

User Guide for DRHBc Mass Table Calculation

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Outline

□ Introduction

□ How to calculate a nucleus

□ How to collect results

□ Notice

Introduction

- The **DRHBc code** is a numerical program based on Fortran, and can solve the deformed relativistic Hartree-Bogoliubov equation with a Dirac Woods-Saxon basis.
- The first version of the DRHBc code was developed by Prof. Shan-Gui Zhou and his collaborators, starting from 1998.
- The latest released version of DRHBc code for mass table calculations is **Code_DRHBc_202112**.

[DRHBc Mass Table Collaboration, PRC 106,014316 \(2022\)](#)

The updated **Code_DRHBc_202401** will be released soon.

What do we need to do?

- Principal investigators need to (i) submit **calculations**, (ii) check the **outputs**, and (iii) summarize the results into a **table**, including binding energy, deformation, rms radius, etc.

- If you found something interesting or have new ideas based on DRHBc, it is encouraged to discuss them with collaborators and publish papers.


E.g., halo, shape coexistence, new magic number, alpha decay, proton emission, recent experimental data ...














































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Files of DRHBc code

Input file



 dir.dat	 drhblib.f	 potel.f
 readme_dir.dat	 drhbws.f	 prep.f
 ana.f	 ecm_mic.f	 reader.f
 basis.f	 erot.f	 rungdi.f
 broyden.f	 expect.f	 rungdo.f
 can.f	 field.f	 sort.f
 canws.f	 gaussj.f	 splout.f
 ccom.f	 gordon.f	 start.f
 default.f	 inout.f	 startws.f
 densave.f	 iter.f	 paramet.for
 densit.f	 jmat.f	 change.log
 densit_can.f	 lam.f	 makefile
 densit_canws.f	 lev_can.f	 mpireadme
 densit_lev.f	 mpi.f	
 diagm.f	 norm_check.f	
 dirac0.f	 pair.f	

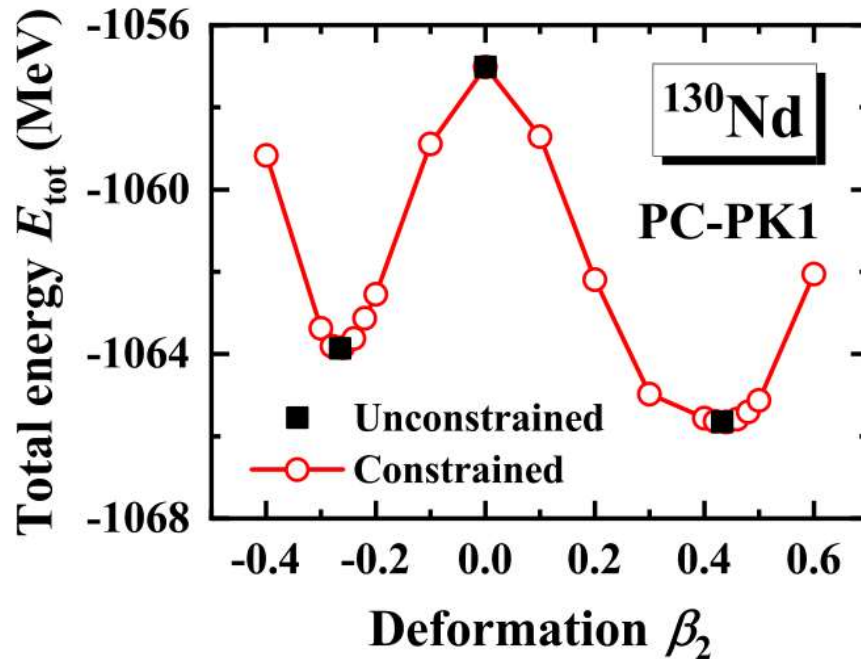
How to submit a calculation

- Compile the code, modify input file, and run 1drhbws.

- **Example 1:**
Calculate ^{20}Ne , with initial deformation $\beta_0 = 0.4$.

Constrained calculation

- In a constrained calculation, the deformation is constrained to a given value, not determined by iteration.



Potential energy curve (PEC)

- **Example 2:**
Calculate ^{20}Ne , with deformation constrained to $\beta_{2,\text{cst}} = 0.35$.

Calculation with given initial potentials

- In some cases, we need to do calculations starting from a given potential file dir.wel.

- **Example 3:**
Calculate ^{20}Ne , starting from converged potential.

Blocking effect for odd nucleus

- When neutron or proton number is odd, the blocking effect of the odd nucleon should be considered.

