User's manual for `Chaconne.f`

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1 Introduction

Halos are exotic, loosely-bound, nuclear structures observed in some neutron-rich nuclei far from stability [1]. They are observed mostly close to the neutron dripline when one or two valence neutrons sit in an s or p orbital. In that case, these valence neutrons decouple from the core of the nucleus and, thanks to their loose binding, their wave function extends far into the classically-forbidden region. They hence form a diffuse halo around a rather compact core. Being located far from stability, their lifetimes are usually very short. They are therefore difficult to study through usual spectroscopic techniques. An indirect way to infer key information about their structure is reactions. In the *breakup* reaction, the nucleus under study is sent on a target and the events in which the halo neutrons dissociate from the core are measured. This reaction therefore reveals the internal structure of the nucleus. Because of the fragile nature of the projectile, its cross section should be large and hence measurable at radioactive-ion beam facilities.

`Chaconne` is a Fortran computer code that implements the Coulomb-Corrected Eikonal model of breakup reactions (CCE) for one-nucleon halo nuclei (proton halos are also possible and supported in this code) [2]. It is based on the eikonal approximation of the reaction, which is valid at intermediate and high energy, viz. for beam energies $> 40A$MeV. The CCE includes a correction of the Coulomb contribution to breakup [3, 4, 5], which diverges at the usual eikonal approximation [2, 6].

The reaction is described in a few-body model of the collision: the projectile P is seen as a two-body core (c) - fragment (f) system impinging on a target T, whose internal structure is neglected. The core contains most of the projectile nucleons, while the fragment is a neutron, a proton or any cluster of nucleons loosely bound to the core. The c-f system is described within an effective single-particle Hamiltonian

$$H_0(\boldsymbol{r}) = -\frac{\hbar^2}{2\mu_{cf}}\Delta_{\boldsymbol{r}} + V_{cf}(r), \tag{1}$$

where $\mu_{cf} = m_c m_f/(m_c + m_f)$ is the c-f reduced mass, $\boldsymbol{r}$ is the relative coordinate of the fragment to the core, and V_{cf} is an effective potential simulating the interaction between the core and the fragment.

The interaction of both constituents of the projectile with the target is modelled by optical potentials V_{cT} , and V_{fT}.

Within that three-body model, describing the reaction reduces to solving the Schrödinger equation with the following three-body Hamiltonian

$$H(\boldsymbol{R},\boldsymbol{r}) = -\frac{\hbar^2}{2\mu_{PT}}\Delta_{\boldsymbol{R}} + H_0(\boldsymbol{r}) + V_{cT}(R_{cT}) + V_{fT}(R_{fT}), \tag{2}$$

where $\mu_{PT} = m_P m_T/(m_P + m_T)$ is the P-T reduced mass (with $m_P = m_c + m_f$) and $\boldsymbol{R}$ is the relative coordinate of the projectile centre of mass to the target. We look for the eigenstates of Hamiltonian (2) Ψ, which exhibit the boundary condition with the projectile in its ground state impinging on the target

$$\Psi(\boldsymbol{R}, \boldsymbol{r}) \underset{Z\to-\infty}{\longrightarrow} e^{iKZ}\phi_0(\boldsymbol{r}), \tag{3}$$

where the Z axis is chosen along the incoming beam.

`Chaconne` solves that Schrödinger equation within the CCE [2]. The input file (Sec. 2) provides the conditions of the reaction (projectile structure, target, beam energy etc.) and the numerical parameters for the numerical resolution of the equation (number of points in the different discretisations, parameters of the potentials V_{cf}, V_{cT} , and V_{fT} etc.). In the output file (Sec. 3), the breakup cross section can be provided as a function of various observables: c-f relative energy E, momentum for the c-f motion parallel to the beam $p_\parallel$, or scattering angle of the c-f centre of mass.

