PPRPA Code

Version 1, 2015

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1 Introduction

Calculations of nuclear structure and transitions are still an important research topic. There are a number of well-known codes such as OXBASH [1]. The purpose of this paper is to present an improved version of a computer program for calculating nuclear structure and transition densities. The main advantage is its user friendly interface build using Intel® Visual Fortran Composer XE 2013 for Windows. The program will be useful for research students and also for teaching undergraduate and postgraduate courses in nuclear structure.

This manual describes the version 1, 2015 of Particle-Particle Random Phase Approximation (PPRPA) code that can be used on Windows PCs. PPRPA code is a graphical user interface (GUI) Fortran program for carrying out the calculations of nuclear structure of nuclei having closed core ± 2 nucleons. The

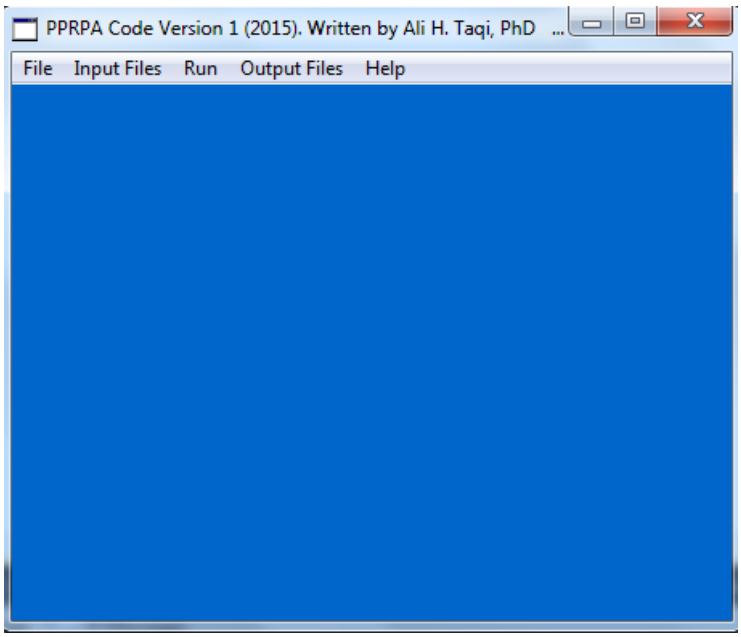
program has been constructed in the total angular momenta and isospin (JT) scheme to solve the particle–particle (pp) and hole–hole (hh) Tamm-Dancoff Approximation (TDA) and Random Phase Approximation (RPA). The Hamiltonian is to be daigonalized with a given input model space, single-particle energies and interaction. Space function has been expanded to include orbits s, p, d, f, g and h, but the current version of the code allows the user to test 20 orbits only. The single-particle density, charge density distribution and transition density are calculated in the basis of the harmonic oscillator (HO). We have also significantly improved the capabilities of the program as far as plotting of the functions and the associated densities through the call of module file for DISLIN Fortran 90- Version 10.5 [2].

[1] B. A. Brown and W. D. M. Rae, Nushell@MSU, MSU-NSCL report (2007).

[2] Helmut Michels, Max Plank Institute for Solar System research, http://www.max-planck-innovation.de

2 Setup

Make a directory and extract compressed file PPRPA.rar on it. Executable file PPRPA (Type: Application) initialize the code and the following interface window will appear. If you get any message of missing files, please setup the Redistributable Libraries Packages for Intel® Composer XE compiler (obtained in utilities folder involved with the code package). The redistributable library packages are for the end users who use applications that are built with Intel Compilers.



3 How to use the code

We describe here how to use the code. The input files contains the values need to be modified according to the studied nucleus before running the code, after that many output files will be created.

3.1 Input Files

Choosing (`Input files`) will open a sub-menu which consist a number of files:

Particle shells (p_shells.dat)**:** This contains a list of particle orbits (occupied states) set as follows:

Line 1: `m` (number of orbits)

Line 2: `I, n, l, 2j` (`I` is a label of orbit, `n, l, j` are principle, orbital and total quantum numbers)

.

Line `m: I, n, l, 2j`

Hole shells (h_shells.dat)**:** This contains a list of hole orbits (unoccupied states) set as follows:

Line 1: `m`

Line 2: `I, n, l, 2j`

.

Line `m: I, n, l, 2j`

Interaction (files.dat)**:** This contains a list of parameters for interaction set as follows:

- If one intends to perform the calculations with using modified surface delta interaction (msdi):

  Line 1; `1`

  Line 2: `msdi`, `correction` (`correction` is a factor to be multiplied by two-body matrix, default value is 1.0)

Line 3: `A0, A1, B, C` (`A0, A1, B` and `C` are msdi interaction parameters)

- Or using interaction file in isospin formalism (see Appendix A for provided sample of spsdpfmw.int). Note, the input file could be a number of files each one is specific for a certain shell:

  Line 1: `m` (number of files)

  Line 2: `name of file 1, correction`

  .

