SPOMC Computational Code

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The SPOMC code calculates elastic scattering cross sections based on the São Paulo potential (SPP) [1] as the real part of the optical potential. In this manuscript, we provide a summary of the theoretical framework and information about the use of the SPOMC.

I. SPP

The SPP has been successful in describing the elastic scattering and peripheral reaction channels for several heavy-ion systems in a very wide energy region. Within this model, the nuclear interaction is connected with the folding potential through [1]:

$$V_N(R,E) = V_F(R)\; e^{-4\mathrm{v}^2/c^2}\;, \tag{1}$$

where c is the speed of light and v is the local relative velocity between the two nuclei,

$$\mathrm{v}^2(R,E) = \frac{2}{\mu}\;[E - V_C(R) - V_N(R,E)]\;, \tag{2}$$

and V_C is the Coulomb potential (which is also calculated through folding procedures). The folding potential depends on the matter densities of the nuclei involved in the collision:

$$V_F(R) = \int \rho_1(\vec{r_1})\;\rho_2(\vec{r_2})\;V_0\;\delta(\vec{R} - \vec{r_1} + \vec{r_2})\;d\vec{r_1}\;d\vec{r_2}, \tag{3}$$

with $V_0 = -456$ MeV fm^3. The use of the matter densities and delta function in Eq. (3) corresponds to the zero-range approach for the folding potential, which is equivalent [1] to the more usual procedure of using the frozen M3Y effective nucleon-nucleon interaction with the nucleon densities of the nuclei (instead of the matter densities).

We assume a two-parameter Fermi (2pF) distribution to describe the nuclear densities:

$$\rho(r) = \frac{\rho_0}{1 + exp\left(\frac{r-R_0}{a}\right)}, \tag{4}$$

In Ref. [1], we presented an extensive systematics for the densities of heavy nuclei. We found that the radii of the charge and matter densities can be well represented by:

$$R_0 = 1.76Z^{1/3} - 0.96 \text{ fm}, \tag{5}$$

$$R_0 = 1.31A^{1/3} - 0.84 \text{ fm}. \tag{6}$$

The charge and matter distributions present average diffuseness values of $a = 0.53$ fm and $a = 0.56$ fm, respectively. Within the context of the systematics for the densities, the SPP has no adjustable parameter. This systematics has been based on theoretical calculations with the Dirac-Hartree-Bogoliubov model and also on experimental results for charge distributions. Of course, small deviations around these average values are expected due to the effects of the structure of the nuclei. In Ref. [1], these variations were analysed and standard deviations of $\sigma_R = 0.07$ fm and $\sigma_a = 0.025$ fm relative to the average radius and diffuseness values, respectively, were found. So, there is room to treat R_0 and a as adjustable parameters. In Ref. [1] we have demonstrated that the barrier height is more affected by variations in the diffuseness value than in the radius. Thus, in the SPOMC code only the diffuseness value can be modified. The systematics for the densities has been obtained considering results for heavy ions. Therefore, the SPZPM is not appropriate for systems involving light nuclei such as proton or neutron. For ^{4}He, the code assumes that the corresponding matter density has similar shape as the charge one, which has been determined by electron scattering experiments.

For the imaginary part of the optical potential, the code can work with two models. It can use a Woods-Saxon shape or $W(R) = N_I \times V_N(R)$. The latter model has been applyed for several systems in a wide energy range (see Ref. [2]). It has been found that $N_I = 0.78$ is an average value that works very well for most cases.

II. INPUT

SPOMC.for has been built using FORTRAN 77 with double-precision, and it can be compiled within the LINUX environment. If no problems occur, the CPU time is very small. The input parameters should be provided in an input file (SPOMC.dat). The code can calculate the chi-square that corresponds to an experimental angular distribution. In this case, a further input file (SPOMC.ent) is necessary, where center of mass angles, elastic cross section data (ratio to Rutherford), and corresponding uncertainties are given. The results of the calculations are provided in an output file (SPOMC.out).

The SPOMC.dat file must provide the following parameters:

Elab,AP,ZP,AT,ZT
Rmax,Lmax,dr
Ide1,Ide2,am1,ac1,am2,ac2
Iopw,NI,W0,ri0,ai
I1,I2,L1,L2,dang,Ichi

Elab=laboratory energy.
AP=number of nucleons of projectile (real variable).
ZP=number of protons of the projectile (real variable).
AT, ZT = the same for the target nucleus.
Rmax= matching radius (the nuclear interaction can be neglected for $R > Rmax$).
Lmax= number of partial waves.
dr= step-size for integration.
Ide1 and Ide2 are options for the densities of projectile and target, respectively. Ide=0 represents 2pF distributions with radii from the systematics. Ide=1 is used for ^{4}He.
am1 and ac1 are matter and charge diffuseness of the projectile. am2, ac2 are for the target.
Iopw indicates the model for the imaginary part of the optical potential. Iopw=2 represents Woods-Saxon, while Iopw=1 is for $W(R) = N_I \times V_N(R)$. The values of NI, W0, ri0 and ai must always be given. The code will select the paremeters that correspond to the option Iopw.
The other parameters correspond to print options. I1 different from zero will provide the densities. I2 different from zero gives the potentials. L1 corresponds to the partial-wave for which the code provides the effective potential (nuclear plus Coulomb plus centrifugal parts). A negative value for L1 should be used if you do not want the effective potential to be printed. L2 is the partial-wave to print the corresponding elastic scattering wave-function (negative = do not print). Dang is the angular step-size assumed in the elastic scattering angular distribution. If Ichi is different from zero, a chi-square will be calculated (for the data set of the SPOMC.ent file).

The SPP has been based on the systematics for the nuclear densities. The average diffuseness value of this systematics is $a = 0.56$ fm. As already commented, small deviations around this average value are expected due to the effects of the structure of the nuclei. In Ref. [1], these variations were analysed and standard deviation of $\sigma_a = 0.025$ fm was found. A realistic value for the diffuseness should not be too far from the average value. Thus, the code will run with any diffuseness value that you want, but if this value is more than two standard deviations far from the average value a warning will be printed in the output file.
As described in Ref. [2], $N_I \approx 0.8$ works well for most cases. However, this value has not been obtained from fundamental grounds. Thus, there is room to assume N_I as an adjustable parameter.
The code provide warnings if problems are found in the numerical calculations. Even so, the convergence of the results should be tested by changing the Rmax, Lmax and dr parameter values.
If you have any problem with the SPOMC, please do not hesitate of writing me.

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[1] L. C. Chamon, B. V. Carlson, L. R. Gasques, D. Pereira, C. De Conti, M. A. G. Alvarez, M. S. Hussein, M. A. Cândido Ribeiro, E. S. Rossi Jr., C. P. Silva, Phys. Rev. **C 66**, 014610 (2002).
[2] M. A. G. Alvarez, L. C. Chamon, M. S. Hussein, D. Pereira, L. R. Gasques, E. S. Rossi Jr., C. P. Silva, Nucl. Phys. **A 723**, 93 (2003).