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MOMDIS: a Glauber model computer code for knockout reactions ☆

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Abstract

A computer program is described to calculate momentum distributions in stripping and diffraction dissociation reactions. A Glauber model is used with the scattering wavefunctions calculated in the eikonal approximation. The program is appropriate for knockout reactions at intermediate energy collisions (30 MeV $\leqslant E_{\rm lab}$/nucleon $\leqslant$ 2000 MeV). It is particularly useful for reactions involving unstable nuclear beams, or exotic nuclei (e.g., neutron-rich nuclei), and studies of single-particle occupancy probabilities (spectroscopic factors) and other related physical observables. Such studies are an essential part of the scientific program of radioactive beam facilities, as in for instance the proposed RIA (Rare Isotope Accelerator) facility in the US.

Program summary

Title of program: MOMDIS (MOMentum DIStributions)
Catalogue identifier: ADXZ_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADXZ_v1_0
Computers: The code has been created on an IBM-PC, but also runs on UNIX or LINUX machines
Operating systems: WINDOWS or UNIX
Program language used: Fortran-77
Memory required to execute with typical data: 16 Mbytes of RAM memory and 2 MB of hard disk space
No. of lines in distributed program, including test data, etc.: 6255
No. of bytes in distributed program, including test data, etc.: 63 568
Distribution format: tar.gz
Nature of physical problem: The program calculates bound wavefunctions, eikonal S-matrices, total cross-sections and momentum distributions of interest in nuclear knockout reactions at intermediate energies.
Method of solution: Solves the radial Schrödinger equation for bound states. A Numerov integration is used outwardly and inwardly and a matching at the nuclear surface is done to obtain the energy and the bound state wavefunction with good accuracy. The S-matrices are obtained using eikonal wavefunctions and the "t-$\rho\rho$" method to obtain the eikonal phase-shifts. The momentum distributions are obtained by means of a Gaussian expansion of integrands. Main integrals are performed with the Simpson's method.
Typical running time: Almost all CPU time is consumed by calculations of integrals, specially for transverse momentum distributions which involves multiple integral loops. It takes up to 30 min on a 2 GHz Intel P4-processor machine.

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Keywords: Direct reactions; Momentum distributions; Unstable nuclear beams; Breakup; Stripping; Diffraction dissociation

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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[1] "Neutron saturated nuclei are the closest one can get to having a neutron star in the laboratory. The study of drip-line nuclei has progressed remarkably by observing nuclear reactions caused by radioactive fragments." P. Gregers Hansen, Nature 334 (1988) 194.

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1. Introduction

Single-nucleon knockout reactions with heavy ions, at intermediate energies and in inverse kinematics, have become a specific and quantitative tool for studying single-particle occupancies and correlation effects in the nuclear shell model [1]. The high sensitivity of the method has allowed measurements on rare radioactive species available in intensities of less than one atom per second for the incident beam. The experiments observe reactions in which fast, mass A, projectiles collide peripherally with a light nuclear target, typically ^{9}Be or ^{12}C, producing residues with mass $(A-1)$, in the following referred to as the core (c) of the assumed two-body system of core plus nucleon. The final state of the target and that of the struck nucleon are not observed, but instead the energy of the final state of the residue can be identified by measuring coincidences with decay gamma-rays emitted in flight. Referred to the center-of-mass system of the projectile, the transferred momentum is $\mathbf{k}_c$. In the sudden approximation and for the stripping reaction, defined below, this must equal the momentum of the struck nucleon before the collision. The measured partial cross-sections to individual final levels provide spectroscopic factors for the individual angular-momentum components j. In complete analogy to the use of angular distributions in transfer reactions, the orbital angular momentum l is in the knockout reactions revealed by the distributions of the quantity $\mathbf{k}_c$.

The early interest in momentum distributions came from studies of nuclear halo states, for which the narrow momentum distributions in a qualitative way revealed the large spatial extension of the halo wave function [2]. It was shown by Bertulani and McVoy [3] that the longitudinal component of the momentum (taken along the beam or z-direction) gave the most accurate information on the intrinsic properties of the halo and that it was insensitive to details of the collision and the size of the target. In contrast to this, the transverse distributions of the core are significantly broadened by diffractive effects and by Coulomb scattering. For experiments that observe the nucleon produced in elastic breakup, the transverse momentum is entirely dominated by diffractive effects, as illustrated [4] by the angular distribution of the neutrons from the reaction ^{9}Be(^{11}Be, ^{10}Be + n)X. In this case, the width of the transverse momentum distribution reflects essentially the size of the target.

The cross-section for the production of a given final state of the residue has two contributions. The most important of the two, commonly referred to as stripping or inelastic breakup, represents all events in which the removed nucleon reacts with and excites the target from its ground state. The second component, called diffractive or elastic breakup [5], represents the dissociation of the nucleon from the residue through their two-body interactions with the target, each being at most elastically scattered. These events result in the removed nucleon being present in the forward beam with essentially the beam velocity, and the target remaining in its ground state. These processes lead to different final states, they are incoherent, and their cross-sections must be added in measurements where only the residue is observed. General expressions for the total and differential cross-sections for the two components have been given by Hussein and McVoy [6] and further developed by other authors in studies of reactions with halo nuclei (see, e.g., Ref. [7]).

In a subsequent development, the knockout method was extended to non-halo states [8–15]. For these, involving more deeply-bound nucleons, the one-nucleon absorption cross-sections are much smaller than the free-nucleon reaction cross-section on the same target; a ratio that gives a measure of how much the nucleon wave function is "shielded" from the target by the bulk of the core. This required a more elaborate theoretical treatment based on the elastic S-matrices S_c and S_n [16, 17] of the core and nucleon. Other advanced theoretical treatments by Bonaccorso and collaborators [18–20] have shown the relevance of transfer to the continuum in eikonal methods for stripping and diffraction dissociation.

The code described in this article is based on the work presented in Ref. [21] and on previous works, as those mentioned above. The code calculates single-particle bound state wavefunctions and eikonal S-matrices. Using these wavefunctions and S-matrices, one obtains single-particle cross-sections after integration over momentum and summation over the m_l substates. As shown in Ref. [21], the use of this code demonstrates (i) that the transverse momentum distributions are quantitatively and even qualitatively different from the parallel momentum distributions, and (ii) can serve to extract angular-momentum information from the angular distributions of the residues. The code is also of importance for calculating acceptance corrections in experiments, and one can evaluate the correlations between longitudinal and radial components [21].

