a brief manual for AGPC-NPA

Y. Lei(雷杨)*[a] and Y. Lu(路毅)[b]

[a]School of National Defense Science and Technology, Southwest University of Science and Technology, Mianyang 621010, China
[b]College of Physics and Engineering, Qufu Normal University, 57 Jingxuan West Road, Qufu, Shandong 273165, China

July 8, 2020

Abstract

AGPC-NPA是被AGPC（Algorithm for General Pair Configuration）算法充分优化的M-scheme配对近似（nucleon-pair approximation，NPA）计算程序。本文主要向已有壳模型计算经验的核物理学者示例性地介绍这种程序的使用方法。

AGPC-NPA is an M-scheme Nucleon-Pair Approximation (NPA) calculation program, which has been fully optimized with the AGPC (Algorithm for General Pair Configuration) algorithm. This paper mainly aims to introduce the usage of this program to the nuclear physicists who already have experience in the shell-model calculations.

Contents

*leiyang19850228@gmail.com

1 Introduction

上世纪末本世纪初，陈金泉、赵玉民等给出了这种角动量守恒的集体对组态重叠与矩阵元递归计算公式，并发展为配对壳模式（Nucleon-Pair Shell Model, NPSM），亦称壳模型配对近似（Nucleon-Pair Approximation of shell model, NPA）[1]。最近何秉承、罗延安等也提出使用M-scheme思想来进行NPA计算[2]。AGPC-NPA则是在这些工作的基础之上引入我们称之为AGPC算法的优化方法，进而形成的程序。我们可以看到这一程序在减少计算耗时方面有优势。

At the end of the last century and early this century, Chen, Zhao and their collaborators proposed a recursive formalism for those collective pair configurations with angular-momentum conservation, and further developed the Nucleon-Pair Shell Model (NPSM), also known as Nucleon-Pair Approximation (NPA) [1]. Recently, He and Luo's collaborators also proposed M-scheme NPA framework [2]. AGPC-NPA code is based on these work, where the AGPC algorithm is introduced. We can see that this program has advantages in reducing computational time.

2 basic concept of NPA

这一章节是对NPA模型的简要介绍，读者或从文献[1]得到更加详尽的信息。NPA模型空间的构建基石为一系列精心优化的角动量-宇称守恒的"集体对"。这样的NPA集体对定义为：

This section provides a brief introduction to the NPA model. One may found more detail from Ref. [1]. In the NPA, the model space is constructed with several optimal "collective pairs" with definite angular-momentum and parity. The NPA collective pair is defined as

$$A_M^{L\dagger} = \sum_{ab} y(ab;L) A_M^{L\dagger}(ab),\ A_M^{L\dagger}(ab) = (c_a^\dagger \times c_b^\dagger)_M^{(L)}, \tag{1}$$

其中L与M这样的集体对所携带的角动量与其三分量。a和 b代表球形单粒子基矢的量子数，$\{nljm\}$。$\times$表示为两个单粒子的角动量耦合。$y(ab;L)$为该NPA集体对的结构系数。它可以用矩阵的形式进行表达，同时有反对称性

where L and M is the angular-momentum and its projection to principal axi, a and b represent the quantum numbers of spherical single-particle basis, $\{nljm\}$, $\times$ means the angular-momentum coupling, and $y(ab;L)$ is the

structural coefficient of this NPA collective pair. $y(ab;L)$ can be written in matrix format, and has anti-symmetric property as

$$y(ab;L) = -(-)^{L-j_a-j_b} y(ba;L) \tag{2}$$

与集体对定义类似，NPA中的单体算符定义为

Similarly to collective pair, the one-body operator of NPA is defined as

$$Q^k_\kappa = \sum_{ab} \mathcal{q}(ab;k)(c^\dagger_a \times \tilde{c}_b)^k_\kappa, \tag{3}$$

其中$\mathcal{q}(ab;k)$为相应的结构系数，$\tilde{c}_{j_b m_b} = (-)^{j_b-m_b} c_{j_b-m_b}$，为$c_{j_b m_b}$的时间反演态。

where $\mathcal{q}(ab;k)$ is the structural coefficient, $\tilde{c}_{j_b m_b}$ is the time-reversal partner of $c_{j_b m_b}$ with $\tilde{c}_{j_b m_b} = (-)^{j_b-m_b} c_{j_b-m_b}$.

