*) : NQIN, DQIN, QOIN, NKFIN
Line 2 (*) : AKFIN
Lines 3–7 (*) : isoscalar amplitudes $\{A_0, B_0, C_0, E_0, F_0\}$
Lines 8–12 (*) : isovector amplitudes $\{A_1, B_1, C_1, E_1, F_1\}$.

9.5.4. NFORCE = 'TEFF'

This option permits empirical medium modifications to be applied to a free interaction. Separate parametrizations for the real and imaginary parts of any component of the effective interaction are based upon the generic function

$$t_i(q,\kappa_F) = [S - d\kappa_F^\alpha]\, t_i(q,0) + \kappa_F^\gamma q^\delta \sum_{n=1}^{N} a_n \left[1 + (\frac{q}{\mu_n})^2\right]^{-\beta} \tag{188}$$

where $\kappa_F = k_F/1.33$ and where the index i distinguishes various components. If we consider these components to be appropriate Fourier transforms of Yukawa expansions, the natural exponents β are 1 for central, 2 for spin-orbit, and 3 for tensor interactions. Similarly, we use $\delta = 2$ for tensor interactions and $\delta = 0$ otherwise. These defaults are used if input Lines 2 or 3 are terminated after N. We have found that theoretical G-matrices may be accurately reparametrized using unit scale factors $S = 1$ and exponents $\alpha = \gamma = 3$ for real parts and $\alpha = \gamma = 2$ for imaginary parts of each component.

The input structure is described below. Note that lines 1-3 are repeated NCOMP times. Separate parametrizations are read for the real part and then the imaginary part of each $\{\texttt{COMP(i)}, \texttt{i} = 1, \texttt{NCOMP}\}$, when COMP is a character label drawn from the CNAME array listed in Sec. 9. Following these parameters, the subroutine FORCEP is called upon to establish the interaction $t_i(q,0)$ upon which the parametrization is based. If this interaction is itself density dependent, the free interactions are obtained by extrapolation to zero density. Components which are not parametrized according to (*) are obtained from FORCEP.

Line 0 (*)	: NCOMP	
Line 1 (*)	: COMP	
Line 2r (*)	: $S, d, \alpha, \gamma, N, \beta, \delta$	for real part
Line 3r (*)	: $\{\mu_i, a_i, i = 1, N\}$	for real part (if N¿0)
Line 2i (*)	: $S, d, \alpha, \gamma, N, \beta, \delta$	for imag part
Line 3i (*)	: $\{\mu_i, a_i, i = 1, N\}$	for imag part (if N¿0)
Line 4 (*)	NFORCE for zero–density interaction	
Line 5	input needed for NFORCE selection	

9.5.5. `NFORCE = 'FILE'`

The input required to describe the empirical effective interaction can become rather cumbersome. When many calculations are anticipated for the same interaction model, it is sometimes more convenient to collect the interaction parameters in a single common file than to reproduce a long input section in many files. The `'FILE'` option is provided for this purpose. When invoked, the next line of input is simply a file name. The remainder the `FORCEP` input is then obtained from that file.

Line 0 `(A)`: `FILNAM`

10. OPTIONS FOR `MODE='CALC'`

10.1. General Description

After distorted waves for the initial and final channels have been calculated and stored in scratch files during the elastic scattering steps, DWA calculations can be performed for a variety of options. The available options were listed in Sec. 4.4.1 and their specific input structure is described in the subsections below. Many options require interaction or transition density information. Detailed input to the relevant subroutines are described in Secs. 7.4 and 9, respectively.

10.2. Folding Model

Folding model calculations require an effective interaction. The input is obtained from the subroutine `INITF` and is described in Sec. 9.3. The simplest situation occurs, of course, when the same interaction is used for both elastic and inelastic scattering consistently. The interaction input required at this stage then reduces to only two lines.

The folding routine loops through `NJT` values of the J-transfer `JT`. Repeated values are permitted, but `BORN` routines add these contributions incoherently. For each J-transfer, `FOLD` calls the transition density subroutine `TRDEN` described in Section VI. Scale factors that multiply the calculated scattering potentials can be useful for testing or for exploratory purposes. These factors are initialized to unity for each ΔJ and changes can be skipped by using a slash (/) to terminate input for that line. Normal-parity transitions require 9 scale factors, applied in the order

`FJC,FJ,FJD,FJL,FJS,FLS1,FLS2,FLS3,FLS4`

Abnormal-parity transitions require 5 scale factors, applied in the order

`FJS,FLS1,FLS2,FLS3,FLS4`

For detailed formulae specifying the scattering potentials, consult the `LEA` formalism report.