2. Bound states

The computer code MOMDIS calculates various quantities of interest for knockout reactions of the type

$$(c+v)+T \to c+X. \tag{1}$$

The internal structure of nucleus c, the valence particle v and of the target T is not taken into account. The initial state of the projectile nucleus $P = c + v$ is obtained by the solution of the Schrödinger equation for the relative motion of c and v in a nuclear + Coulomb potential. Particles c, v, and P have intrinsic spins labeled by I_c, I_v and J, respectively. The corresponding magnetic substates are labeled by M_c, M_v and M. The orbital angular momentum for the relative motion of $c + v$ is described by l and m. In most situations of interest, particle v is a nucleon and c is a "core" nucleus. Thus it is convenient to couple angular momenta as $\mathbf{l}+\mathbf{I}_v = \mathbf{j}$ and $\mathbf{j}+\mathbf{I}_c = \mathbf{J}$, where $\mathbf{J}$ is the channel spin. Below we also use the notation $\mathbf{s}$, instead of $\mathbf{I}_v$, for the intrinsic spin of particle v.

The bound state wavefunctions of P are specified by

$$\Psi_{JM}(\mathbf{r}) = R^J_{lj}(r)\mathcal{Y}^l_{JM} = \frac{u^J_{lj}(r)}{r}\mathcal{Y}^l_{JM}, \tag{2}$$

where r is the relative coordinate of c and v, $u^J_{lj}(r)$ is the radial wavefunction and $\mathcal{Y}^l_{JM}$ is the spin-angle wavefunction

$$\mathcal{Y}^l_{JM} = \sum_{m,M_c} \langle jmI_cM_c|JM\rangle |jm\rangle |I_cM_c\rangle,$$
$$\text{with } |jm\rangle = \sum_{m_l,m_s} Y_{lm_l}(\hat{\mathbf{r}})\chi_{m_s} \tag{3}$$

where χ_{m_s} is the spinor wavefunction of particle v and $\langle jmI_cM_c|JM\rangle$ is a Clebsch–Gordan coefficient.

The ground-state wavefunction is normalized so that

$$\int \mathrm{d}^3r \left|\Psi_{JM}(\mathbf{r})\right|^2 = \int_0^\infty \mathrm{d}r \left|u^J_{lj}(r)\right|^2 = 1. \tag{4}$$

The wavefunctions are calculated using a spin-orbit potential of the form

$$V(\mathbf{r}) = V_0(r) + V_S(r)\ (\mathbf{l}\cdot\mathbf{s}) + V_C(r), \tag{5}$$

where $V_0(r)$ and $V_S(r)$ are the central and spin-orbit interaction, respectively, and $V_C(r)$ is the Coulomb potential of a uniform distribution of charges:

$$V_C(r) = \begin{cases} \frac{Z_cZ_ve^2}{r} & \text{for } r > R_C, \\ \frac{Z_cZ_ve^2}{2R_C}(3 - \frac{r^2}{R_C^2}) & \text{for } r < R_C, \end{cases} \tag{6}$$

where Z_i is the charge number of nucleus $i = v, c$.

The nuclear potential is assumed to have a Woods–Saxon form plus a spin-orbit interaction,

$$V_0(r) = V_0 f_0(r), \quad \text{and}$$
$$V_S(r) = -V_{S0}\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} f_S(r)$$

with

$$f_i(r) = \left[1 + \exp\left(\frac{r - R_i}{a_i}\right)\right]^{-1}. \tag{7}$$

The spin-orbit interaction in Eq. (7) is written in terms of the pion Compton wavelength, $\hbar/m_\pi c = 1.414$ fm. The parameters V_0, V_{S0}, R_0, a_0, R_{S0}, and a_{S0} are adjusted so that the ground state energy E_B (or the energy of an excited state) is reproduced.

The bound-state wavefunctions are calculated by solving the radial Schrödinger equation

$$-\frac{\hbar^2}{2m_{ab}}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2}\right]u^J_{lj}(r) + \left[V_0(r) + V_C(r) + \langle \mathbf{s}.\mathbf{l}\rangle V_{S0}(r)\right]u^J_{lj}(r) = E_i u^J_{lj}(r), \tag{8}$$

where $\langle \mathbf{s}\cdot\mathbf{l}\rangle = [j(j+1) - l(l+1) - s(s+1)]/2$. This equation must satisfy the boundary conditions $u^J_{lj}(r=0) = u^J_{lj}(r=\infty) = 0$ which is only possible for discrete energies E corresponding to the bound states of the nuclear + Coulomb potential.

3. Unitarity, stripping and diffraction dissociation

Using eikonal waves for scattering wave functions, one gets

$$\Psi^{(-)*}(\mathbf{r})\Psi^{(+)}(\mathbf{r}) = S(b)\exp(i\,\mathbf{q}\cdot\mathbf{r}), \tag{9}$$

where $S(b)$ is the scattering matrix

$$S(b) = \exp\left[i\,\chi(b)\right], \quad \text{with } \chi(b) = -\frac{1}{\hbar \mathrm{v}}\int_{-\infty}^{\infty} \mathrm{d}z\, U_{\mathrm{opt}}(r), \tag{10}$$

and $U_{\mathrm{opt}}(\mathbf{r})$ is the appropriate optical potential for the core + target and the neutron (or proton) + target scattering. In Eq. (10) $\chi(b)$ is the eikonal phase, and $r = \sqrt{b^2 + z^2}$, where b is often interpreted as the impact parameter. This interpretation arises from a comparison of the results obtained with eikonal wavefunctions with those obtained in with classical particles colliding with a fixed impact parameter b [22]. Nonetheless, the eikonal wavefunction is a quantum scattering state and b is the transverse coordinate associated to them. Thus wave-mechanical effects, like smearing and interference, are accounted for properly.