NPA或者说壳模型同类核子哈密顿量总可以写作

Thus, the NPA or shell-model Hamiltonian of like nucleon can be formally written as

$$\begin{aligned} H_{\text{like nucleon}} = &\sum_{jm} \varepsilon_j c^\dagger_{jm} c_{jm} + \sum_{yL} G_L(y) \sum_M A^{L\dagger}_M(y) A^L_M(y) \\ &+ \sum_{qk} F_k(\mathcal{q}) \sum_\kappa Q^k_\kappa(\mathcal{q}) Q^{k\dagger}_\kappa(\mathcal{q}), \end{aligned} \tag{4}$$

其中加和的三项分别对应于单体项、多极对力、多极相互作用。ε为单粒子能级，G_{LM}与$F_{k\kappa}$分别为多极对力与多极相互作用的强度。其中对结构系数矩阵y、$\mathcal{q}$的遍历是为了兼顾所有两体相互作用自由度。而质子中子相互作用为

where the three terms corresponds to one-body, multipole pairing and multipole-multipole interaction. ε is the single-particle energy, G_{LM} and $F_{k\kappa}$ corresponds to the two-body interaction strengths of multipole pairing and multipole-multipole interaction. The traversal of the structural coefficient matrix y and $\mathcal{q}$ is to take all the two-body degrees of freedom into account. While, the proton-neutron interaction reads

$$H_{\pi\nu} = \sum_{\mathcal{q}_\pi \mathcal{q}_\nu k} F_k(\mathcal{q}_\pi \mathcal{q}_\nu) \sum_\kappa Q^k_{\kappa\pi}(\mathcal{q}_\pi)(-)^\kappa Q^k_{-\kappa\nu}(\mathcal{q}_\nu) \tag{5}$$

一个k秩的球张量可能会有如下对称性:

ome spherical tensor in NPA, O, with rank k could has the symmetry of

$$(O^k_\kappa)^\dagger = \pm(-)^{k-\kappa} O^k_{-\kappa}. \tag{6}$$

我们称这种对称性为“轭密操作对称性”。并不是所有球张量都具有这一对称性，但是NPA计算可以受益于这种对称性。

We called as “conjugate symmetry”. We note not all the tensor has such symmetry. However, the NPA calculation could always benefit from it.

3 code structure and compilation

AGPC-NPA程序主要可以执行两个阶段的多体计算：能谱的计算与本征态单体算符矩阵元的计算。这两阶段的计算分别由名为“spectra_out.cpp”以及“tran_out.cpp”文件中的主函数完成。这两个CPP文件的编译依赖于MKL[3]与ARPACK[4]代数包。我们假定使用者在linux环境下，都使用GCC编译器套件，且已将MKL与ARPACK函数库装入默认路径。那么相应的编译命令为：

The AGPC-NPA program performs two types of calculations for many-body problem: the calculation of the nuclear low-lying spectrum, and the calculation of the one-body operator's matrix elements for eigenstates of Hamiltonian. These two calculations are carried out by the main functions in "spectra_out.cpp" and "tran_out.cpp" CPP files. The compilation of these two CPP files relies on MKL[3] and ARPACK [4] libraries. Assuming that the users already have the GCC compiler suite installed in linux, with pre-compiled MKL and ARPACK libraries in default paths, corresponding compilation commands of these two CPP files are:

```
1 $g++ spectra_out.cpp -lmkl_rt -larpack -O3 -o spectra.
    out
2 $g++ tran_out.cpp -lmkl_rt -O3 -o tran.out
```

如果使用者的计算环境并非完全与我们一致，则可能需自行对编译命令进行修改。编译成功后，当前路径下应存在着“spectra.out”与“tran.out”两个可执行文件。

If the users' computing environment is not exactly the same as ours, she/he may need to modify the compilation command accordingly. If the compilation is successful, there should be two executables named “spectra.out” and “tran.out” in the current path, .

4 spectrum calculation

4.1 input files

NPA的能谱计算都需要3方面输入信息：单粒子空间、组成配对基矢的集体对、哈密顿量。同时程序使用者还需要明确哪些计算所得的能级是需要呈现的。在AGPC-NPA中，使用者将通4个文本格式的输入文件来告知程序这些信息：

Energy spectrum calculation of NPA requires three types of input: single-particle space, collective pairs that constructs many-body basis, and the Hamiltonian. In the mean time, the user should also clarify which calculated energy levels need to be presented in the final results. In the AGPC-NPA, all the information is organized in four input files in text format:

4.1.1 sps.dat

在sps.dat中，使用者需要明确计算的单粒子空间。一个典型的中子50-82壳、质子50-82壳的单粒子空间描述如下所示：

In sps.dat file, the user needs to clarify the single particle space for NPA calculation. A typical single particle space within the 50-82 major shell can be described in text format as:

```
 1  2
 2  5
 3  1  3  5  7  11
 4  0  4  4  8  10
 5  4  4  4  4  5
 6  0  0  1  0  1
 7  2
 8  5
 9  1  3  5  7  11
10  0  4  4  8  10
11  4  4  4  4  5
12  0  0  1  0  1
```