2 Input File

An example of an input file for `Chaconne` is given here for the collision of ^{11}Be on ^{208}Pb at 69AMeV, similar to what has been used in Ref. [2]. Please note that it is a mere example, the convergence is by no means ensured and the optical potentials considered here should not be seen as reliable. This example should run quickly on a laptop (a few seconds) and give you the output file shown in Sec. 3. The details on each input variable are provided below.

```
197.32705359 1.43996518 20.736              * csts:hc,e2,hm
10.0 1.0 4 0 0 1                            * Masses,charges,spins:Ac,Af,Zc,Zf,iSc,iSf
2 2                                         * c-f potential:ntypo,Njpo
-39.74 2.585 0.6 21.0 2.585 0.6 2.585       *odd Vp,rp,ap,Vpp,rpp,app,rC
-62.52 2.585 0.6 21.0 2.585 0.6 2.585       *even Vp,rp,ap,Vpp,rpp,app,rC
2                                           * Nel:nb of bound states
1 1 0 -0.504 0 1 1 -0.184                   * bound states:NR,J,l, E0 (ground state first)
208.0 82 69.0                               * Collision:Ata,ZT,E/A
10 100.0 2                                  * P-T potential:npotN,bmaxN,lamax
-70.0 -58.9 0 7.43 7.19 1 1.04 1.00 1 8.08 * cT:V,W,WD,rR,rI,rD,aR,aI,aD,rC
-29.46 -13.4 0 6.93 7.47 1 0.75 0.58 1 1   * fT:V,W,WD,rR,rI,rD,aR,aI,aD,rC
1000 100.0 6 18                             * radial and angular meshes:Nr,rm,Nt,Np
20 1.0 300 0.1                              * meshes in Z and s:NZ,hZ,Ns,hs
2 100.0 0.05                                * mesh in b:Nzb,bmax,hbpol
0 0.5                                       * bmin, hb
30.0 1                                      * bmin, hb
10 0.1 0.1                                  * NE,E0,hE
50 0.1 0.1                                  * CDM: Nth,th0,hth
11                                          * lec=0:Pbu;1:dE;2:dpp;3:dt.eik:+0;CCE:+10
Be11Pbexample                               * output file
```

Physical constants

`* csts:hc,e2,hm`

`hc` is $\hbar c$ expressed in MeV fm, `e2` is $e^2/4\pi\epsilon_0$, also in MeV fm, and `hm` is $\hbar^2/2m_N$ in MeV fm^2, where m_N is the mass unit in which the masses of the core, halo nucleon, and target are expressed (e.g. the nucleon mass, like in this example, or the atomic mass unit, for which `hm` ≈ 20.9008 MeV fm^2).

Projectile constituents

`* Masses,charges,spins:Ac,Af,Zc,Zf,iSc,iSf`:

`Ac` and `Af` are the masses of the core and the halo nucleon expressed in unit m_N (see above); these are real number, but in practice they should simply be seen as the c and f mass numbers. `Zc` and `Zf` are the corresponding charges, expressed in unit e; they are integers. `iSc` and `iSf` are the spins of the core and the valence nucleon; these are integer numbers, so twice the spin if it is half-integer and its actual value if it is integer. For a spin 1/2 halo neutron, `iSf` should be set to 1. Note that in the current status of the code, the spin of the core is implicitly assumed to be nil. Therefore `iSc` is read but not considered in the model of the projectile, see below.

Core-fragment potential V_{cf}

Two forms of the c-f interactions are implemented in this code.

1. A usual Woods-Saxon form with a spin-orbit coupling term:

$$V_{cf}(r) = V_p\ f(r, r_p, a_p) + \boldsymbol{l}\cdot\boldsymbol{S_f}\ V_{pp}\frac{1}{r}\frac{\partial}{\partial r}f(r, r_{pp}, a_{pp}) + V_C(r, r_C), \tag{4}$$

   where $\boldsymbol{l}$ is the c-f relative orbital angular momentum and $\boldsymbol{S_f}$ the fragment spin, to which it is coupled. V_C is the Coulomb potential [see Eq. (6)]. The Woods Saxon form reads

$$f(r, r_0, a) = \left[1 + \exp\left(\frac{r - r_0}{a}\right)\right]^{-1}. \tag{5}$$

   The Coulomb potential V_C has a point-sphere expression:

$$V_C(r, r_C) = \begin{cases} \frac{Z_c Z_f}{2r_C}\frac{e^2}{4\pi\epsilon_0}\left(3 - \frac{r^2}{r_C^2}\right) & r < r_C \\ \frac{Z_c Z_f}{r}\frac{e^2}{4\pi\epsilon_0} & r \geq_C \end{cases} \tag{6}$$

2. A Gaussian form with central and surface terms:

$$V_{cf}(r) = V_p\ g(r, r_p, a_p) + V_{pp}\ r^2 g(r, r_{pp}, a_{pp}) + V_C(r, r_C), \tag{7}$$

   with the Gaussian form

$$g(r, r_0, a) = \exp\left[-\left(\frac{r - r_0}{a}\right)^2\right]. \tag{8}$$

   The Coulomb interaction is the point-sphere potential (6).