As seen in Eq. (10), in the eikonal approximation, the phase shift is linear in the interaction. Then, according to Glauber [23], the S-matrix for $P(c+v)+T$ can be written as

$$\widehat{S}_P = \widehat{S}_v\widehat{S}_c, \tag{11}$$

where the $\widehat{S}$ is still an operator since it refers to a particle inside the projectile and this depends upon parameters that have to be averaged over by the ground state wave function of projectile, ϕ_0. The elastic breakup cross-section can be easily calculated (the observed particle is c)

$$\sigma_{\mathrm{el.bup}} = \sum_{\mathbf{k}} \left|\langle\phi_{\mathbf{k}}|\widehat{S}_v\widehat{S}_c|\phi_0\rangle\right|^2, \tag{12}$$

where $\phi_{\mathbf{k}}$ is wave function that represents the continuum of c and v. Since

$$\int |\phi_{\mathbf{k}}\rangle\langle\phi_{\mathbf{k}}|\mathrm{d}\mathbf{k} + |\phi_0\rangle\langle\phi_0| = 1,$$

the above expression can be simplified

$$\sigma_{\mathrm{el.bup}} = \int \langle\phi_0|\widehat{S}^*_v\widehat{S}^*_c|\phi_{\mathbf{k}}\rangle\langle\phi_{\mathbf{k}}|\widehat{S}_v\widehat{S}_c|\phi_0\rangle\,\mathrm{d}\mathbf{k} = \langle\phi_0|\left|\widehat{S}_v\right|^2\left|\widehat{S}_c\right|^2|\phi_0\rangle - \left|\langle\phi_0|\widehat{S}_v\widehat{S}_c|\phi_0\rangle\right|^2. \tag{13}$$

In so far as the inelastic break up is concerned, one realizes that the detected particle must reach the detector intact and thus one must use a survival probability to guarantee this. This survival probability is $|\widehat{S}_c|^2$. On the other hand, the interacting fragment v is removed (stripped) and the probability for this to happen is $(1 - |\widehat{S}_v|^2)$. Identifying the transmission coefficient T_v with $1 - |\widehat{S}_v|^2$, we can write for the inelastic break up the following expression [6]

$$\sigma_{\mathrm{in.bup}} = \frac{\pi}{k^2}\sum\langle\phi_0|\left(1 - \widehat{T}_c\right)\widehat{T}_v|\phi_0\rangle. \tag{14}$$

The above cross-section is also called the v removal cross-section with the notation σ_{-v}. Of course one may have the removal of the core (less probable owing to the Coulomb barrier between the charged core and the target)

$$\sigma_{-c} = \frac{\pi}{k^2}\sum\langle\phi_0|\left(1 - \widehat{T}_v\right)\widehat{T}_c|\phi_0\rangle. \tag{15}$$

The sum of σ_{-v} and σ_{-c} gives

$$\sigma_{-v}+\sigma_{-c}=\frac{\pi}{k^2}\sum\langle\phi_0|\widehat{T}_c+\widehat{T}_v-2\widehat{T}_v\widehat{T}_c|\phi_0\rangle. \tag{16}$$

Summing the above with the *total absorption* of P, described here by $\sigma_{-P}\equiv\sigma_{\rm abs}=(\pi/k^2)\sum\langle\phi_0|\widehat{T}_v\widehat{T}_c|\phi_0\rangle$, gives

$$\begin{aligned}&\sigma_{-v}+\sigma_{-c}+\sigma_{-P}\\&\quad=\frac{\pi}{k^2}\sum\langle\phi_0|\widehat{T}_c+\widehat{T}_v-\widehat{T}_v\widehat{T}_c|\phi_0\rangle\\&\quad=\frac{\pi}{k^2}\sum\langle\phi_0|\big(1-|S_c|^2|S_v|^2\big)|\phi_0\rangle\\&\quad=\sigma_{\rm reaction},\end{aligned} \tag{17}$$

which confirms unitarity.

The expressions for $\sigma_{\rm el.bup}$, Eq. (13), and $\sigma_{\rm in.bup}$, Eq. (14), have been used by several authors to analyze the data on halo nuclei. It has been common to call $\sigma_{\rm el.bup}=\sigma_{\rm dif}$, the *diffractive break-up* cross-section and $\sigma_{\rm in.up}=\sigma_{\rm strip}$ the *stripping* cross-section [5,9,24–27]. The cross-sections also depend on the single particle occupancy probability which can be accounted for multiplying them by spectroscopic factors S_i [1].

4. Eikonal S-matrices

In the optical limit of the Glauber theory and the "t-$\rho\rho$" approximation (explained in detail in Ref. [28]), the eikonal phase is obtained from the nuclear ground state densities and the nucleon–nucleon cross-sections by the relation [22] (here we drop the operator notation)

$$S(b)=\exp\big[i\chi(b)\big],\quad\text{with}$$
$$\chi_N(b)=\frac{1}{k_{NN}}\int_0^\infty {\rm d}q\, q\rho_p(q)\rho_t(q)f_{NN}(q)J_0(qb), \tag{18}$$

where $\rho_{p,t}(q)$ is the Fourier transform of the nuclear densities of the projectile and target, and $f_{NN}(q)$ is the high-energy nucleon–nucleon scattering amplitude at forward angles, which can be parametrized by [29]

$$f_{NN}(q)=\frac{k_{NN}}{4\pi}\sigma_{NN}(i+\alpha_{NN})\exp(-\beta_{NN}q^2). \tag{19}$$

In this equation σ_{NN}, α_{NN}, and β_{NN} are parameters which fit the high-energy nucleon–nucleon scattering at forward angles. These parameters were originally obtained for $E_N\geqslant 100$ MeV/nucleon [29]. We use an additional set of parameters which have been shown to reproduce the nucleon–nucleon scattering data in the energy region 30 MeV $\leqslant E_N\leqslant$ 2200 MeV [22]. The nucleon–nucleon amplitude $f_{NN}(q)$ which enters Eq. (18) is of course not the same as the one expressed in Eq. (19) for the free nucleon–nucleon scattering. Medium modifications (e.g., isospin average, etc.) have to be taken into account. As shown in Ref. [28], the largest medium effect is due to Pauli-blocking [30]. The code MOMDIS allows (optional) one to include Pauli blocking effects in the nucleon–nucleon cross-section σ_{NN}, according to Refs. [28,30].