  Line m: `name of file m, correction`

Single particle energies (SpEnergy.dat)**:** This contains a list of single particle energies set as follows:

Line 1: `m` (number of orbits)

Line 2: `I, ε` (`I` is a label of orbit and ε is a single particle energy)

.

Line `m: I, ε`

General (RPAPP11.dat)**:** This contains the general input parameters as follows:

Line 1: `jA, jZ, core, shift` (`jA` is a mass number, `jZ` is an atomic number, `core` is a number of closed core nucleons, if `jA=core+2` the code will do the particle-particle pp calculations, but if `jA=core-2` the hole-hole hh calculations will be done. `Shift` is energy required to zeroing ground)

Line 2: `vmode` (`vmode` is a calculation mode set to either `tda` or `rpa`)

Line 3: `cmode, m` (if `cmode` set to `allj`, the calculations will automatically run for all possible J, T and parity, then the program will bypass `m`. But if `cmode` set to `onlyj`, the calculations will run for `m` specified J, T and parity)

Line 4: `J, T, parity` (`J` is total angular momenta, `T` is isospin and `parity` set to 1.0 or -1.0)

.

Line m: `J, T, parity`

Single-particle HO density (spDinput.dat)**:** This contains the input parameters of single-particle harmonic-oscillator (HO) potential wave and density functions set as follows:

Line 1: `n, l, brms, rmax` (`n` is a principle quantum number, `l` is an orbital quantum number, `brms` is root-mean square (rms) charge radii of HO potential and `rmax` is the upper limit of radius `r`).

Line 2: `jplot` (set `jplot=1` for plotting a graph, or `=0` to skip plot).

Line 3: `jplottype` (set `jplottype`=0 for plotting a function rR, or `=1` to plot density r^2R^2)

Line 4: `Xtitle` (`Xtitle` is the title of the x-axis).

Line 5: `Ytitle` (`Ytitle` is the title of the y-axis).

Line 6: `Gtitle` (`Gtitle` is the title of the graph).

Line 7: `joptions` (set `joptions=0` for automatic graph parameters, or `=1` for reading parameters of the following).

Line 8: `XA, XE, XOR, XSTEP, YA, YE, YOR, YSTEP`

(`XA, XE` are the lower and upper limits of the X-axis. `XOR, XSTEP` are the first X-axis label and the step between labels. `YA, YE` are the lower and upper limits of the Y-axis. `YOR, YSTEP` are the first Y-axis label and the step between labels).

Line 9: `XNDIG, YNDIG` (number of digits after the decimal point displayed in labels, -1 defines integer labels, 0 defines integer labels followed by a decimal point, n (1, 2,..) defines the number of digits after the decimal point. The last digit will be rounded up).

Line 10: `GridOn` (`1`=grid on, `0`=grid off).

Line 11: `FileF` (is a character string that defines the file format (extension), like: `XWIN` (defines a window for graphical output), `pdf, eps, ps, gif, tiff, png, bmp`).

Line 12: COLOR defines the colors used for plotting).

Line 13: TickOn, TickNo (1=Tick on, 0=Tick off and TickNo is the number of ticks).

Charge density distribution (CDDinput.dat)**:** This contains the input parameters of calculations of charge density distribution in the basis of HO wave function set as follows:

Line 1: A, Z, brms, rmax

Line 2: n, l, 2j, OccNo (OccNo is the occupation probability of the state $n\ell j$. Hence, we set OccNo = 0.0 or 1.0 for closed shell nuclei and 0<OccNo< 1 for open shell nuclei with partially filled state).

Line 3: n, l, 2j, OccNo

.

Line m: 0 0 0 0 0.0 (stop).

Line m+1: jplot (set jplot=1 for plotting a graph, or =0 to skip plot).

Line m+2: Xtitle (Xtitle is the title of the x-axis).

Line m+3: Ytitle (Ytitle is the title of the y-axis).

Line m+4: Gtitle (Gtitle is the title of the graph).

Line m+5: joptions (set joptions=0 for automatic graph parameters, or =1 for reading parameters of the following).

Line m+6: XA, XE, XOR, XSTEP, YA, YE, YOR, YSTEP

(XA, XE are the lower and upper limits of the X-axis. XOR, XSTEP are the first X-axis label and the step between labels. YA, YE are the lower and upper limits of the Y-axis. YOR, YSTEP are the first Y-axis label and the step between labels).

Line m+7: XNDIG, YNDIG (number of digits after the decimal point displayed in labels, -1 defines integer labels, 0 defines integer labels followed by a decimal

point, n (1, 2,..) defines the number of digits after the decimal point. The last digit will be rounded up).

Line m+8: GridOn (1=grid on, 0=grid off)

Line m+9: FileF (is a character string that defines the file format (extension), like: XWIN (defines a window for graphical output), pdf, eps, ps, gif, tiff, png, bmp).

