# User's manual for `Boscos.f`

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## 1 Introduction

The program `Boscos` is a small Fortran 90 computer code that solves the Schrödinger equation to compute bound states or stationary continuum states in the continuum for two pointlike particles, 1 and 2, interacting through a local real potential. Such a two-body system is described by the Hamiltonian

$$H(\boldsymbol{r}) = -\frac{\hbar^2}{2\mu}\Delta + V(r), \tag{1}$$

where $\mu = M_1 M_2/(M_1+M_2)$ is the reduced mass of particles 1 and 2 (of masses $M_1$ and $M_2$, respectively), $\boldsymbol{r}$ is their relative coordinate and $V$ is the local potential that simulates their interaction. That potential may include a spin-orbit coupling term.

In partial wave $slj$, where $s$ is the total spin of the system, $l$ is the orbital angular momentum and $j$ is the total angular momentum, the program solves the radial Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u_{slj}(r) + \left[\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V(r)\right] u_{slj}(r) = E\ u_{slj}(r). \tag{2}$$

The negative-energy states (i.e. with $E < 0$) correspond to bound states. Since they are discrete, in addition to the partial-wave quantum numbers $s$, $l$, and $j$, they are identified with the number of nodes in the radial wave function $n$. `Boscos` provides, if they exist, the binding energy and ANC of a given set of bound states of a local potential. The code can also provide the radial wave function for one of these states.

The positive-energy states ($E > 0$) correspond to the continuum states describing the particles 1 and 2 moving around each other freely. `Boscos.f` computes the phaseshift in required partial waves at different energies on a uniform grid. It can also provide the wave function for a bin state in the continuum obtained by integration of radial wave functions over a set of energies in the continuum.

After compilation, e.g., through the command

```
gfortran Boscos.f -o Boscos.out
```
(3)

the program can be executed through

```
Boscos.out < Be11BS.dat
```
(4)

In the following sections are examples of an input file and an output files, with a detailed explanations of their variables and structures.

## 2 Input File

An example of an input file for `Boscos` is given here for the archetypical one-neutron halo nucleus $^{11}$Be described as a neutron loosely bound to an inert $^{10}$Be core assumed in its $0^+$ ground state. The $^{10}$Be-n potential has the Woods-Saxon form developed in Ref. [1]. 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 21.000 2.585 0.6 2.585 * (j,l),Vp,rp,ap,VLS,rls,als,rC
-62.52 2.585 0.6 21.000 2.585 0.6 2.585 * (j,l),Vp,rp,ap,VLS,rls,als,rC
2                                       * Nel:nb of bound states
1 1 0 0 1 1                             * bound states:NR,J,l
20000 100 1e-6                          * radial mesh:Nru,rmu,eps
1 1.0 1.0                               * Energies:NE,E0,hE
0                                       * lec 0:E,10:wf 1st state,100:phaseshift,110 bin
Be11testBS                              *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` $\approx 20.9008$ MeV fm$^2$).

**Nucleus 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 calculation.

**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:

$$V_{cf}(r) = V_p\ f(r, r_p, a_p) + \boldsymbol{l}\cdot\boldsymbol{S_f}\ V_{pp}\frac{1}{r}\frac{\partial}{\partial r}f(r, r_{pp}, a_{pp}) + V_C(r, r_C), \tag{5}$$

   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. (7)]. The Woods Saxon form reads

$$f(r, r_0, a) = \left[1 + \exp\left(\frac{r - r_0}{a}\right)\right]^{-1}. \tag{6}$$

The Coulomb potential $V_C$ has a point-sphere expression:

$$V_C(r, r_C) = \begin{cases} \frac{Z_c Z_f}{2r_C} \frac{e^2}{4\pi\epsilon_0} \left(3 - \frac{r^2}{r_C^2}\right) & r < r_C \\ \frac{Z_c Z_f}{r} \frac{e^2}{4\pi\epsilon_0} & r \geq_C \end{cases} \tag{7}$$

2. A Gaussian form with central and surface terms:

$$V_{cf}(r) = V_p \; g(r, r_p, a_p) + V_{pp} \; r^2 g(r, r_{pp}, a_{pp}) + V_C(r, r_C), \tag{8}$$

with the Gaussian form

$$g(r, r_0, a) = \exp\left[-\frac{(r - r_0)^2}{2a^2}\right]. \tag{9}$$

The Coulomb interaction is the point-sphere potential (7).