In Eq. (18) the quantities $\rho_p(q)$ and $\rho_t(q)$ are calculated from the radial density distributions, usually [1] taken to be of Gaussian shapes for light nuclei, and of Fermi shapes for heavier nuclei with parameters taken from experiment. For cases where more accuracy is needed, it is possible to take the density distributions directly from Hartree–Fock calculations. A set of experimental values of density parameters was published in Ref. [31]. These are useful, in particular in parametrizing the densities of stable nuclei.

For the Coulomb part of the optical potential the integral in Eq. (10) diverges. One solves this by using $\chi=\chi_N+\chi_C$, where χ_N is given by Eq. (10) without the Coulomb potential and writing the Coulomb eikonal phase, χ_C as

$$\chi_C(b)=2\eta\ln(kb), \tag{20}$$

where $\eta=Z_pZ_te^2/\hbar{\rm v}$, Z_p and Z_t are the charges of projectile and target, respectively, v is their relative velocity, k their wavenumber in the center of mass system. Eq. (20) reproduces the exact Coulomb scattering amplitude when used in the calculation of the elastic scattering with the eikonal approximation [22]:

$$\begin{aligned}f_C(\theta)=&\frac{Z_pZ_te^2}{2\mu v^2\,\sin^2(\theta/2)}\\&\times\exp\big\{-i\eta\ln\big[\sin^2(\theta/2)\big]+i\pi+2i\phi_0\big\},\end{aligned} \tag{21}$$

where $\phi_0=\arg\Gamma(1+i\eta/2)$. This is convenient for the numerical calculations since, as shown below, the elastic scattering amplitude can be written with the separate contribution of the Coulomb scattering amplitude included. Then, the remaining integral (the second term on the right-hand side of Eq. (26) below) converges rapidly for the scattering at forward angles. Although the Coulomb phase in Eq. (20) diverges at $b=0$, this does not pose a real problem, since the strong absorption suppresses the scattering at small impact parameters. It is also easy to correct this expression to account for the finite charge distribution of the nucleus. For example, assuming a uniform charge distribution with radius R the Coulomb phase becomes

$$\begin{aligned}\chi_C(b)=2\eta\Big\{&\Theta(b-R)\ln(kb)+\Theta(R-b)\\&\times\Big[\ln(kR)+\ln\Big(1+\sqrt{1-b^2/R^2}\Big)\\&-\sqrt{1-b^2/R^2}-\frac{1}{3}(1-b^2/R^2)^{3/2}\Big]\Big\},\end{aligned} \tag{22}$$

where Θ is the step function. This expression is finite for $b=0$, contrary to Eq. (20). If one assumes a Gaussian distribution of charge with radius R, appropriate for light nuclei, the Coulomb phase becomes

$$\chi_C(b)=2\eta\Big[\ln(kb)+\frac{1}{2}E_1(b^2/R^2)\Big], \tag{23}$$

where the error function E_1 is defined as

$$E_1(x)=\int_x^\infty\frac{e^{-t}}{t}\,{\rm d}t. \tag{24}$$

This phase also converges as $b\to 0$. In Eq. (22) $R=R_p+R_t$, while in Eq. (23) $R=\sqrt{R_p^2+R_t^2}$, where R_p and R_t are the

respective projectile and target radius. The cost of using the expressions (22) and (23) is that the Coulomb scattering amplitude becomes more complicated than (21). Moreover, it has been proven [22] that the elastic and inelastic scattering cross-sections change very little by using Eqs. (22) or (23), instead of Eq. (20).

In calculations involving stripping the final state Coulomb interaction between the core and the target is taken into account by using the eikonal-Coulomb phase shift of (20) in the calculation of S_c. However in the calculation of diffraction dissociation both S_c and S_n are calculated using the eikonal-Coulomb phase shift of (20).

5. Elastic cross-sections

The calculation of elastic scattering amplitudes using eikonal wave functions, Eq. (9), is very simple. They are given by [22]

$$f_{\rm el}(\theta) = ik\int_0^\infty db\, b J_0(qb)\big\{1-\exp\big[i\chi(b)\big]\big\}, \tag{25}$$

where $q = 2k\sin(\theta/2)$, and θ is the scattering angle. The elastic scattering cross-section is $d\sigma_{\rm el}/d\Omega = |f_{\rm el}(\theta)|^2$. For numerical purposes, it is convenient to make use of the analytical formula, Eq. (21), for the Coulomb scattering amplitude. Thus, if one adds and subtracts the Coulomb amplitude, $f_C(\theta)$ in Eq. (25), one gets

$$f_{\rm el}(\theta) = f_C(\theta) + ik\int_0^\infty db\, b J_0(qb)\exp\big[i\chi_C(b)\big] \times\big\{1-\exp\big[i\chi_N(b)\big]\big\}. \tag{26}$$

The advantage in using this formula is that the term $1-\exp[i\chi_N(b)]$ becomes zero for impact parameters larger than the sum of the nuclear radii (grazing impact parameter). Thus, the integral needs to be performed only within a small range. In this formula, χ_C is given by Eq. (20) and $f_C(\theta)$ is given by Eq. (21), with

$$\phi_0 = -\eta C + \sum_{j=0}^{\infty}\left(\frac{\eta}{j+1} - \arctan\frac{\eta}{j+1}\right), \tag{27}$$

and $C = 0.5772156\ldots$ is the Euler's constant.

The elastic cross-section can be expressed in terms of the transverse momentum by using the relationships $d\Omega \simeq d^2k_\perp/k^2$, and $k_\perp \simeq q = 2k\sin(\theta/2)$, valid for high-energy collisions.