The input structure is listed below in schematic form. Lines 3-5 are repeated `NJT` times.

Line 1 : Obtain interaction from subroutine INITF.
Line 2 (*) : NJT = number of J-transfers.
Line 3 (*) : JT = J-transfer.
Line 4 : Obtain transition density from subroutine TRDEN.
Line 5 (*) : Scale factors for scattering potentials.

10.3. Collective Model

The collective model can be used for a single normal-parity multipole with $\Delta L = \Delta J$. Separate models can be used for the Coulomb and nuclear potentials. The multipolarity and the models are selected on Line 1.

If OPTZ='NONE', Coulomb excitation is neglected and no further input is required for that part of the potential. If OPTZ='SHELL', the δ-shell model is used for Coulomb excitation. For this choice, the radius of the shell and the Coulomb matrix element must be supplied on the next line. Alternatively, if OPTZ='FOLD', the Coulomb potential will be folded with the transition charge density, ρ_{ch}. This density is obtained from input to the subroutine TRMODEL, as described in Sec. 7.5.

Two options are available for the nuclear potential. The simplest and most consistent approach is deform the optical potential previously used for elastic scattering. This option is chosen by OPTU='DERIV' and requires two lines of input. The first specifies the deformation procedure and the second specifies the deformation lengths δ_V, δ_W, δ_{VSO}, and δ_{WSO} for each potential. Alternatively, the deformed Woods-Saxon model is chosen by OPTU='WSAX' and requires deformation parameters ($\beta's$) and Woods-Saxon parameters.

Line		restriction	variables	description
1	(*)		LT	= multipolarity
			OPTZ	= option for Coulomb potential
			OPTU	= option for nuclear potential
2a	(*)	OPTZ='SHELL'	RZ	= radius of charged shell
			ZL	= Coulomb matrix element
2b	(*)	OPTZ='FOLD'	DENMOD	= model for ρ_{ch}
2c		OPTZ='FOLD'	input for DENMOD selection	See Sec. 7.5
3a	(*)	OPTU='DERIV'	KD	= deformation type (see Sec. 2.5.1)
			RSURF	= surface radius (not reduced)
3b	(*)	OPTU='DERIV'	$\{\delta_V, \delta_W, \delta_{VSO}, \delta_{WSO}\}$	deformation lengths
3c	(*)	OPTU='WSAX'	$\{\beta_V, \beta_W, \beta_{VSO}, \beta_{WSO}\}$	deformation parameters
3d	(*)	OPTU='WSAX'	V, RV, AV	Woods-Saxon parameters
			W, RW, AW	volume absorption
			VSO, RVSO, AVSO	real spin–orbit
			WSO, RWSO, AWSO	imag spin–orbit

11. INPUT FOR MODE='TWOPOT': DWA CONTRIBUTIONS TO ELASTIC SCATTERING

This routine calculates nonspherical contributions to elastic scattering in distorted-wave approximation (DWA). The DWA scattering amplitudes are added to elastic amplitudes according to the two-potential formula. For example, the quadrupole contribution to elastic scattering from a deformed nucleus can be estimated in DWA. The results are generally comparable to, though much faster than, a coupled-channels calculation. The perturbative scattering potential can be obtained from either the folding model or from the collective model.

Line 1 (*): Option = 'FOLD' or 'COLLECTIVE'.
Line 2 (*): Folding model option.

The input for the folding model was described in Sec. 10.2 and for the collective model in Sec. 10.3.

12. INPUT FOR LINEAR EXPANSION OPTIONS

12.1. General Description

The fitting and grid routines described in Sec. 5 all require reaction model input from one or more secondary input files assigned sequentially to logical unit number LUN5. This information is used to direct the construction of files containing overlap integrals for each basis function of a linear expansion. These overlap integrals are constructed by subroutines with names of the form AMPx where x distinguishes the various models. The subroutine MAKEX then reads the file of overlap integrals and produces a file of X-amplitudes in the manner outlined in Sec. ??.

Among the FITMOD choices listed below, {G,N, D, and P} fall in this category. Other choices of FITMOD pass through the generic fitting routine NAFIT, which does not interpret the fitted parameters in as much detail as the FITx routines. However, the choices {S, T, and Y} have not been used recently and have been disabled in the present version.