在上文第1行输入的是价中子个数。第2行为中子单粒子轨道的个数。第3行逐项描述了每一个中子单粒子轨道的总角动量。这些总角动量都乘以2，以整数方式进行描述。比如说，在上述sps.dat文件中，中子最后一个轨道的总角动量用整数11表达，其对应的单粒子总角动量即为$11/2\hbar$。如果无特别说明，AGPC-NPA输入文件与程序中的角动量均乘以2表达。第4行为轨道角动量。第5行为主量子数；第6行主要明确的是未配对中子可能占据的单粒子轨道。在此行中，如果某一轨道的数值为0，则未配对核子不能占据此轨道；如为1，则可以占据。这一行输入只对奇数核子系统有效，但是在偶数核子系统计算中也必须占位输入（这是为此后的谱因子或β衰变计算留有的接口）。而后按相同规则列出质子的输入量。该文件中的中子与质子的输入顺序可以互换。

In line 1, the number of valence neutrons is represented. Line 2 provides the number of neutron single-particle orbits. Line 3 describes the total angular momentum of each neutron single particle-orbit one by one. These total angular momentums are multiplied by 2, and thus can be always described as integers. For example, according to line 3, the total angular momentum of the last neutron orbit is expressed by integer 11, and the corresponding single-particle total angular momentum is $11/2\hbar$. Unless otherwise stated, all the AGPC-NPA input/output files adopt the same convention for the angular momentum expression, i.e., a multiplication factor of 2. The 4th line declares the orbital angular momentum of each orbit. Line 5 provides the principal quantum number. Line 6 clarifies the single particle orbit that unpaired neutrons may occupy in an odd-neutron system. In this line, five (the number of neutron single-particle orbits) integers are inputed with values of

0 or 1. If it's 0, the unpaired neutron can not corresponding orbit, vice versa. Line 6 is only valid for the odd nuclear system, but in even-nucleon system calculations, one also needs to input five arbitrary integers herein, just in case for further β-decay or spectroscopic-factor calculations. The input for proton single-particle space is then listed according to the same rules. The input order of the neutrons and protons in this file is interchangeable.

4.1.2 P.dat

在P.dat中，使用者需要明确计算所使用的NPA集体对种类与结构，其具体的描述格式示例如下：

In P.dat file, the user needs to clarify the collective pairs' angular momentum, parity, maximum number and their structural coefficient matrix in the NPA calculation as:

```
2
0 0 -1
0.2013247629888237 0.0 0.0 0.0 0.0
0.0 0.3329935007849622 0.0 0.0 0.0
0.0 0.0 0.1150256931337728 0.0 0.0
0.0 0.0 0.0 0.0919393566416904 0.0
0.0 0.0 0.0 0.0 0.3531862020833097
4 0 1
0.0 -0.397 -0.234 0.0 0.0
0.397 -0.450 0.139 -0.210 0.0
-0.234 -0.139 -0.150 -0.040 0.0
0.0 -0.210 0.040 -0.114 0.0
0.0 0.0 0.0 0.0 -0.731
2
0 0 -1
0.0420145450157065 0.0 0.0 0.0 0.0
0.0 0.0714145509316199 0.0 0.0 0.0
0.0 0.0 0.1556621455431875 0.0 0.0
0.0 0.0 0.0 0.5313406310744926 0.0
0.0 0.0 0.0 0.0 0.0784167956503778
4 0 -1
0.0 -0.397 -0.234 0.0 0.0
0.397 -0.450 0.139 -0.210 0.0
-0.234 -0.139 -0.150 -0.040 0.0
0.0 -0.210 0.040 -0.114 0.0
0.0 0.0 0.0 0.0 -0.731
```

在上文第1行输入1个整数，对应于中子的NPA集体对种类数目。第2行开始逐项描述每一种NPA集体对的具体信息。这些信息依次为集体对的角动量、宇称、最大容许个数，以及对结构系数矩阵。其中角动量、宇称、