6. Momentum distributions

Following Ref. [6], the stripping reaction $(c+v)+A\to c+X$, where c corresponds to a specified final state of the core, is given by

$$\frac{d\sigma_{\rm str}}{d^3k_c} = \frac{1}{(2\pi)^3}\frac{1}{2J+1}\sum_M\int d^2b_v\big[1-|S_v(b_v)|^2\big] \times\left|\int d^3r\, e^{-i\mathbf{k}_c\cdot\mathbf{r}} S_c(b_c)\Psi_{JM}(\mathbf{r})\right|^2, \tag{28}$$

and where $\mathbf{r}\equiv(\boldsymbol{\rho},z,\phi) = \mathbf{r}_v - \mathbf{r}_c$, so that

$$b_c = |\boldsymbol{\rho}-\mathbf{b}_v| = \sqrt{\rho^2+b_v^2-2\rho b_v\cos(\phi-\phi_v)} = \sqrt{r^2\sin^2\theta + b_v^2 - 2r\sin\theta b_v\cos(\phi-\phi_v)}. \tag{29}$$

Assuming an independence of the bound state wave functions on spin (i.e. no spin-orbit term), Eq. (28) can be recast to

$$\frac{d\sigma_{\rm str}}{d^3k_c} = \frac{1}{(2\pi)^3}\frac{1}{2l+1}\sum_m\int d^2b_v\big[1-|S_v(b_v)|^2\big] \times\left|\int d^3r\, e^{-i\mathbf{k}_c\cdot\mathbf{r}} S_c(b_c)\psi_{lm}(\mathbf{r})\right|^2, \tag{30}$$

where the single-particle bound state wave functions for the subsystem $(c+v)$ is specified by $\psi_{lm}(\mathbf{r}) = R_l(r)Y_{lm}(\hat{\mathbf{r}})$, where $R_l(r)$ is the radial wave function. The code MOMDIS uses Eq. (30) (and the subsequent ones below) to obtain the momentum distributions. But it also allows one to calculate and use radial wavefunctions with a spin-orbit potential term which is useful in some cases.

The cross-sections for the longitudinal momentum distributions are obtained by integrating Eq. (28) over the transverse component of $\mathbf{k}_c$, i.e. over $\mathbf{k}_c^\perp$, and using

$$\int d^2\mathbf{k}_c^\perp \exp\big[-i\mathbf{k}_c\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')\big] = (2\pi)^2\delta(\boldsymbol{\rho}-\boldsymbol{\rho}'). \tag{31}$$

One gets

$$\frac{d\sigma_{\rm str}}{dk_z} = \frac{1}{(2\pi)^2}\frac{1}{2l+1}\sum_m\int_0^\infty d^2b_v\,\big[1-|S_v(b_v)|^2\big] \times\int_0^\infty d^2\rho\,\big|S_c(b_c)\big|^2\left|\int_{-\infty}^{\infty} dz\,\exp[-ik_z z]\psi_{lm}(\mathbf{r})\right|^2, \tag{32}$$

where k_z represents the longitudinal component of $\mathbf{k}_c$.

For the transverse momentum distribution in cylindrical coordinates $k_\perp = \sqrt{k_x^2+k_y^2}$, one uses in Eq. (28)

$$\int_{-\infty}^{\infty} dk_z\,\exp\big[-ik_z(z-z')\big] = 2\pi\delta(z-z'), \tag{33}$$

and the result is

$$\frac{d\sigma_{\rm str}}{d^2k_\perp} = \frac{1}{2\pi}\frac{1}{2l+1}\int_0^\infty d^2b_v\,\big[1-|S_v(b_v)|^2\big] \times\sum_{m,p}\int_{-\infty}^{\infty} dz\left|\int d^2\rho\,\exp(-i\mathbf{k}_c^\perp\cdot\boldsymbol{\rho})S_c(b_c)\psi_{lm}(\mathbf{r})\right|^2. \tag{34}$$

The code MOMDIS also allows to calculate the transverse momentum distributions in terms of the projection onto one of the Cartesian components of the transverse momentum. This can be obtained directly from Eq. (34), i.e.

$$\frac{d\sigma_{str}}{dk_y} = \int dk_x \frac{d\sigma_{str}}{d^2k_\perp}(k_x, k_y). \tag{35}$$

The total stripping cross-section can be obtained by integrating either Eq. (32) or Eq. (34). For example, from Eq. (32), using Eq. (33), one obtains

$$\sigma_{str} = \frac{2\pi}{2l+1}\int_0^\infty db_v\, b_v\big[1-|S_v(b_v)|^2\big] \times \int d^3r \left|S_c\Big(\sqrt{r^2\sin^2\theta + b_v^2 - 2r\sin\theta b_v\cos\phi}\Big)\right|^2 \times \sum_m \big|\psi_{lm}(\mathbf{r})\big|^2. \tag{36}$$

Using the explicit form of the spherical harmonics

$$Y_{lm}(\hat{\mathbf{r}}) = (-1)^m\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}P_{lm}(\cos\theta)e^{im\phi} = C_{lm}P_{lm}(\cos\theta)e^{im\phi} \tag{37}$$

and

$$\mathbf{k}_c\cdot\mathbf{r} = k_\perp r\sin\theta\cos(\phi_k-\phi) + k_\parallel r\cos\theta, \tag{38}$$

part of the integral in (28) is shown to be of the form [21]

$$\mathcal{F}_{lm}(k_\perp, k_z, b_v) = \int d^3r\, e^{-i\mathbf{k}_c\cdot\mathbf{r}}S_c(b_c)\psi_{lm}(\mathbf{r}) = C_{lm}\int dr\, r^2\sin\theta\, d\theta\, d\phi \times \exp\big\{-i\big[k_\perp r\sin\theta\cos(\phi_k-\phi)+k_\parallel r\cos\theta\big]\big\} \times S_c\Big(\sqrt{r^2\sin^2\theta + b_v^2 - 2r\sin\theta b_v\cos(\phi-\phi_v)}\Big) \times R_l(r)P_{lm}(\cos\theta)e^{im\phi}. \tag{39}$$

To simplify the calculations we can express $S_c(b_c)$ as an expansion in terms of integrable functions. The S-matrices can be well described by the expansion

$$S_c(b_c) = \sum_j^N \alpha_j \exp\big[-b_c^2/\beta_j^2\big], \quad \text{with } \beta_j = \frac{R_L}{j}. \tag{40}$$

Good fits for realistic S-matrices are obtained with $N = 20$, i.e. with 20 complex coefficients α_j and $R_L = 10$–20 fm, depending on the size of the system. Since the real part of the S-matrices has the usual behavior of $S_c(b_c)\sim 0$ for $b_c \ll R$, and $S_c(b_c)\sim 1$ for $b_c \gg R$, where R is a generic nuclear size, one of the coefficients of the expansion in Eq. (40) is $\alpha_j = 1$, and $\beta_j = \infty$, which we take as the $j = 0$ term in the expansion.