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 $l$s, while the second corresponds to the even $l$s.

`*(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. (5)–(9).

**Information about the bound states of the projectile**

`* Nel:nb of bound states`

Number of bound states to be computed, or number of partial waves in which the phaseshift is required (integer).

`* bound states:  NR,J,l.`

On one line are given for each bound state the number of radial node (integer), the total angular momentum `J` (integer, multiplied by two if $S_f$ is half integer), and the orbital momentum `l` (integer). If the phaseshifts are required, they correspond to the partial waves in which the phaseshifts have to be computed. In that case, `NR` is read but not considered.

**Discretisation mesh**

`* radial mesh:Nru,rmu,eps`

`Nru` gives the number of points on the uniform radial mesh used to compute the bound and continuum $c$-$f$

states (integer). `rmu` is the last point of the mesh $r_{\max}$ given in fm (real). `eps` is the numerical accuracy required (real number)

**Selection of the output**

`* NE,E0,hE`: mesh in the $c$-$f$ continuum energies $E$ at which the phaseshift is requested. It is also used to build the continuum bin wave function when `lec` = 110 (see below). `NE` is the number of energies (integer), `E0` is the lowest energy at which the phaseshift is computed (real in MeV), and `hE` is the step size in energy (real in MeV).

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

For `lec` =

- 0: `Boscos` computes the energies and ANCs of the bound states listed above.
- 10: in addition, `Boscos` provides in the file with extension `.dfo` the radial wave function of the first state listed above.
- 100: `Boscos` computes continuum states.
  When `NE` $> 1$ its provides the phaseshifts in all the partial waves given below `Nel`. The values are listed in the output file with the extension `.dep`. If `NE` $= 1$ then the wave function of the continuum state at that energy `E0` is provided in the first partial wave listed below `Nel`.
- 110: a continuum bin wave function is built by integration of single continuum wave functions over the energy range provided above. The corresponding radial wave function is provided in the file with extension `.dfo`.

`* 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 `Boscos` depends on `lec`. The output file is named by adding an extension to the name given in input.

If `lec` = 0 no output file is added: the results of the calculations (binding energies and ANCs) are printed in the standard output.

When `lec` = 10, the extension `.dfo` is added. That file is structured in columns. The first column gives the radius $r$ in fm. The second gives the (reduced) radial wave function $u_{slj}$ of the first state listed below `Nel`. The third column contains the asymptotic behaviour of the wave function, viz. a Whittacker function multiplied by the ANC (in fm$^{-1/2}$). The fourth column contains the effective potential $V(r) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}$ in MeV.

When `lec` = 100:

- If `NE` $> 1$, the extension `.dep` is added. The output file is also structured in columns. The first one contains the energy $E$ in MeV. The second one contains the phaseshift in radian. The third one contains the numerical derivative of the phaseshift with energy obtained with a Simpson method (in rad/MeV). The fourth columns contains a function of the phaseshift that enables one to infer the scattering lenth: $-\tan\delta_{lj}/k^{2l+1}$.
- If `NE` $= 1$, the extension `.dfo` is added. That file is structured in columns. The first column gives the radius $r$ in fm. The second gives the (reduced) radial wave function $u_{slj}$ of the continuum state

computed at that sole energy `E0` within the first partial wave listed below `Nel`. The third column contains the asymptotic behaviour of the wave function: $\cos\delta_{lj}F_l(\eta,kr) + \sin\delta_{lj}G_l(\eta,kr)$, where $F_l$ and $G_l$ are the regular and irregular Coulomb wave functions. The fourth column contains the regular Coulomb wave function at that energy.

When `lec` = 110, the extension `.dfo` is added. That file exhibits two columns. The first gives the radius $r$ in fm. The second gives the (reduced) radial wave function $u_{slj}$ of the bin continuum state corresponding to the first partial wave listed below `Nel`.

# References


[1] P. Capel, G. Goldstein, and D. Baye. Time-dependent analysis of the breakup of $^{11}$Be on $^{12}$C at 67$A$ MeV. *Phys. Rev. C*, 70:064605, Dec 2004.