最大容许个数用三个整数进行表达，如第2行所示。角动量乘以2进行表达。宇称如表达为0，即为正宇称；1即为负宇称。AGPC-NPA中所有的输入文件均沿用这样的宇称输入约定。最大容许个数如为-1，表示程序对该集体对在基矢中的个数不设限制，否则程序会忽略所有超过集体对最大容许个数的基矢。NPA集体对的对结构系数矩阵由单粒子轨道数的平方个浮点数进行描述。其具体输入顺序应与sps.dat文件中的单粒子轨道输入相匹配。当一种中子集体对输入完成后，按相同的规则输入另一种中子集体对，直至所有集体对输入完成。比如说在上述P.dat文件就在第1行明确将要输入2种中子集体对。第1种集体对的角动量、宇称、最大容许个数位于于第2行，对应于角动量$J = 0$，宇称为正（0）。这实际上就是NPA中常用的S对。S对最大容许个数表为"-1"，对应于程序对中子S对的个数不作限制。在第3-7行之间，输入了S对的NPA对结构系数矩阵。紧接着，在第8行输入第2种中子集体对的角动量、宇称、最大容许个数。该集体对的角动量表为"4"对应于$J = 2$，宇称表为"0"对应于正宇称。这是NPA中常用的D对。最大容许个数为1，计算中NPA基矢只能出现不多于1数的D对。在其后的第9到13行列出了该D对的对结构系数。在完成中子输入后，第14到26行按相同的输入规则再次输入质子集体对的信息。在此我们强调，由于集体对个数与单粒子轨道的个数是可变化的，P.dat中的输入内容并不固定于某一具体行，但总是有序的。在P.dat中，中子与质子的输入顺序是可交换的，但应与sps.dat匹配。

The first line of P.dat declares the numbers of neutron collective pairs introduced to the NPA calculations. For example, according to line 1 of the above P.dat file, it is clear that two neutron collective pairs will be inputted. From line 2, one begins to describe the information of each collective pair one by one. These information is in order of angular momentum, parity, the maximum number in basis, and the structure coefficient matrix, i.e., "$y(ab; L)$" defined in Eq. (**??**). The angular momentum, parity and maximum number are expressed with three integer in one line, as shown in line 2. The parity can be "0" or "1", corresponding to positive parity or negative parity, respectively. All input files in the AGPC-NPA follow this parity input convention. The maximum number of a collective pair, as "-1", means that there is no limit on the number of this collective pair in one basis, or it should be a non-negative integer. If the number of this collective pair in some NPA basis is larger than such a integer, this basis would be omitted in the NPA calculation. The first neutron collective pair described above has angular momentum, parity and maximum number of "0 0 -1", correspoding to $J^\pi = 0^+$ collective pair, as usully called "S" pair. One sees there is not limit on S-pair number in one basis. The structure coefficient matrix of the NPA collective pair is described with float matrix with the dimension of single-particle-orbit number, which has be declared in sps.dat, as shown in lines 3-7. After than, there is another collective pair inputted in following lines 8-13, with angular momentum, parity, and maximum number of "4 0 1". That's a $J^\pi = 2^+$ D pair. Each basis could have at most 1 D pair. After the neutron input, lines 14-26 declare the information of proton collective

pair, with the same input convention. In P.dat, the input order of neutrons and protons is exchangeable, but should be matched to sps.dat.

4.1.3 ham.dat

在ham.dat中，使用者需要明确计算所使用的哈密顿量参数与结构其具体描述格式示例如下：

In ham.dat, the Hamiltonian adopted is described, including strength parameters and structure as:

```
0.332  0.0  1.655  2.434  0.242
2.99  2.708  0.962  0.0  2.793
2
-0.1  0  0
0.707  0.0  0.0  0.0  0.0
0.0  1.0  0.0  0.0  0.0
0.0  0.0  1.225  0.0  0.0
0.0  0.0  0.0  1.414  0.0
0.0  0.0  0.0  0.0  1.732
-0.02  4  0
-0.0  1.335  1.635  0.0  -0.0
-1.335  1.388  -0.908  1.717  -0.0
1.635  0.908  1.817  0.572  -0.0
0.0  1.717  -0.572  2.141  -0.0
-0.0  -0.0  -0.0  -0.0  3.142
1
-0.01  4  0
-0.0  1.335  1.635  0.0  -0.0
-1.335  1.388  -0.908  1.717  -0.0
1.635  0.908  1.817  0.572  -0.0
0.0  1.717  -0.572  2.141  -0.0
-0.0  -0.0  -0.0  -0.0  3.142
1
-0.11  0  0
0.707  0.0  0.0  0.0  0.0
0.0  1.000  0.0  0.0  0.0
0.0  0.0  1.225  0.0  0.0
0.0  0.0  0.0  1.414  0.0
0.0  0.0  0.0  0.0  1.732
0
1
0.07  4  0  1
-0.0  1.335  1.635  0.0  -0.0
-1.335  1.388  -0.908  1.717  -0.0
1.635  0.908  1.817  0.572  -0.0
```

```
0.0  1.717  −0.572  2.141  −0.0
−0.0  −0.0  −0.0  −0.0  3.142
−0.0  1.335  1.635  0.0  −0.0
−1.335  1.388  −0.908  1.717  −0.0
1.635  0.908  1.817  0.572  −0.0
0.0  1.717  −0.572  2.141  −0.0
−0.0  −0.0  −0.0  −0.0  3.142
```