- **Example 4:**
Calculate ^{21}Ne , with initial deformation $\beta_{\text{ini}} = 0.2$.

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What results are needed

- The head of the DRHBc mass table for **even-even** nuclei:

A	N	E_b^{cal} (MeV)	$E_{b+\text{rot}}^{\text{cal}}$ (MeV)	E_b^{exp} (MeV)	S_{2n} (MeV)	S_{2p} (MeV)	R_n (fm)	R_p (fm)	R_m (fm)	$R_{\text{ch}}^{\text{cal}}$ (fm)	$R_{\text{ch}}^{\text{exp}}$ (fm)	β_{2n}	β_{2p}	β_2	λ_n (MeV)	λ_p (MeV)
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- Therefore, the following results should be extracted:
 - ✓ E_{tot} , E_{cm} , E_{rot}
 - ✓ β_{2n} , β_{2p} , β_2
 - ✓ r_n , r_p , r_m , r_c
 - ✓ λ_n , λ_p
 - ✓ blocked orbital
- **Example 5:**
Extract the results of a calculation.

Procedure to find the ground state

- To correctly find the ground state of a nucleus, firstly one needs to find where is the corresponding deformation minimum.
- Either of the two methods can be applied:

Method 1

- For each nucleus, independently perform the calculations with 11 initial deformations ($\beta_0 = -0.4, -0.3, \dots, 0.6$).
- Take the result with the **lowest** E_{totcm} as the ground state.

Method 2

- For each nucleus, construct the PEC, and determine the deformation minima.
- Perform unconstrained calculations near the minima, and find the ground state.



One can contact HKU team for more details.

Data collection

- Based on the calculations, summarize a data table and determine ground-state properties according to Etotcm.
- One can use a bash script (or other tools) as an assistant.
- **Example 6:**
Determine the ground states for $^{159,161}\text{Cs}$.

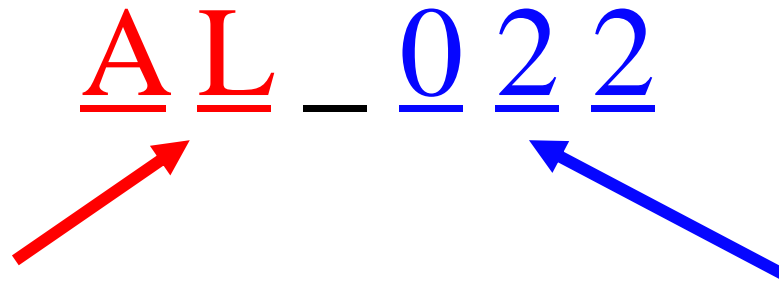
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Nuclide symbol

```
l6      = 10
rmax    = 20.00
xstep   = 0.10
maxi    = 101      902      ! max iteration step
xmix    = 0.4
inin    = 1        ! 1: start from DWS potential, 0: start from dir.wel
levin   = 1
AL 022  ! nuclide symbol
beta    = 0.40      0      ! [1st] initial deformation; [2nd] NNTC
match0  = 25
Ecut    = 300.000   10000.000
ibry ist = 1      40
iext ire = 0      0      1
Neu. blk = 2      1      1      1      ! [1st] 0:no block, 1:orbit-fix, 2:auto; [2nd-4th], m, ip, lb
Pro. blk = 2      1      1      1      ! [1st] 0:no block, 1:orbit-fix, 2:auto; [2nd-4th], m, ip, lb
Trap CAN
```

- Notice the format of the nuclide symbol:



Element name: 2 characters, all capitalized. Mass number: 3 characters

- For the one-letter element, e.g., I - 107

Legendre expansion truncation

- The Legendre expansion truncations in different nuclear regions are different.

They are modified in the file `paramet.for`.

$$\lambda_{\max} = \begin{cases} 6, & (8 \leq Z \leq 70) \\ 8, & (71 \leq Z \leq 100) \\ 10, & (101 \leq Z \leq 120) \\ \text{checks in progress} & (Z \geq 121) \end{cases}$$

- **Example 7:**
Unconstrained calculations for superheavy nucleus ^{300}Og ($Z = 118$).

Notices on convergence

- In a few cases, the iteration does not converge after maxi steps, and they should **NOT** be taken as the ground state. Empirically, about 10% calculations fail to converge.
- For an odd system, due to the blocking effect, the calculation may be more difficult to converge and consume more time.
- If the unconverged point is the possible ground state, then **constrained calculations** are needed for confirmation.

Thanks for your attention!