FITMOD	x	interpretation
'TEFF	G	empirical effective interaction
'NEUTRON'	N	neutron transition density
'DENSITY'	D	general transition density model
'PEREY'	P	Perey factor
'SHELL'	S	spectroscopic amplitudes
'YUKAWA'	Y	Yukawa expansion of free interaction
'TFACTOR'	T	linear density dependence

Each of these routines begins by initializing the reaction, kinematics, ground–state density, optical potentials, and distorted waves. The common input for this initialization phase is outlined below, with references to the sections which describe the details. Note that the exit optical potential is not needed for elastic scattering. The subsequent input varies with the choice of FITMOD and is described in the following subsections.

step	description	subroutine	section
1	initialization of DWA calculation	INITDW	Sec. 6.1
2	ground–state densities	GSDEN	Sec. 7.2
3	self–consistent wave number	SCWK	Sec. 6.6
4	incident optical potential	OPTN	Sec. 8
5	exit optical potential	OPTN	Sec. 8
6	FITMOD dependent input	AMPx	below

12.2. Input to AMPG: Empirical Effective Interaction

The input needed for AMPG is described below. In principle, items 6b abd 6c are repeated NJT times, but even though NJT is presently limited to a single angular momentum transfer, it is read anyway.

6a NJT number of J–transfers
6b JT J–transfer
6c transition densities from TRDEN, Sec. 7.4

12.3. Input to AMPN: Neutron Transition Density

The subroutine AMPN governs the formation of an amplitude file for fitting neutron matter densities to inelastic scattering data. The first item of input is the interaction model, as described by subroutine INITF. The expansion begins with a term representing the proton transition density alone. This term requires the input:

Line 3	:	Input to INITF (see Section VIII.C)
Line 4 (*)	:	MODELP = model for proton transition density
		FORMFF = governs unfolding of proton form factor
Line 5	:	Input required by MODELP.

A detailed description of the options for densities may be found in Sec.VI.E.1. Note that only parametrized densities are permitted here.

The second term of the model represents a neutron density equal to the proton density just described. These first two terms can then be used for scale factor analyses which fit a proportionality factor between ρ_n and ρ_p. No input is needed for this term.

The remaining NTERMS of the model represent a linear expansion of ρ_n, with ρ_p set to zero. The information needed for these terms has already been obtained from INITDEN. Therefore, AMPD will produce an amplitude file with NTERMS+2 entries.

12.4. Input to AMPD: General Transition Density

The subroutine AMPD governs the formation of amplitude files for arbitrary transition densities and hence is more general than AMPN. Also, it is often desirable to represent fixed components of the structure model as independent terms in the expansion. Hence, we provide for two sets of input. First, the subroutine TRDEN can be used to generate NSET1 independent sets of overlap integrals. These terms may represent different J-transfers, for example. Then NSET2 independent transition densities can each be expanded in different radial bases. Hence, the set of Lines 4-5 is repeated NSET1 times and the set of Lines 6-9 is repeated NSET2 times. If either NSET1 or NSET2 is zero, the corresponding input is omitted.

Line 3 (*) NSET1, NSET2
Line 4 (*) J-transfer
Line 5 input to TRDEN (refer to Sec. VI for details)
Line 6 (*) J-transfer
Line 7 (*) DENNAM, ISOMOD
Line 8 (*) DENMOD
Line 9a (*) PGE $\Longrightarrow$ NTERMS, α
Line 9b (*) LGE $\Longrightarrow$ NTERMS, b
Line 9c (*) FBE $\Longrightarrow$ NTERMS, $R_{\max}$

For normal-parity transitions, DENNAM, the density to be expanded, can be chosen from the list {RJ, RSJ, RJD, RLS, RLSJ1, RLSJ2, RLSJ3} where the variable names are interpreted in Ref. ??. For abnormal parity, DENNAM can be selected from the list {RSJLL, RSJLU, RLJLL, RLJLU}. The isospin mode ISOMOD can assume the values 'ISOSCALAR', 'ISOVECTOR', 'PROTON', or 'NEUTRON'. The radial expansions DENMOD presently available are {'PGE', 'LGE', 'FBE'}. The total number of sets of overlap integrals written to disk is then

$$\mathtt{NAMP} = \mathtt{NSET1} + \sum_{\mathtt{i}=1}^{\mathtt{NSET2}} \mathtt{NTERMS(i)} \tag{189}$$

12.5. Input to AMPP: Perey Factor

The subroutine AMPP produces amplitudes that can be used to model a damping factor similar in spirit to the Perey factor. The factor

$$P(\rho) = \sum_{n=0}^{N-1} a_n \left(\frac{\rho}{0.16}\right)^n \tag{190}$$

is used to modify the scattering potential. First, the subroutine INITF is used to initialize the interaction. Next, we read the number of terms N in the Perey expansion. Then, the subroutine TRDEN is used to initialize the transition density. Note, that AMPP is presently restricted to normal-parity excitations of a spinless target.