The parameters of either of these forms are provided through the following lines of the input file.

`* c-f potential:ntypo,Njpo`

`ntypo` fixes the form of the potential and `Njpo` the number of lines in which it is provided; both are integer.

For a Woods Saxon form of the potential, `ntypo` should be chosen to be either 1 or 2, and for a Gaussian form, either 11 or 12.
When `ntypo` = 1 or 11, the potential is given by partial wave. Each of the following `Njpo` −1 lines gives the potential in a definite partial wave, identified by its total angular momentum j and orbital angular momentum l. The expression of the potential in all other partial waves is given in the next, viz. `Njpo`$^{\text{th}}$, line. To use the same potential in all partial waves, one simply chooses this option (`ntypo` = 1 or 11) with `Njpo` = 1.
If `ntypo` = 2 or 12, the potential is given for odd- and even-l partial waves. In that case `Njpo` is automatically set to 2 by the program, the first following line corresponds to the odd ls, while the second corresponds to the even ls.
`*(J,l),Vp,rp,ap,Vpp,rpp,app,rC`: V_{cf} potential parameters.
`J` and `l` are the total angular and orbital momenta of the considered partial wave (they are integer and the value of `J` is multiplied by two if the fragment spin is half integer). These two numbers must not be included in the `Njpo`$^{\text{th}}$ line, nor if `ntypo` = 2. The other parameters are real and correspond to the descriptions given in Eqs. (4)–(8).

Information about the bound states of the projectile

`* Nel:nb of bound states`
Number of bound states to be considered in the reaction calculation (integer).
`* bound states: J,l, E0 (ground state first).`
On one line are given for each bound state the total angular momentum `J` (integer, multiplied by two if S_f is half integer), the orbital momentum `l` (integer), and an estimate of the energy `E0` relative to the fragment-separation threshold (negative real). The initial bound state must be listed first.

Information about the collision

`* Collision: AT,ZT,E/A.`
`AT` is the target mass in m_N unit (real number, but as for c and f it should seen as the mass number of the target), `ZT` is its charge (integer), and `E/A` is the kinetic energy per nucleon of the projectile in the laboratory frame expressed in MeV (real number).

Projectile-target optical potentials

`* P-T potential: npotN,bmaxN,lamax:projectile-target potentials.`
`npotN` fixes the type of projectile-target potentials (integer)

- 0: mere point-point Coulomb potentials
- 10: Coulomb + nuclear interactions
  (optical potentials given in the next two lines)
- 20: Real Gaussian potential (no Coulomb)

When `npotN` = 10, `bmaxN` is the maximum impact parameter for which the nuclear optical potential is considered in the calculation (real number; in fm). For larger impact parameters, the nuclear interaction is neglected, and only the point-point Coulomb potentials are used.
`lamax` is the largest multipole used in the calculation of the eikonal phases (integer).
`*c/fT:V,W,WD,rR,rI,rD,aR,aI,aD,rC`
Parameters of the optical potentials. These two lines contain the parameters of the optical potentials that simulates the interaction between the projectile constituents and the target (real numbers). These potentials exhibit a usual Woods-Saxon form:

$$V_{xT}(r) = V\ f(r, r_R, a_R) + i\ W_I\ f(r, r_I, a_I) + i\ W_D\ a_D\ \left|\frac{\partial}{\partial r} f(r, r_D, a_D)\right| + V_C(r, r_C), \tag{9}$$

where V_C is the point-sphere Coulomb potential (6), and f is the Woods-Saxon form (5).