The expansion (40) allows to calculate analytically many of the integrals in Eq. (28), and one gets (see Appendix of Ref. [21])

$$\frac{d\sigma_{str}}{k_\perp\, dk_\perp\, dk_z} = \frac{2\pi}{2l+1}\int_0^\infty db_v\, b_v\big[1-|S_v(b_v)|^2\big] \times \sum_{m,p} C_{lm}^2\big|\mathcal{A}_{lmp}(k_\perp, k_z, b_v)\big|^2, \tag{41}$$

where

$$\mathcal{A}_{lmp}(k_\perp, k_z, b_v) = \sum_j \alpha_j \exp\big[-b_v^2/\beta_j^2\big] \times \int_0^\infty d\rho\, \rho J_p(k_\perp\rho)\exp\big[-\rho^2/\beta_j^2\big]I_{m-p}\left(\frac{2\rho b_v}{\beta_j^2}\right) \times \int_{-\infty}^\infty dz\, \exp[-ik_z z]R_l(r)P_{lm}(\cos\theta). \tag{42}$$

The first term of Eq. (42), with $\beta_j = \infty$ and $\alpha_j = 1$ can be calculated using $I_\alpha(0) = \delta_\alpha$.

Using the integral of Eq. (33) in Eq. (41) one gets for the *transverse momentum distribution*

$$\frac{d\sigma_{str}}{d^2k_\perp} = \frac{2\pi}{2l+1}\int_0^\infty db_v\, b_v\big[1-|S_v(b_v)|^2\big] \times \sum_{m,p} C_{lm}^2\int_{-\infty}^\infty dz\,\big|\mathcal{D}_{lmp}(k_\perp, b_v, z)\big|^2, \tag{43}$$

where

$$\mathcal{D}_{lmp}(k_\perp, b_v, z) = \sum_{j=0}^N \alpha_j \exp\big[-b_v^2/\beta_j^2\big] \times \int_0^\infty d\rho\, \rho J_p(k_\perp\rho)\exp\big[-\rho^2/\beta_j^2\big]I_{m-p}\left(\frac{2\rho b_v}{\beta_j^2}\right) \times R_l(r)P_{lm}(\cos\theta). \tag{44}$$

The momentum distributions from diffractive dissociation have nearly the same shape as those from stripping [21]. The code MOMDIS uses the equations of this section to obtain the momentum distributions renormalized so that their integral over momentum yields the total knockout cross-section, Eqs. (13) and (14).

For cases where the magnetic quantum number m differs from zero, we weight the differential cross-section with the multiplicity of 2, so that the sum over all m components gives the total cross-section. The two-dimensional momentum distribution does not depend on the azimuthal angle. It is convenient to present it as a function of the parallel and the transverse momentum with the definition

$$\frac{d^2\sigma_{str}}{dk_\perp\, dk_z} = 2\pi k_\perp\frac{d^3\sigma_{str}}{d^2k_\perp\, dk_z}, \tag{45}$$

which normalizes to the total cross-section when the integration is extended over the negative k_z-axis.

7. Computer program and user's manual

7.1. Distribution

The package is distributed in a tar.gz file and, under UNIX systems, can be unpacked as follows:

gunzip *filename*.tar.gz
tar -xvf *filename*.tar

Unpacking the file generates two files, a README file, the Fortran source, MOMDIS.FOR, and a directory, testdata. This directory contains sample input files for a typical run of MOMDIS and files containing the expected output.

Option 1—Eigenfunctions and energies
input file, a_bound.txt; output file, bound.out

Option 2—S_matrices—Sn
input file, a_sn.txt; output file, s_sn.out.

Option 2—S_matrices—Sc
input file, a_sc.txt; output file, s_sc.out

Option 3—Momentum distributions
input file, a_bound.txt; bound.out, s_sn.out, s_sc.out
output file, sigma.out

The MOMDIS.FOR program file is in DOS format. To use on a Unix system it should first be converted.

dos2unix -ascii MOMDIS.FOR MOMDIS.f

It can be compiled using the command

g77 -o MOMDIS.exe MOMDIS.f

and run using the command

./MOMDIS.exe

The screen output produced from each of the sample runs mentioned above is shown in the README file contained in the distribution.

7.2. Fortran code

The units used in the program are fm (femtometer) for distances and MeV for energies. The output cross-sections are given in millibarns (mb), mb/(MeV/c), and mb/(MeV/c)^2.

The program is very fast, except for transverse and double-differential momentum distributions, and does not require a complicated input. It is divided in 3 modules:

Module 1 Calculates of energy and wavefunction of bound states.
Module 2 Calculates S-matrices.
Module 3 Calculates momentum distributions. If one chooses option Module 3, other options follow: **1**—for longitudinal momentum distributions, Eq. (32), **2**—for transverse momentum distributions, Eq. (43), **3**—for projected transverse momentum distributions, Eq. (35), **4**—for double differential momentum distributions, Eq. (45), and **5**—for elastic scattering cross-section of the core with the target, using Eq. (26).

7.3. Sample input file

A sample input file is shown below. It is prepared to study the reaction $^{15}\mathrm{C} + {}^{9}\mathrm{Be} \to {}^{14}\mathrm{C} + X$ at 103 MeV/nucleon laboratory energy. The rows starting with a symbol "*" are not read as input and can be used in the input file at free will. They are well suited to remind the user of the input procedure. For more details on how to prepare an input file see the **readme** file located at the end of the Fortran code. With the sample input below the code calculates the *bound-state wave function*. To obtain *S-matrices*, one needs to comment with a "*" the input lines (4th and 5th rows) for bound-state wavefunction and delete the "*" from the input lines for S-matrices. The comments in the following two input lines depend upon the option parameters $\mathrm{I_{SMAT}}$, $\mathrm{I_{DPROJ}}$, and $\mathrm{I_{DTARG}}$. For *momentum distributions*, only the first three rows of the sample file (see Table 1) are used.