Line m+10: COLOR (defines the colors used for plotting.)

Line m+11: TickOn, TickNo (1=Tick on, 0=Tick off, and TickNo is the number of ticks.)

Transition density (TrDinput.dat)**:** This contains the input parameters for calculating transition density based on HO potential wave function using amplitudes of PPRPA calculations set as follows:

Line 1: jA, jZ, vmode, brms, rmax

Line 2: Jf, Tf, JPf, kf (J, T, JPf is parity [set 0 or 1 for +Ve or –Ve parity], and k [state number] of the final state).

Line 3: Ji, Ti, JPi, ki [initial state parameters].

Line 4: ep, en (ep and en are effective charges of proton and neutron).

Line 5: jplot (set jplot=1 for plotting a graph, or =0 to skip plot).

Line 6: Xtitle (Xtitle is the title of the x-axis).

Line 7: Ytitle (Ytitle is the title of the y-axis).

Line 8: Gtitle (Gtitle is the title of the graph).

Line 9: joptions (set joptions=0 for automatic graph parameters, or =1 for reading parameters of the following).

Line 10: XA, XE, XOR, XSTEP, YA, YE, YOR, YSTEP

(XA, XE are the lower and upper limits of the X-axis. XOR, XSTEP are the first X-axis label and the step between labels. YA, YE are the lower and upper limits of the Y-axis. YOR, YSTEP are the first Y-axis label and the step between labels).

Line 11: XNDIG, YNDIG (number of digits after the decimal point displayed in labels, -1 defines integer labels, 0 defines integer labels followed by a decimal point, n (1, 2,..) defines the number of digits after the decimal point. The last digit will be rounded up).

Line 12: GridOn (1=grid on, 0=grid off).

Line 13: FileF (is a character string that defines the file format (extension), like: XWIN (defines a window for graphical output), pdf, eps, ps, gif, tiff, png, bmp).

Line 14: COLOR defines the colors used for plotting).

Line 15: TickOn, TickNo (1=Tick on, 0=Tick off, and TickNo is the number of ticks).

3.2 Run

Choosing (Run) will give you two alternatives,

1) **Run PPRPA:** execute the whole PPRPA program,
2) **Calculate:** also gives you two alternatives,
   i) **Single-particle density:** the calculations will run for a single-particle HO wave and density function.
   ii) **Charge density distribution:** the calculations will run for a charge density distribution.
   iii) **Transition density:** do the calculations of transition density

If the file format is "xwin", the graph of the created file will be displayed in a window.

3.3 Output files

Choosing (Output files) will open a sub-menu which consist a number of files:

Eigenvalues: Display the `eigenvalues.txt` file of the calculated eigenvalues.

Eigenvectors: Display the `eigenvctors.txt` file of the calculated eigenvectors.

Configurations: Display the `configurations.txt` file of the all possible configurations as well as some details of the calculations, like matrices of TDA and RPA.

Other files: Shows the name and the location of all the created files in a specific folder for each energy.

Density files: will give you two alternatives,

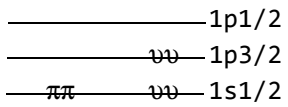
i) **Single-particle density:** Display the file `CCDout.dat` for the calculated charge density distribution.

ii) **Charge density distribution:** Display the file `CCDout.dat` for the calculated charge density distribution.

iii) **Transition density:** Shows the name and the location of the created file in a specific folder for the calculated transition density.

4 Example Run

The nucleus $^{6}_{2}He_{4}$ is an example of two-particle nucleus with two neutrons in 1p shell.



Example run input:
Particle shells:

```
2
2 1p3
3 1p1
```

Hole shells:

```
1
1 1s1
```

Interaction:

```
1
msdi 1.0
1.0 1.0 0.0 0.0   msdi interaction parameters A0, A1, B and C

Or, write the names of interaction files. We provided the files of wbp
interaction:
3
```

```
spsdpfmw.int   1.0  correction=Matrix elements*(18/A)^(0.3) for sd-shell
spsdpfpb.int   1.0
0s0f1p0.int    1.0
```

Single particle energies:

```
3
1 -23.0     *1s1/2
2 0.0        *1p3/2
3 6.0       *1p1/2
```

General:

```
6 2 4 0.0  (A, Z, CORE, GROUND ENERGY)
rpa
allj  0    (allj:  all possible J, T and parity)
```

Single-particle density:

```
1 0 1.7 7        (n, l, brms, rmax)
1
1
1s Radial HO Density
r(fm)
Density in (1/fm)
1
1=input parameters
0.0 10.0 0.0 1.0 0.0 0.6 0.0 0.1
-1 1
1
xwin
red
1   10
```