Line 3 : Input to INITF (see Section VIII)
Line 4 (*) : N
Line 5 : Input to TRDEN (see Section VI).

12.6. Input to AMPY: Yukawa Expansion of Free Interaction

The subroutine AMPY produces amplitudes which can be used to seek density-independent modifications to the t-matrix. Corrections to each of the four interactions { Ret_{00}^C, Imt_{00}^C,

Ret_0^{LS}, Imt_0^{LS} } are represented by a delta function plus two Yukawa terms. The functional forms are

$$V^Z = S^Z V_0^Z \tag{191}$$
$$t^C = S^C t_0^C + 4\pi \left[(A_0^C + iB_0^C) + (A_1^C + iB_1^C) Y^C(\frac{q}{\mu_1}) + (A_2^C + iB_2^C) Y^C(\frac{q}{\mu_2}) \right] \tag{192}$$
$$\tau^{LS} = S^{LS} \tau_0^{LS} + 2\pi \left[(A_0^{LS} + iB_0^{LS}) + (A_1^{LS} + iB_1^{LS}) Y^{LS}(\frac{q}{\mu_3}) + (A_2^{LS} + iB_2^{LS}) Y^{LS}(\frac{q}{\mu_4}) \right] \tag{193}$$

where

$$Y^C(x) = (1 + x^2)^{-1} \tag{194}$$
$$Y^{LS}(x) = (1 + x^2)^{-1} \tag{195}$$

and where V_0^Z, t_0^C, and τ_0^{LS} are Coulomb, central, and spin-orbit contributions to the t-matrix for isoscalar normal-parity transitions. Fifteen sets of overlaps are written to the amplitude file in the order S^Z, S^C, A_0^C, B_0^C, A_1^C, B_1^C, A_2^C, B_2^C, S^{LS}, A_0^{LS}, B_0^{LS}, A_1^{LS}, B_1^{LS}, A_2^{LS}, B_2^{LS}.

The routine begins by initializing the interaction via subroutine `INITF`. It then reads two central Yukawa ranges followed by two spin-orbit Yukawa ranges. Finally, the transition density is obtained from subroutine `TRDEN`.

Line 3: Input to `INITF` (see Section VIII)
Line 4: $\{\mu_i\}$.
Line 5: Input to `TRDEN` (see Section VI).

12.7. Input to `AMPT`: Linear Density Dependence

Another useful way to model density-dependent modifications of the effective interaction is to apply separate correction factors to each of the four interaction components { Ret_{00}^C, Imt_{00}^C, Ret_0^{LS}, Imt_0^{LS}}, assuming that these factors are linear in the local density. Hence, we modify component i according to

$$t_i(q, k_F) = \left(a + b(k_F/1.33)^3\right) * t_i(q, 0). \tag{196}$$

Note that if the rearrangement factor is requested, the coefficient of b is effectively doubled.

The routine begins by initializing the t-matrix via `INITF`. The transition density is then established by `TRDEN`. Overlap integrals are written for 9 terms, beginning with Coulomb excitation and then cycling through a and b for each of the four interactions in the order prescribed.

Line 3: Input to `INITF` (see Section VIII)
Line 4: Input to `TRDEN` (see Section VI).

13. INPUT TO PWEE: PLANE-WAVE (E, E')

Although electron scattering form factors are printed during the course of most calculations of nucleon scattering, it is sometimes useful to calculate these form factors without the added burden of nucleon scattering. The choice `MODE='ESCAT'` provides this opportunity.

The subroutine `PWEE` calculates longitudinal and transverse form factors for `NJT` values of the J-transfer `JT`. `PWEE` will also compute total form factors for `NEE` laboratory angles. For each multipole, the separated form factors and the form factors for each angle are written into a plot file `PLTFIL` for later processing by graphics programs.