A more specific description follows. **Row 1:** Z_P, A_P = projectile charge and mass numbers, Z_T, A_T = target charge and mass numbers, E_{lab} = laboratory energy per nucleon (MeV). **Row 2:** Z_{CORE}, A_{CORE} = projectile core (^{14}C) charge and mass number. **Row 3:** S^2C = Spectroscopic factor. **Row 4:** Single-particle bound state quantum numbers. n_0 = nodes of the wave function (exclude origin), j_0 = total angular momentum, l_0 = orbital angular momentum. **Row 5:** Parameters of the Woods–Saxon potential used to calculate wavefunction following Eq. (5). V_0 = depth of central potential, V_{SO} = depth of spin-orbit potential, R_0 = radius parameter of the central potential, A = diffuseness of the central potential, R_{SO} = radius parameter of the spin-orbit potential, A_{SO} = diffuseness of the spin-orbit potential, R_C = Coulomb radius parameter (usually, $R_C = R_0$). **Row 6:** $I_{\mathrm{SMAT}} = 0$, or 1. If $I_{\mathrm{SMAT}} = 0$, S-matrix is for valence particle + target. If $I_{\mathrm{SMAT}} = 1$, S-matrix is for core + target. **Row 7:** $I_{\mathrm{POT}} = 0$, 1, or 2. If $I_{\mathrm{POT}} = 0$, optical potential is a Woods–Saxon, with real and imaginary parts, $V + iV_I$. If $I_{\mathrm{POT}} = 1$, optical potential is entered from an external, user provided, file. If $I_{\mathrm{POT}} = 2$, the optical potential is built with the t-$\rho\rho$ method. **Row 8:** If $I_{\mathrm{POT}} = 0$, enter V_0 [V_I] = real part [imaginary] (both > 0) of Woods–Saxon potential. R_0 [R_{0I}] = radius parameter ($R = R_0(A_P^{1/3} + A_T^{1/3})$). d [d_I] = diffuseness. **Row 9:** Enter names of the input files for the real (FILE1) and imaginary (FILE2) parts of the potential. In the input files, the first row must give the number of the remaining rows which form an ordered list of r (in fm) × V [V_I] (in MeV) in steps of a constant value of Δr. **Row 10:** If $I_{\mathrm{POT}} = 2$, enter the following options: $I_{\mathrm{PAULI}} = 0$ for no Pauli correction of nn cross-sections, $I_{\mathrm{PAULI}} = 1$ for Pauli correction of NN cross-sections. **Row 11:** Enter options for projectile and target densities. I_{DPROJ}, $I_{\mathrm{DTARG}} = 1, 2, 3, 4, 5$. If $I_{\mathrm{DPROJ}} = 1$,

Table 1

	6,	15,	4,	9,	103			Z_P,	A_P,	Z_T,	A_T,	E_{lab}		
	6,	14						A_{CORE},	Z_{CORE}					
	1							S^2C						
	1,	0.5	0					n_0,	j_0,	l_0				
	−61.85,	2.67,	0.6,	0.	2.4,	0.6,	2.67	V_0,	R_0,	A,	V_{SO},	R_{SO},	A_{SO},	R_C
	1							I_{SMAT}						
	2							I_{POT}						
*	50.,	1.067,	0.8,	58.,	1.067,	0.8		V_0,	R_0,	D,	V_I,	R_{0I},	D_I	
*	rp.in	ip.in						FILE1	FILE2					
	0							I_{PAULI}						
	1,	1						I_{DPROJ}	I_{DTARG}					
	1.73,	1.38,	1.					α,	$\beta(b)$,	ω				
*	2.,	1.,	1.,	1.				c,	a,	b,	ω			
*	2.,	1.,	1.,	0.				c,	a,	ω,	I_{DER}			
*	pd.in,	0.6						FILE3	α_p					
	1.93,	0.,	0.					α,	$\beta(b)$,	ω				
*	2.,	1.,	1.,	1.				c,	a,	b,	ω			
*	2.,	1.,	1.,	0				c,	a,	ω,	I_{DER}			
*	td.in,	0.6						FILE4	α_p					

projectile density is a three-parameter Gaussian density

$$G(r) = \left[1 + b\left(\frac{r}{\alpha}\right)^{\omega}\right] \exp\left(-\frac{r^2}{\alpha^2}\right). \tag{46}$$

If $I_{\text{DPROJ}} = 2$, projectile density is a two-parameter Yukawa

$$Y(r) = r^{\omega} \frac{1}{\beta r} \exp(-\beta r). \tag{47}$$

If $I_{\text{DPROJ}} = 3$, projectile density is a four-parameter Fermi function

$$F(r) = \left[1 + b\left(\frac{r}{\alpha}\right)^{\omega}\right] \frac{1}{[1 + \exp(\frac{r-c}{\alpha})]}. \tag{48}$$

If $I_{\text{DPROJ}} = 4$, projectile density is a power of the Fermi function ($I_{\text{DER}} = 0$), or its derivative ($I_{\text{DER}} = 1$)

$$S(r) = \frac{1}{[1 + \exp(\frac{r-c}{\alpha})]^{\omega}}, \quad \text{or} \quad \frac{\mathrm{d}S}{\mathrm{d}r}. \tag{49}$$

If $I_{\text{DPROJ}} = 5$, projectile density is a calculated from liquid-drop model. If $I_{\text{DPROJ}} = 10$, projectile density is from an input file. **Row 12:** In case $I_{\text{DPROJ}} = 1$ or 2, enter here Gaussian or Yukawa density parameters for the projectile, according to Eqs. (46) and (47), respectively. **Row 13:** If $I_{\text{DPROJ}} = 3$ enter the four parameter of the Fermi function, Eq. (48). **Row 14:** If $I_{\text{DPROJ}} = 4$, enter Fermi density parameters for the projectile and its power, as in Eq. (49). **Row 15:** If $I_{\text{DPROJ}} = 10$, enter name (FILE3) of the input file where the projectile density is to be found and α_p is the proton size parameter to be used in a folding of the input distribution with the proton Gaussian density, $\rho_p(r) = (\pi a^2)^{-3/2} \exp(-r^2/a^2)$. In the input file FILE3, the first row must give the number of the remaining rows which form an ordered list of r (in fm) × ρ_{PROJ} (in fm^{-3}) in steps of a constant value of Δr. **Rows 16, 17, 18 and 19:** Same as the previous four rows, but for the target (depending upon the option I_{DTARG}).