Charge density distribution:

```
6 2 1.7 6         (A, Z, brms, rmax)
1 0 1 1.          (n, l, 2j, occupation number)
1 1 3 0.25
0 0 0 0.
1
Charge Density Distribution
r(fm)
Density in (Ze.1/fm^3)
1
0.0 6.0 0.0 1.0 0.0 0.08 0.0 0.02
-1  2
1
xwin
red
0   10
```

Transition density: We need firstly to run PPRPA to obtain eigenvalues and eigenvectors.

```
6 2 rpa 1.7 7  (A, Z, mode, brms, rmax)
2 1 0 1     (Jf, Tf, JPf, kf, where the dada read from the file He2101.rpa)
0 1 0 1     (Ji, Ti, JPi, ki, where the dada read from the file He0101.rpa)
1.0 0.0     (ep, en)
1
Transition Charge Density
r(fm)
Density (e/fm^3)
1
0.0 7.0 0.0 1.0 0.0 0.016 0.0 0.002
-1  3
0
xwin
red
0   10
```

Example run output:

Eigenvalues:

```
He6

 ___________________________________________
J= 0(3)=  45.0694351 MeV     T=1, parity=+
J= 0(2)=  11.1311865 MeV     T=1, parity=+
J= 0(1)=  -2.2006216 MeV     T=1, parity=+
 ___________________________________________________
J= 1(1)=   6.0000000 MeV     T=1, parity=+
 ___________________________________________________
J= 2(2)=   5.2565713 MeV     T=1, parity=+
J= 2(1)=  -0.4565713 MeV     T=1, parity=+
 -------------------------------------------
```

Eigenvectors:

```
He6
J= 0  T=1  Parity=+
 -----------------------------------------------
Created file: He6\He0103.rpa       ENERGY=  45.0694  MM=M1+M2=  3
  a  b   Vectors(T=0)  Vectors(T=1)
  2  2   0.00000E+00  -0.29176E-01
  3  3   0.00000E+00  -0.28117E-01
  1  1   0.00000E+00   0.99918E+00
Created file: He6\He0102.rpa       ENERGY=  11.1312  MM=M1+M2=  3
  a  b   Vectors(T=0)  Vectors(T=1)
  2  2   0.00000E+00  -0.10968E+00
  3  3   0.00000E+00   0.99366E+00
  1  1   0.00000E+00   0.24759E-01
Created file: He6\He0101.rpa       ENERGY=  -2.2006  MM=M1+M2=  3
  a  b   Vectors(T=0)  Vectors(T=1)
```

```
  2  2   0.00000E+00   0.99354E+00
  3  3   0.00000E+00   0.10887E+00
  1  1   0.00000E+00   0.32075E-01
____ END FOR J= 0 T=1 Parity=+  _____


J= 1  T=1  Parity=+
 ------------------------------------------------
Created file: He6\He1101.rpa       ENERGY=   6.0000  MM=M1+M2=  1
  a  b   Vectors(T=0)  Vectors(T=1)
  2  3   0.00000E+00   0.10000E+01
____ END FOR J= 1 T=1 Parity=+  _____


J= 2  T=1  Parity=+
 ------------------------------------------------
Created file: He6\He2102.rpa       ENERGY=   5.2566  MM=M1+M2=  2
  a  b   Vectors(T=0)  Vectors(T=1)
  2  2   0.00000E+00  -0.99509E-01
  2  3   0.00000E+00   0.99504E+00
Created file: He6\He2101.rpa       ENERGY=  -0.4566  MM=M1+M2=  2
  a  b   Vectors(T=0)  Vectors(T=1)
  2  2   0.00000E+00   0.99504E+00
  2  3   0.00000E+00   0.99509E-01
____ END FOR J= 2 T=1 Parity=+  _____


J= 3  T=1  Parity=+
 ------------------------------------------------
 There are no possible states
____ END FOR J= 3 T=1 Parity=+  _____


J= 0  T=1  Parity=+
 ------------------------------------------------
 There are no possible states
____ END FOR J= 0 T=1 Parity=+  _____


J= 1  T=1  Parity=+
 ------------------------------------------------
 There are no possible states
____ END FOR J= 1 T=1 Parity=+  _____

J= 2  T=1  Parity=+
 ------------------------------------------------
 There are no possible states
```

```
____ END FOR J= 2 T=1 Parity=+  _____

J= 3  T=1  Parity=+
 ------------------------------------------------
 There are no possible states
____ END FOR J= 3 T=1 Parity=+  _____

J= 0  T=1  Parity=-
 ------------------------------------------------
 There are no possible states
____ END FOR J= 0 T=1 Parity=-  _____

J= 1  T=1  Parity=-
 ------------------------------------------------
 There are no possible states
____ END FOR J= 1 T=1 Parity=-  _____

J= 2  T=1  Parity=-
 ------------------------------------------------
 There are no possible states
____ END FOR J= 2 T=1 Parity=-  _____

J= 3  T=1  Parity=-
 ------------------------------------------------
 There are no possible states
____ END FOR J= 3 T=1 Parity=-  _____
```