Line 1 (A) `PLTFIL`
Line 2 (*) description of transition using subroutine `READST`
Line 3 (*) `RMAX, DR`
Line 4 (*) `NQB, DQB`
Line 5 (*) `KCOM, KTM, DEFALPHA`
Line 6 (*) `NEE` = number of angles (repetitions of Line 7)
Line 7 (*) `EEANG` = angle for total form factor
`FFLABL` = label used within `PLTFIL` for this angle
Line 8 (*) `NJT` = number of multipoles (repetitions of Lines 9-10)
Line 9 (*) `JT` = J-transfer
Line 10 (*) transition density using subroutine `TRDEN`

14. INITIALIZATION OF COUPLED-CHANNELS CALCULATIONS USING INITCC

Many of the input items have already been explained in earlier sections. See Sec. 6.1 for additional information about many of the items on Lines 6 – 13 and Sec. 4.3.4 for an explanation of Line 16. If `OPTIONS='NONE'` or `OPTIONS=' '`, the kinematics options are read from Line 2 using the format described in Sec. 6.2; otherwise that information is obtained from the specified file and Line 2 is omitted. The laboratory kinetic energy is included on Line 6 for `MODE='SPECTD'` or `MODE='TRANSP'`, but is omitted for other choices of `MODE`, whereas the other items should always be present. To minimize the variation among similar input sections, some items are read by `INITCC` that may not be actually be used. For example, acceptance averaging parameters are read even though acceptance averaging has not yet been implemented for coupled-channels calculations. Similary, Lines 9 and 13 are read but ignored. Thus, much of the input for these types of calculations remains quite similar to the input for single–shot calculations, as described in Sec. 4.4.1.

Lines 15 – 20 are repeated for each channel. Note that if the file name for optical potential input is `SAME` (without quotes because `(A)` format is used), the current optical potential will be the same as the last.

Three types of coupled-channels models are presently available. If `CCMODEL='SRM'`, all channels are assumed to belong to the ground–state rotational band of a symmetric rotor; the input required on Line 4 to specify the deformation parameters is described in Sec. 14.1 and no further input is needed on Line 21. If `CCMODEL='VIB1'`, all channels are assumed to belong to a vibrational system; the input required on Line 4 to specify the phonon properties is described in Sec. 14.2 and no further input is needed on Line 21. Otherwise, CCMODEL='MICROSCOPIC' requires input for each coupling potential to be described at the location reserved by Line 21 in the primary input file (LUN1). This input describes the coupling scheme includes file names for secondary input files (LUN5) containing the detailed input for each coupling potential. At present the coupling potentials may be obtained either from the folding model for nucleon–nucleus scattering or from collective models, as described in Sec. 14.4.

1	(A) OPTIONS	file name for interaction options
2	(*)	kinematics options if OPTIONS='NONE'
3	(*) CCMODEL	coupled-channels model
4		input needed for CCMODEL selection
5	(*) METHOD(I), I=1,6	6 character variables specifying numerical methods
6	(*) TLAB	lab kinetic energy (read ONLY for MODE='SPECTD' or MODE='TRANSP'
	LMAX	maximum angular momentum
	NSTATE	number of coupled channels
	NPASS	maximum number of iterations
	CCONV	convergence criterion
7	(*) RMAX, DR, RZMAX	radial mesh parameters
8	(*) NQF, LQ	mesh parameters for folding model
9	(*) NQB, DQB	mesh parameters for Born calculations
10	(*) NTH, DTH, THO	angular mesh
11	(*) NXTRA, DTHETAO, DPHIO	mesh for acceptance averaging (not implemented)
12	(*) CPRNTF, CPRNTR, CPRNTQ, CPRNTP, CPRNTO	print options
13	(*) CBORN1, CFOLD, CBORN2, CDWBA, CPART	calculation options
14	(*) CPLTEL, CPLTB1, CPLTB2, CPLTU, CPLTDW	plot options
15	(*) STATE	state label
16	(*) PZI, PMI, TZI, TMI, ITI, IPARI, EXC	state description
17	(*) NPHONON	number of phonons (only for CCMODEL='VIB1')
18	(*) LPHONON(I), I=1,NPHONON	phonon multipolarities (only for CCMODEL='VIB1')
19	(A) FILNAM	file name for optical model input
20	(A) POTFIL	plot file for potentials, if CPLTU='PLOT U'
21		input needed for CCMODEL selection

14.1. Input for CCMODEL='SRM': symmetric rotor model

The multipole potentials for the symmetric rotor model are obtained from deformed optical potentials by Legendre projection, according to Eq. (75). The maximum λ used in the Legendre projection, LAMMAX, determines the largest possible J–transfer and may be greater than the maximum ℓ used in the deformation of the optical potential. The deformation of each component of the optical potential is performed according to Eq. (37), but several variations are available. If DEFMODE='UNIFORM', all potentials are assumed to share a common set of deformation parameters, BETAO(I), I=1,NBETA, entered on a single instance of Line 4c. Note that only even multipoles are considered, so that β_ℓ =BETAO(I) with ℓ =2*I. The deformation of the Coulomb potential may be omitted by choosing CDEFORMZ = 'NO DEFORM

Z' (or, in fact, anything other than 'DEFORM Z'). If DEFMODE='GENERAL', each potential is permitted to have independent deformation parameters, in which case Line 4c is repeated for U^Z, ReU^C, ImU^C, ReU^{LS}, and ImU^{LS}. Note that in this case a line is read for U^Z even if CDEFORMZ = 'NO DEFORM Z'.