7.4. Eigenfunctions and energies

Option 1 calls the subroutine **EIGEN**. The potential parameters to build the Woods–Saxon are entered in the input file. In the sample file above, the ground state of ^{15}C is calculated. It is assumed to be a $1s1/2^+$ s-wave ($n = 1$, $l = 0$, $j = 0.5$). This is just one of the possible single particle occupancies in the ground state of ^{15}C. The spectroscopic factor can be adjusted to account for the occupancy probability of this single-particle configuration.

The calculations are mainly done in the subroutine **BOUNDWAVE** which solves the Schrödinger equation for the bound-state problem. When Woods–Saxon potentials are used they are constructed in the routine **POTENTIAL**.

The output of the wavefunction will be printed in **EIGEN.TXT** and another file specified by the user, which will be ready for use later.

7.5. S-matrices

Option 2 calls subroutine **SMAT**. If this option is used the input rows for the bound-state wavefunction should be commented with a "*". Here one has to specify if one wants S_v or S_c and if the optical potentials are entered in a separate file or built with the "t-$\rho\rho$" approximation. If the later is chosen, one has to enter the options for the nuclear densities. An option is given to include, or not, the effect of Pauli blocking on the in-medium nucleon–nucleon cross-section.

7.6. Momentum distributions

Option 3 calls for calculation of momentum distributions. In this case, only the general input (charges, masses and bombarding energy) are used. All subsequent rows may be commented, or not. One can then choose to calculate $\mathrm{d}\sigma/\mathrm{d}p_z$, $\mathrm{d}^2\sigma/\mathrm{d}p_t^2$, $\mathrm{d}\sigma/\mathrm{d}p_y$, $\mathrm{d}^2\sigma/\mathrm{d}p_t\,\mathrm{d}p_z$, or σ_{elast}.

8. Routines included with the code distribution

EIGEN finds eigenvalue and eigenfunction of a system composed of a valence particle with charge Z1 and a nucleus with charge Z2. The nuclear potential is a Woods–Saxon, with spin-orbit and Coulomb components.

BOUNDWAVE solves the radial Schrodinger equation for bound states.

POTENT constructs potentials to be used in the calculation of bound state wavefunctions. Uses routine **OMP_WS** which constructs the Woods–Saxon potential.

SMAT computes the eikonal S-matrices for heavy ion collisions. The S-matrices are functions of the impact parameter b. The program is appropriate for heavy ion bombarding energies $E_{\rm lab} > 30$ MeV/nucleon.

CROSS. If IOPT = 1, this routine calculates $\mathrm{d}\sigma/\mathrm{d}p_z$. If IOPT = 2, 3, 4 and 5, it calculates $\mathrm{d}^2\sigma/\mathrm{d}p_t^2$, $\mathrm{d}\sigma/\mathrm{d}p_y$, $\mathrm{d}^2\sigma/\mathrm{d}p_t\,\mathrm{d}p_z$, or $\sigma_{\rm elast}(\theta)$, respectively.

COMPDIF is used in the calculation of the total diffraction dissociation cross-section, Eq. (13).

GAUST calculates the sum over the Gaussian expansion for $\mathrm{d}\sigma/\mathrm{d}p_y$, where p_y is one of the components of the transverse momentum.

GAUSLT is similar to GAUST, but calculates $\mathrm{d}^2\sigma/\mathrm{d}p_t\,\mathrm{d}p_z$.

FINTEG calculates $\int_{-\infty}^{\infty}\mathrm{d}z\,|R_l(r)|^2 P_{lm}(\cos\theta)$ which is used in several other integrals. **PINTEG** deals with the integral $\int \mathrm{d}\phi |S(\sqrt{r^2\sin^2\theta + b^2 - 2r\sin\theta b\cos\phi})|^2$. **ZINTEG** computes $\int_{-\infty}^{\infty}\mathrm{d}z\exp[-ik_z z]R_l(r)P_{lm}(\cos\theta)$.

COMPL is used in the calculation of the longitudinal momentum distribution, Eq. (32).

SMAT_FIT finds the best expansion parameters α_j to fit S_c with an expansion in Gaussians (Eq. (40)). Uses auxiliary routines **FUNCS**, **LFIT**, **GAUSSJ** and **COVSRT**.

FCOUL and **CP0** are used in the calculation of the Coulomb elastic amplitude, Eq. (21).

SIGNNE and **PHNNE** are used in the calculation of the nucleon–nucleon scattering amplitude, Eq. (19).

PHNUC calculates the eikonal nuclear phase, Eq. (18).

The routines **GAUSS** (Eq. (46)), **YUKAWA** (Eq. (47)), **FERMI** (Eq. (48)), **SAXON** (Eq. (49)) and **DROP** are used to calculate the nuclear densities parametrized as Gaussians, Yukawa, Fermi, Woods–Saxon, and liquid drop functions, respectively. The parametrizations follow Eqs. (46)–(49). **DROP** builds liquid drop model densities for the nuclei, following Ref. [32].

The routines **PLGNDR, BESSJ, BESSJ0, BESSJ1, BESSI, BESSI0** and **BESSI1** calculate Legendre polynomials and Bessel functions.

The other routines in the code are shortly described as follows. **GFV** calculates factorials, **BETWEEN** and **FINFOUT** are interpolating routines, **SKIPCOM** is used to skip comments in the input file, **RSIMP** does Simpson's integrations of tabulated functions, **FOURIER0** calculates Fourier transforms (e.g., in the calculation of the transformed densities of Eq. (18)), **NUCNAME** finds the symbol associated to a given chemical element and **EXCESS** calculates the mass excess with the parameters published in Ref. [33].

9. Things to do

1. Use the sample input file to obtain Fig. 6 of Ref. [21].
2. Modify the input file so as to reproduce all other results published in Ref. [21].
3. Use the overlap function for $\Psi_{JM}(\mathbf{r})$ published in Ref. [34] to reproduce their Fig. 2.

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