Configurations:

```
He6
J= 0  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
 (1p 3/2)(1p 3/2)    2  2
 (1p 1/2)(1p 1/2)    3  3

 Possible Hole-Hole Configurations:
 (1s 1/2)(1s 1/2)    1  1
 Sub-Matrix A
    -2.00000    -1.41421
    -1.41421    11.00000
 Sub-Matrix C
   45.00000
```

```
 Sub-Matrix B
    -1.41421
    -1.00000
 FINAL MATRIX
    -2.00000    -1.41421    -1.41421
    -1.41421    11.00000    -1.00000
    -1.41421    -1.00000    45.00000
____ END FOR J= 0 T=1 Parity=+  _____

J= 1  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
 (1p 3/2)(1p 1/2)    2  3

 Possible Hole-Hole Configurations:
      No possible configurations
 Sub-Matrix A
     6.00000

 FINAL MATRIX
     6.00000
____ END FOR J= 1 T=1 Parity=+  _____

J= 2  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
 (1p 3/2)(1p 3/2)    2  2
 (1p 3/2)(1p 1/2)    2  3

 Possible Hole-Hole Configurations:
      No possible configurations
 Sub-Matrix A
    -0.40000    -0.56569
    -0.56569     5.20000


 FINAL MATRIX
    -0.40000    -0.56569
    -0.56569     5.20000
____ END FOR J= 2 T=1 Parity=+  _____

J= 3  T=1  Parity=+
 ------------------------------------------------
```

```
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 3 T=1 Parity=+  _____

J= 0  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 0 T=1 Parity=+  _____

J= 1  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 1 T=1 Parity=+  _____

J= 2  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 2 T=1 Parity=+  _____

J= 3  T=1  Parity=+
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
```

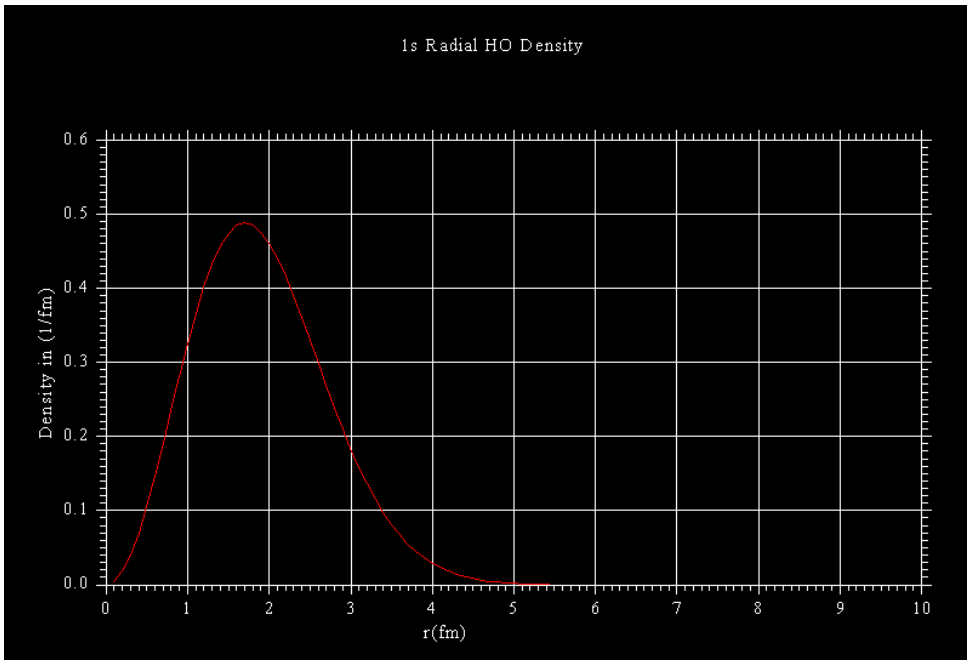
```
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 3 T=1 Parity=+  _____

J= 0  T=1  Parity=-
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations
 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 0 T=1 Parity=-  _____

J= 1  T=1  Parity=-
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 1 T=1 Parity=-  _____

J= 2  T=1  Parity=-
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
____ END FOR J= 2 T=1 Parity=-  _____

J= 3  T=1  Parity=-
 ------------------------------------------------
 ppRPA Calc.

 Possible Particle-Particle Configurations:
      No possible configurations

 Possible Hole-Hole Configurations:
      No possible configurations
```