Two additional DEFMODE options are available when the optical potential is represented by a Woods-Saxon parameterization. If DEFMODE='BETA', each potential shares a common BETA0 array, but the radius used to deform each potential is taken from the Woods-Saxon parametrization, and hence may be different for each. If DEFMODE='DELTA', the β_ℓ used for each term is adjusted so that every term as the same deformation length $\delta_e ll = \beta_\ell R$ as the real central component. Both of these options require only a single instance of Line 4c.

4a	K0	= intrinsic angular momentum projected on symmetry axis
	KD	= deformation exponent K in Eq. (37)
	RSURF	= surface radius R in Eq. (37)
	DEFMODE	= deformation mode
	CDEFORMZ	= 'DEFORM Z' $\Longrightarrow$ deformed Coulomb poential
4b	NBETA	= number of deformation parameters
	LAMMAX	= maximum λ in Legendre projection
4c	BETA0(I), I=1,NBETA	= deformation parameters for ℓ =2*I

14.2. Input for CCMODEL='VIB1': single–phonon vibrational model

Line 4c is repeated for each of NBETA multipolarities.

4a	KD	= deformation exponent K in Eq. (37)
	RSURF	= surface radius R in Eq. (37)
4b	NBETA	= number of deformation parameters
	LAMMAX	= maximum ℓ in deformation, Eq. (37)
4c	LBETA	= phonon multipolarity
	BETAL	= deformation parameter

14.3. Optical model input for coupled channels

The optical model input for each channel is read from a secondary input file. The input is similar to that needed for other modes, and hence can be described in schematic form with references to appropriate sections.

line	variable	description	section
Line 1		input to GSDEN	Sec. 7.2
Line 2		input to SCWK	Sec. 6.6
Line 3 (*)	OPTMOD	optical potential option	Sec. 8
	ZMODE	Coulomb potential option	
	CPEREY	Perey factor option	
Line 4		input needed for ZMODE selection	Sec. 8.2
Line 5		input needed for OPTMOD selection	Sec. 8.1
Line 6		input needed for CKMASS option	Sec. 6.5
Line 7		input needed for CPEREY option	Sec. 6.4

14.4. Input for CCMODEL='MICROSCOPIC': microscopic coupled channels

Microscopic coupled-channels calculations require coupling potentials to be constructed for every pair of states that can be connected by a one–body operator based upon the nucleon–nucleon interaction. Since time–reversal symmetries relate forward and backward amplitudes, for any particular state it is sufficient to specify the transition potentials from any state described previously in the input stream. The current state is treated as a final state and the previous state as the initial state. Therefore, if there are NSTATE channels there will be NSTATE blocks of input. The first block specifies the spherical optical potential and the nonspherical elastic potentials (if needed) for the first channel. The second block specifies the spherical optical potential for the second state, the nonspherical elastic potentials for the second state (if needed), and the coupling between the first and second states. The third block specifies the spherical optical potential for the third state, the nonspherical elastic potentials for the third state (if needed), the coupling between the first and third states, and the coupling between the second and third states. Continuing that pattern, the n^{th} block specifies the spherical optical potential and nonspherical elastic potentials for the n^{th} state and up to $n(n-1)/2$ transition potentials. Note that the convergence may be optimized by arranging the channels in order of importance, with stronger channels appearing before weaker channels.

Each block of input, read from the primary input file (LUN1), has the following structure. These lines are repeated until ISTATE='END' is encountered. The current state is considered a final state with label FSTATE. If ISTATE=FSTATE, the transition potential describes non-spherical elastic potentials, sometimes called reorientation potentials. Other couplings are interpreted as inelastic or charge exchange reactions. States whose couplings are negligible may be omitted. Note that if ISTATE does not correspond to an earlier state a termination conditions occurs.