Discretisation meshes

`* radial and angular meshes:Nr,rm,Nt,Np`

`Nr` gives the number of radial point on the uniform radial mesh used to compute the bound and continuum c-f states (integer). `rm` is the last point of the mesh $r_{\max}$ given in fm (real). `Nt` and `Np` are the number of points on the Lagrange meshes in colatitude θ and azimuthal angle φ used to compute the multipole expansion of the eikonal phases; they should both be even integer.

`* meshes in Z and s:NZ,hZ,Ns,hs`

`NZ` is the number of point on the uniform mesh along the z direction used to compute the eikonal phases from the optical potentials (integer). `hZ` is the corresponding step size in fm (real). To accelerate the calculation, the eikonal phases are calculated on a uniform mesh in the transverse direction s. `Ns` is the number of point in this mesh (integer), while `hs` is the step size in fm (real).

`* b zones: Nzb,bmax,hbpol`. The loop over the impact parameter b is split into different zones, and the step size in b varies between these different zones. `Nzb` is the number of zones (integer), and `bmax` is the last value of b in fm, for which an eikonal phase is evaluated (real). `hbpol` is the value of the step size in fm for the interpolation needed to compute the angular distribution (real). For each of the zones, there is a line with the following parameters:

`* bmin,hb`: discretization parameters in one b zone.

`bmin` is the first impact parameter of the zone, and `hb` is the b step (both are real numbers expressed in fm).

Note that the different zones must be entered in increasing order of b.

Selection of the output

`* NE,E0,hE`: mesh in the c-f continuum energies E at which the breakup cross section is provided in output. If `lec` = 2 or 12 (see below) it corresponds to the mesh in parallel-momentum (actually the corresponding wave number $k_\parallel$ in fm^{-1}).

`NE` is the number of energies (integer), `E0` is the lowest energy at which the breakup cross section is computed (real in MeV), and `hE` is the step size in energy (real in MeV).

`* CDM: Nth,th0,hth`: mesh in the scattering angle of the c-f center of mass at which the angular distribution for the breakup of the projectile is computed.

`Nth` is the number of angles (integer), `th0` is the initial angle of the mesh (real in degree), and `ht` is the step in angle (real in degree).

`* lec`: integer variable that indicates the desired output.

For $0 \leq$ `lec` ≤ 3 the calculation is performed at the usual einkonal approximation. When $10 \leq$ `lec` ≤ 13 the calculation is performed with the Coulomb correction, i.e., within the CCE. For `lec` =

- 0 or 10: breakup probability $P_{\rm bu}$ as a function of the impact parameter b for the first c-f continuum energy provided above (so `E0`); see Eq. (27) of Ref. [2].
- 1 or 11: energy distribution $d\sigma_{\rm bu}/dE$ for the energies provided above; see Eq. (26) of Ref. [2] (in that case, the angular mesh is read but ignored).
- 2 or 12: parallel-momentum distribution $d\sigma_{\rm bu}/dk_\parallel$; see Eq. (28) of Ref. [2]. The values of $k_\parallel$ wave numbers expressed in fm^{-1} are given instead of the energies two lines above. The cross section is provided for $k_\parallel = \pm$[`E0` $+(i_E-1)$ `hE`] $\forall\ i_E = 1$–`NE`. (in that case, too, the angular mesh is read but ignored)
- 3 or 13: breakup angular distribution: $d^2\sigma_{\rm bu}/dEd\Omega$ computed on the angular mesh provided on

the line above; see Eq. (48) of Ref. [6]. If `NE` > 1, then the cross section is integrated over that energy range.

`*` `output file`: name used for the output file. As explained below, an extension is added to that name depending on the value of `lec`.

3 Output File

As seen above, the output of `Chaconne` depends on `lec`. The output file is named by adding an extension to the name given in input.

If `lec` $= 0$ (usual eikonal) or 10 (CCE), the extension `.sdb` is added. That file is structured in columns. The first column gives the impact parameter b in fm. The second column gives the breakup probability at the first energy provided in input (so `E0`); this corresponds to Eq. (27) of Ref. [2]. That value is provided in MeV^{-1}. The next columns correspond to the partial-wave components of that probability for each possible combination of l and j compatible with the value of `lamax` provided in input. They are ordered in increasing value of l from $l = 0$ up to l_0+ `lamax`, where l_0 is the ground-state orbital angular momentum. For each value of l the possible values of j are ordered from the lowest one $(l - S_f)$ to the largest one $(l + S_f)$, with S_f the spin of the fragment f.