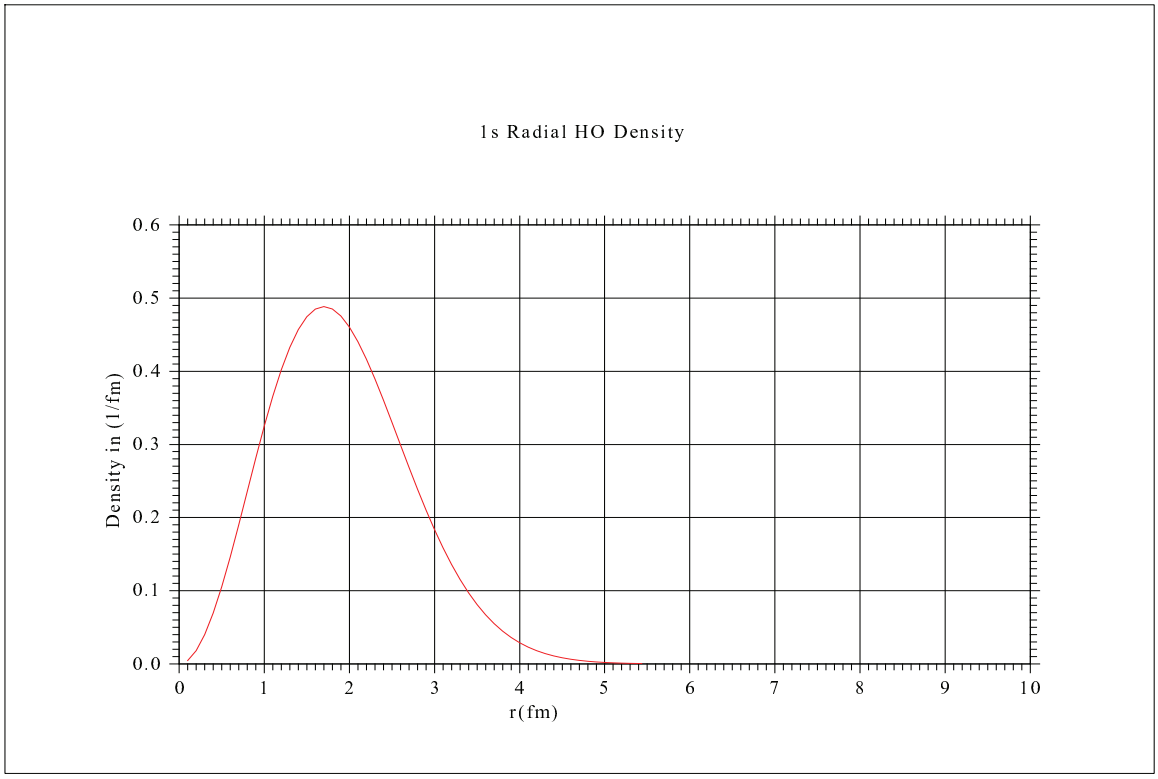
```
____ END FOR J= 3 T=1 Parity=-  _____
```

Other files:

```
He6
Created file: Code Location\He6\He0103.rpa       ENERGY=  45.0694
Created file: Code Location\He6\He0102.rpa       ENERGY=  11.1312
Created file: Code Location\He6\He0101.rpa       ENERGY=  -2.2006
Created file: Code Location\He6\He1101.rpa       ENERGY=   6.0000
Created file: Code Location\He6\He2102.rpa       ENERGY=   5.2566
Created file: Code Location\He6\He2101.rpa       ENERGY=  -0.4566
To open file: File -> Open -> Code location -> select folder -> select
file.
```

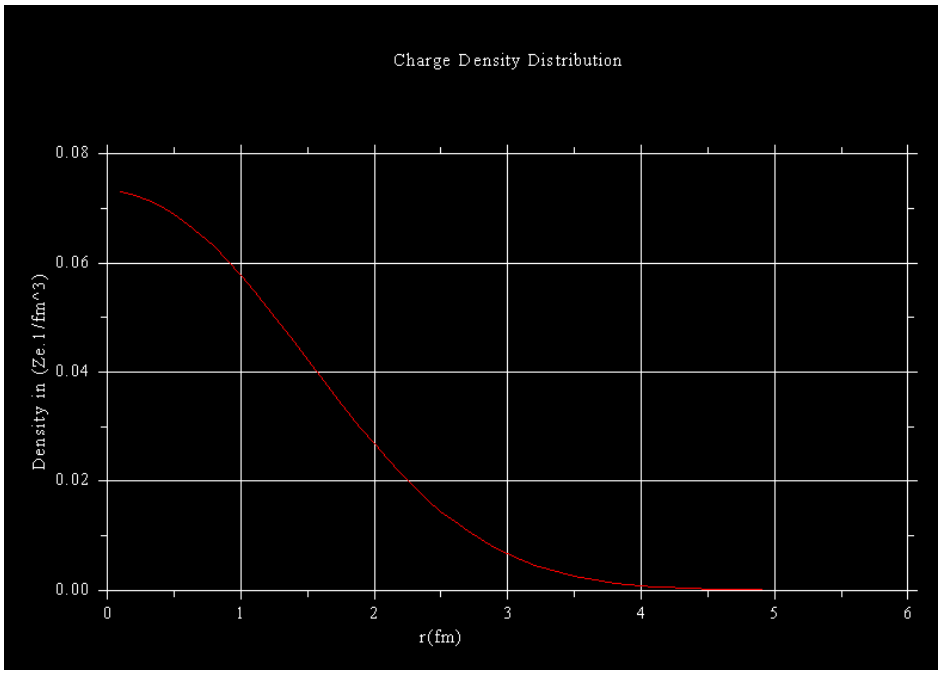
Single-particle density: the result of state-1s HO density are illustrated in the following figure in xwin and eps format, (Data File is spDout.dat and plot file is HO Density.eps)