21a (A) ISTATE state label for a prior (initial) state
21b (A) FILNAM name of file for transition potential input
21c (A) FILNAM name of file for transition potential output

Each pair of coupled channels requires a set of transition potentials that might include several transition operators for each of several J-transfers. A separate pair of secondary input and output files, LUN5 and LUN6, is used for each set of transition potentials. Each secondary input file has the structure outlined below. Note that since we anticipate eventual inclusion of transfer reactions, the integer variable JT is interpreted as twice the J-transfer for the transition. At present two types of transition potential are available. If OPTION='FOLD' the folding model for nucleon–nucleus scattering is employed. If OPTION='DEFORM', collective model potentials are used with Coulomb and nuclear options restricted to OPTZ='SHELL' and OPTU='DERIV' as described in Sec. 10.3.

1 (*) NJT = number of J-transfers
2 (*) JT = twice the J-transfer
3 (*) OPTION = type of potential
4a transition density input from Sec. 7.4
4b folding model input from Sec. 10.2
5a Coulomb deformation input from Line 2a of Sec. 10.3
5b Nuclear deformation input from Lines 3a–3b of Sec. 10.3

15. PSEUDODATA ANALYSIS

Before DWZR and NAFIT were merged into the the integrated LEA package, extensive facilities existed for study the intrinsic sensitivity of a hypothetical data set to the parameters of a model using pseudodata. For example, analysis of pseudodata produced from a known structure model was used to study the sensitivity of proton scattering the neutron transition density, particularly in the interior of the nucleus. However, these facilities have not been used since reorganization of the programs. Therefore, the functionality of these facilities is not known and inexperienced users are discouraged from attempting pseudodata analyses with the present version of LEA. Documentation will be provided when these facilities are restored in a later release.

16. IMPLEMENTATION NOTES

At the University of Maryland the LEA program has been run on both VMS and Unix systems; hence, it should be relatively easy to implement the program on other machines of these types. To compile the sources, the user will have to define a logical name LEA$DIR identifying the location of the include files *.INC. To link the object, it is necessary to use a parameter file with the line ISD_MAX=200. Otherwise, the image will become unreasonably large. Finally, most users will find it necessary to increase the limits on numbers of open files and working sets. For efficient operation on VAXstations, a minimum of 16 MB of memory and a quota of WSEXTENT=6144 is needed. Otherwise, the page-fault rate will become very large for fitting applications.

To compile the sources on other machines, it will be necessary to replace the compiler directives (INCLUDE ...) either with corresponding statements or with the contents of the include files themselves.

The basic distribution package includes the following files.

LEA.FOR	executive main program
LEALIB.FOR	source codes for LEA_LIB
NUCLEON.FOR	source codes for NUCLEON_LIB
NAFIT.FOR	source codes for NAFIT_LIB
JJKLIB.FOR	source codes for JJKLIB
GENERAL.INC	include file containing general parameters and common blocks
NUCLEON.INC	include file containing nucleon scattering information
NAFIT.INC	include file containing fitting parameters and data
DENSITY.INC	include file containing transition density information
PION.INC	include file with skeletal information for future pion code
FL85.DAT	Franey-Love t-matrix
PARIS.G	Paris-Hamburg G-matrix
PARIS.T	Paris-Hamburg t-matrix (Fermi averaging but no Pauli blocking)
NL88.G	Nakayama-Love G-matrix
9BE5M1.INP	sample Born test file
16O1M1.INP	sample LDA calculation

	Sample files for fitting effective interaction
F16O.COM	command file for interaction fit
F16O.INP	input file for interaction fit
TEFF.INP	options file for interaction fit
16O.135	data file
X16O1M1.INP	input files for create X-amplitudes
X16O2P1.INP	
X16O2P3.INP	
X16O3M1.INP	
X16O4P1.INP	
	Sample files for fitting neutron transition density
F2P1.INP	input file for density fit
X2P1.INP	input file for construction of amplitudes
TEFF.135	interaction file
18O.2P1	data file

17. SAMPLE INPUT FILES

Several sample input files are listed below.