When `lec` $= 1$ (usual eikonal) or 11 (CCE), the extension `.sdE` is added to the name provided in input. The file is also structured in columns. The first one gives the c-f continuum energy E. The second one gives the breakup cross section as a function of the relative energy E between c and f after dissociation (see Eq. (26) of Ref. [2]). It is expressed in b MeV^{-1}. The other columns correspond to the partial-wave contributions to that cross section for each possible combination of l and j compatible with the value of `lamax` provided in input. They are ordered in increasing value of l from $l = 0$ up to l_0+ `lamax`, where l_0 is the ground-state orbital angular momentum. For each value of l the possible values of j are ordered from the lowest one $(l - S_f)$ to the largest one $(l + S_f)$.

For `lec` $= 2$ (usual eikonal) or 12 (CCE), the extension `.sdp` is added. The file contains two columns. The first stores the wave number in the direction of the beam $k_\parallel$, expressed in fm^{-1}. The second contains the parallel-momentum distribution $d\sigma_{\rm bu}/dk_\parallel$; see Eq. (28) of Ref. [2]; it is expressed in b fm.

When `lec` $= 3$ (usual eikonal) or 13 (CCE), the extension is `.sdt`. The file is structured in columns. The first one gives the scattering angle θ of the c-f centre of mass in the P-T centre-of-mass frame expressed in degrees. The second one gives the breakup cross section as a function of that angle. If `NE` $= 1$ the angular distribution is given at the first and only one energy `E0` between c and f after dissociation given in input $d^2\sigma_{\rm bu}/dEd\Omega$ [see Eq. (26) of Ref. [2]]. When `NE` > 1 the angular distribution integrated over the energy range given in input. In the former case, the value is given in b MeV^{-1} sr^{-1}, in the latter case its units are b sr^{-1}. The other columns correspond to the partial-wave contributions to that cross section for each possible combination of l and j compatible with the value of `lamax` provided in input. They are ordered in increasing value of l from $l = 0$ up to l_0+ `lamax`, where l_0 is the ground-state orbital angular momentum. For each value of l the possible values of j are ordered from the lowest one $(l - S_f)$ to the largest one $(l + S_f)$.

The output obtained after running `Chaconne` with the input file shown at the beginning of Sec. 2 provides the file `Be11Pbexample.sdE`:

```
0.100 8.68444775D-01 1.36019427D-01 1.19883723D-01 5.99121520D-01 5.33027878D-03 8.08982612D-03 0.00
0.200 1.24425008D+00 1.15146368D-01 1.90178913D-01 9.00423444D-01 1.52142588D-02 2.32870985D-02 0.00
0.300 1.30252587D+00 9.06386246D-02 2.08767849D-01 9.44593615D-01 2.29552442D-02 3.55705411D-02 0.00
0.400 1.22329073D+00 7.12401132D-02 2.01985061D-01 8.79088745D-01 2.75462481D-02 4.34305644D-02 0.00
0.500 1.09719793D+00 5.68295390D-02 1.84876449D-01 7.77846214D-01 2.96916666D-02 4.79540641D-02 0.00
0.600 9.64502630D-01 4.61770681D-02 1.64770496D-01 6.72806854D-01 3.02421721D-02 5.05060393D-02 0.00
0.700 8.41596000D-01 3.82014056D-02 1.44978280D-01 5.76341455D-01 2.98387812D-02 5.22360780D-02 0.00
0.800 7.34250945D-01 3.21186925D-02 1.26852611D-01 4.92223876D-01 2.89024739D-02 5.41532914D-02 0.00
0.900 6.43987240D-01 2.73877457D-02 1.10821086D-01 4.20632860D-01 2.76933410D-02 5.74522081D-02 0.00
1.000 5.71586355D-01 2.36374853D-02 9.68900763D-02 3.60380206D-01 2.63664581D-02 6.43121293D-02 0.00
```

As mentioned before, this output should not be considered reliable. The calculation has not fully converged and the validity of the optical potentials has not been checked.

References

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