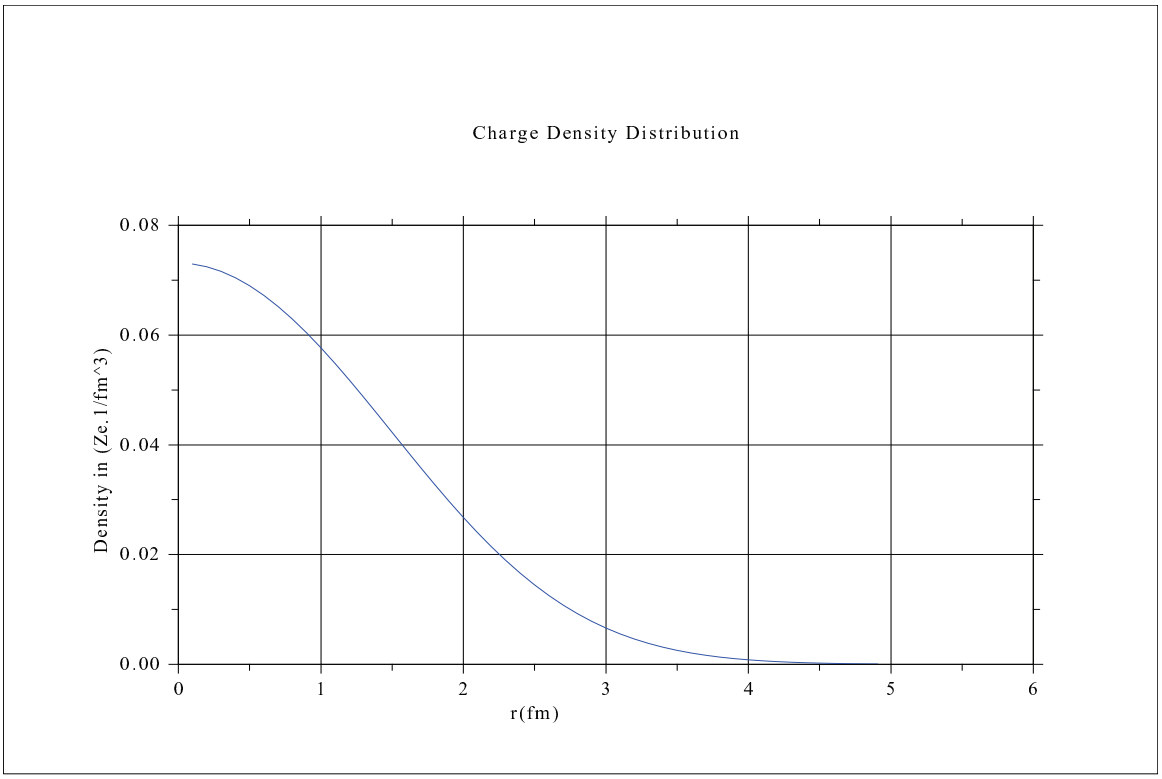




Charge density distribution: the results of ^{6}He, brms=1.7 are illustrated in the following figure in xwin and eps format, (Data File is CDDout.dat and plot file is ChargeD.eps).

The calculated value of the mean square charge radii (read from file CDDout.dat) is $\langle r^2 \rangle^{1/2}$=2.85