17.0.1. Sample $^{16}O(p,p')1_1^-$ *Calculation*

The first sample directs a simple LDA calculation for the 1_1^- state ^{16}O using the Paris-Hamburg G-matrix, consistent distorted waves, and transition densities deduced from electro-excitation measurements.

```
    Sample calculation for 16-O(p,p')1- at 135 MeV

'CALC'
IN:TEFF.135

'16O.0P1'
 1. 1. 1 8. 16. 0 +1
'16O.1M1'
 1. 1. 1 8. 16. 2 -1 -7.117
 135. 30
 12. .1 8.5
 50 2
 50 .1
150 0.75 1.
 0 0.0 0.0

 'NO-CM'  1 .56
 'PRINT F' 'PRINT R' 'PRINT Q' 'PRINT P' 'NO PRINT O'
```

```
 'NO BORN1' 'FOLD' 'NO BORN2' 'DWBA' 'NO PARTIAL'
 'PLOT EL' 'NO PLOT B1' 'NO PLOT B2' 'NO PLOT U' 'PLOT DW'
OU:1601M1.PLT

'ISO'
'FBE-CH' 'NO FOLD'
 13, 8.0
  0.20238E-1  0.44793E-1  0.33533E-1  0.35030E-2 -0.12293E-1
 -0.10329E-1 -0.34036E-2 -0.41627E-3 -0.94435E-3 -0.25771E-3
  0.23759E-3 -0.10603E-3  0.41480E-4
'NONE' 'NO FOLD'

'FOLD' 'FOLD' 'NO PEREY'
/
'SAME' /

'FOLD'
 1
 1
'P-N'
'RJ'
'LGE' 'UNFOLD'
 8 1.8
 619.386E-4 136.488E-4 -57.730E-4 2.520E-4
   2.033E-4   1.693E-4  -1.839E-4 0.582E-4
'LGE' 'UNFOLD'
 8 1.8
 619.386E-4 136.488E-4 -57.730E-4 2.520E-4
   2.033E-4   1.693E-4  -1.839E-4 0.582E-4
/
/
/
```

17.0.2. Sample $^9Be(p,p')\frac{5}{2}^-_1$ Calculation

The second input file directs Born approximation calculations for the $\frac{5}{2}^-_1$ state of ^{9}Be based on Cohen-Kurath wave functions. Three calculations are compared. The `BORN1` calculation uses analytic formulae that neglect density dependence. The `BORN2` calculation uses Fourier transforms of the scattering potentials including density dependence. Finally, the `DWBA` calculations without distorting potentials should give results virtually identical to the `BORN2` calculation. Therefore, this input file provides a stringent test of internal consistency. All three methods are compared with a single input file.

```
  Born approx. tests for 9-Be(p,p')5- at 180 MeV
```

```
'CALC'
NONE

'9BE.3M1'
 1. 1. 1 4. 9. 3 -1
'9BE.5M1'
 1. 1. 1 4. 9. 5 -1 0.0
 180. 30
 12. .1 8.5
 50 2
 50 .1
 90 0. 1.
  0 0. 0.

 'BORN' 'A-WN' 'DW79'  'NO DLAB'  'NO WIGNER' /
 'C-O-M'  1 .567
 'PRINT F' 'PRINT R' 'PRINT Q' 'PRINT P' 'NO PRINT O'
 'BORN1' 'FOLD' 'BORN2' 'DWBA' 'PARTIAL'
 'NO PLOT EL' 'PLOT B1' 'PLOT B2' 'NO PLOT U' 'PLOT DW'
OU:9BE5M1.PLT
OU:9BE5M1.B1
OU:9BE5M1.B2

'ISO'
'MHO' 'UNFOLD'
 1.788 0.62
'MHO' 'UNFOLD'
 1.788 0.62

'NONE' 'NONE' 'NO PEREY'
'SAME' /

'FOLD' 'FOLD'
'LF'
'Q-FOLD' 'D+E' 'ZREA' 'A-WN' 'NO DD' 'NO PRINT' /
FORCES:FL85.DAT
180.
'NO COULX' 'NO CHEON'
 3

 1
'SHELL'
 'Z' 'HO'
 1 1
```

```
'C-O-M' 0.567 'NONE'
 '1P1 ' '1P1 ' 1 -.06573 -.02369 'P-N' 0.
 '1P1 ' '1P3 ' 1  .05896  .11469 'P-N' 0.
 '1P3 ' '1P1 ' 1 -.06496  .10931 'P-N' 0.
 '1P3 ' '1P3 ' 1 -.14208  .17012 'P-N' 0.
 'END' /
/
/
/

 2
'SHELL'
 'Z' 'HO'
 1 1
'C-O-M' 0.567 'NONE'
 '1P1 ' '1P3 ' 2  .24960  .38775 'P-N' 0.
 '1P3 ' '1P1 ' 2 -.23333 -.29015 'P-N' 0.
 '1P3 ' '1P3 ' 2 -.07062 -.34812 'P-N' 0.
 'END' /
 1.6 1. 1.6 1.6 /
 0.7 1. 0.7 0.7 /
/

 3
'SHELL'
 'Z' 'HO'
 1 1
'C-O-M' 0.567 'NONE'
 '1P3 ' '1P3 ' 3  .01805 -.14721 'P-N' 0.
 'END' /
/
/
/
```

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