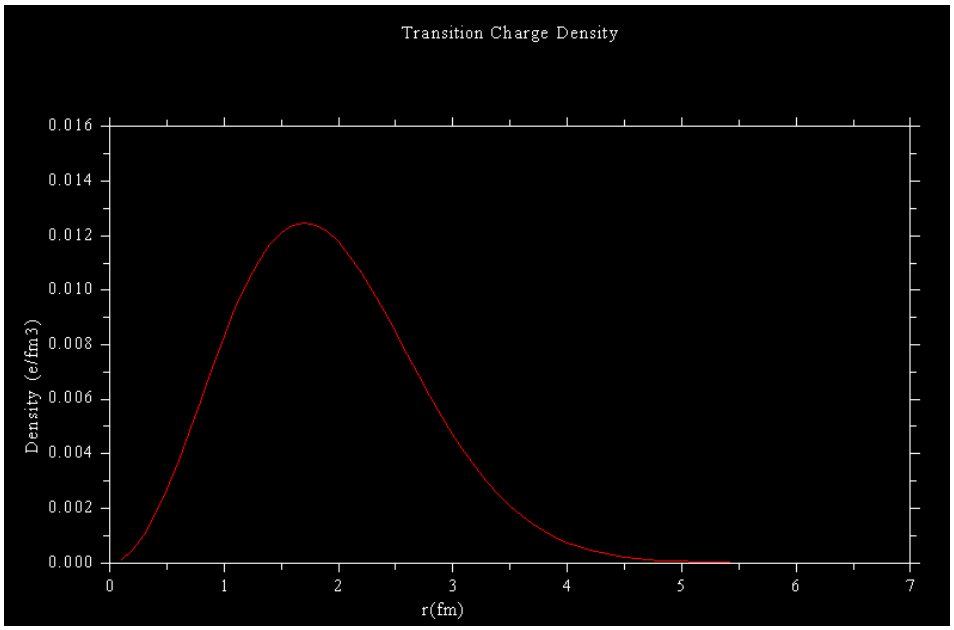


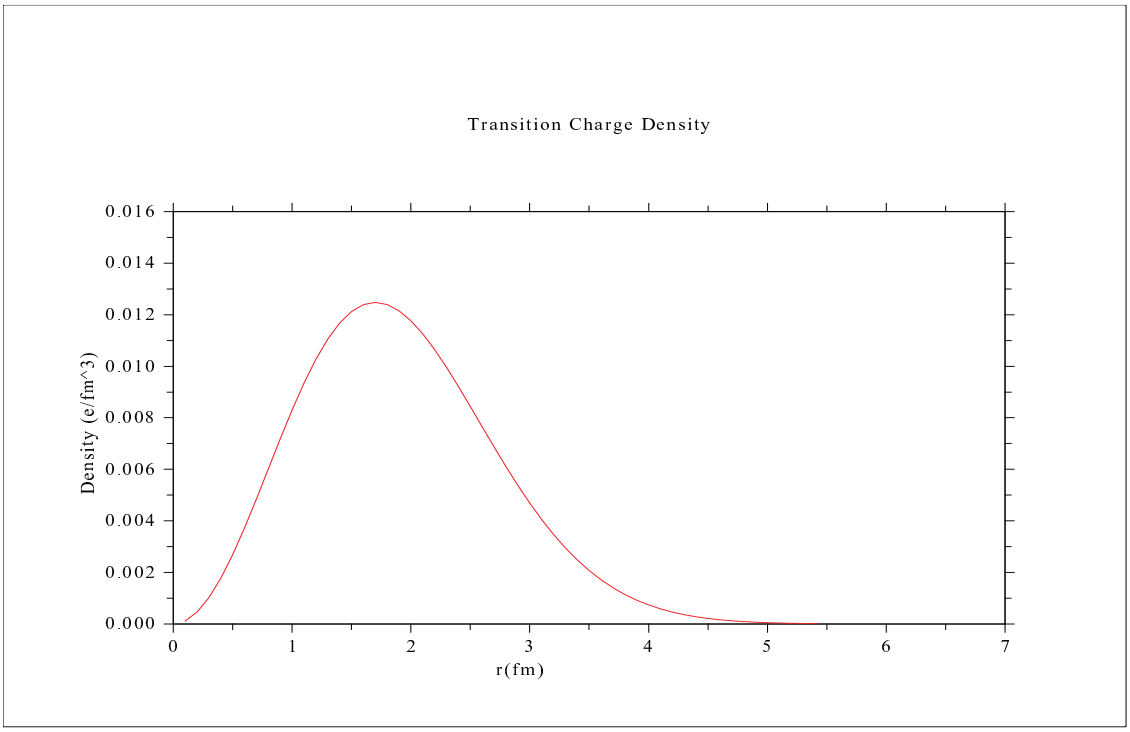


Transition density: the results of J = 2, T = 1, parity = +ve, transition density are illustrated in the following figure in xwin and eps format, (Data Files: TrDinput.dat and He6_Density\He2101.dat, and plot file is TransCD.eps).

The calculated value of the reduced transition probability (read from file Files.txt) is

$B(E2) = 0.22E+02\ e^2fm^4$





Appendix A Sample of interaction file in isospin formalism

```
N                        (N is a number of matrix elements)
j1 j2 j3 j4 J T M   (j1 is angular momenta of particle 1, J is total   angular
                         momenta,  T  is  isospin  and  M  is  two-body  matrix
                         element).

Example: (spsdpfmw.int)
768
   5  5  5  5    0  1    -2.18450
   5  5  5  5    1  0    -1.41510
   5  5  5  5    2  1    -0.06650
   .  .  .  .    .  .      .
   .  .  .  .    .  .      .
   .  .  .  .    .  .      .
```