在以上框中的第1行与第2行分别输入的是中子与质子的单粒子能级。其单粒子能级的顺序应与sps.dat匹配。第3行到第29行输入中子-中子两体相互作用。第3行输入1个整数“2”，表明计算要包括2个形如$\sum_M A^{L\dagger}_M(y)A^L_M(y)$中子-中子多极对力项。其后从第4行开始逐项输入这2个多极对力项的信息。第1个多极对力项信息由第4到第9行给出。其中第4行为1个浮点数“-0.1”、两个整数“0 0”组成，分别对应于该项多极对力的相互作用强度、相应的集体对“$A^{L\dagger}(y)$”秩（$2L=0$）与宇称（表为0有正宇称）。由于$L=0$，这是一个对力项。其后的5-9行对应于$A^{L=0\dagger}$集体对的对结构系数。而后根据相同的规则，在第10-15行中输入第2个中子-中子多体对力项。在多极对力项输入完成后，在第16行输入1个整数“1”，说明计算要包括1个形如$\sum_\kappa Q^k_\kappa(\boldsymbol{q})Q^{k\dagger}_\kappa(\boldsymbol{q})$这样的中子多极相互作用。这1个多极相互作用的详细信息由第17-22行描述，其描述规则与多体对力项描述规则非常类似。第17行也是由1个浮点数“-0.01”，两个整数“4 0”组成，说明这1项中子多极相互作用强度为-0.01；相应的单体算符$Q^k_\kappa(\boldsymbol{q})$的秩为$2k=4$；宇称表为0，即有正宇称。其后的18-22行给出这一单体算符的结构系数矩阵。在完成中子两体相互作用输入后，在第23-30行，按相同规则输入质子两体相互作用。可见本文中的示例只包含有1项质子对力相互作用，也没质子多极相互作用（多体相互作用项数为0 ，见第30行）。在完成同类核子相互作用输入后，在第31-42行输入形如$\sum_\kappa Q^k_{\kappa\nu}(\boldsymbol{q}_\nu)(-)^\kappa Q^k_{-\kappa\pi}(\boldsymbol{q}_\pi)$中子-质子多极相互作用。其中第31行输入1个整数“1”，说明程序仅包含1个中子-质子多极相互作用。而后在第32-42行（逐项，如果有多个多极中子-质子相互作用）输入中子-质子多极相互作用详细信息。其中第32行包含1个浮点数与3个整数。浮点数对应于该相互作用强度，3个整数分别对应于该相互作用中的$Q^k_{\kappa\nu}(\boldsymbol{q}_\nu)$与$Q^k_{-\kappa\pi}(\boldsymbol{q}_\pi)$单体算符的秩、宇称以及轭密特性。注意此处这两个单体算符应该具有一致的角动量、宇称以及轭密特性，否则核相互作用的对称性将被破坏。因此，我们不用分别描述两个算符的秩、宇称以及轭密特性。这里角动量、宇称输入约定与同类核子一致，此处不再冗述。轭密特性可以表为“1”或为“-1”，分别对于应两种不同的共轭对称性$(Q^k_\kappa)^\dagger=(-)^{k-\kappa}Q_{-\kappa}$与$(Q^k_\kappa)^\dagger=-(-)^{k-\kappa}Q_{-\kappa}$。这关系到AGPC-NPA依靠这一对称性对NPA矩阵元计算的具体优化。其后的第33-42行次输入此处中子单体算符与质子单体算符的结构系数矩阵。致此相互作用输入完毕。此处中子与质子的地位是可以互换的，但是需与sps.dat匹配。

In lines 1 and 2 of the box above, the single particle energies of neutron and proton are inputted, respectively. The order of single particle energies should match sps.dat. The neutron-neutron two-body interaction is inputted in line 3 to 29. There is an integer “2” in line 3, which indicates that the calcu-

lation includes two multipole pairing interactions, i.e., the $\sum_M A_M^{L\dagger}(y)A_M^L(y)$ terms in Eq. (4). From line 4, one inputs the information of those multipole pairing interactions one by one. The first neutron multipole pair interaction is presented in lines 4-9. In line 4, there are one float and two integers as "-0.1 0 0", corresponding to the interaction strength, the angular momentum and parity of collective pair $A^{L\dagger}(y)$. One sees that this is a plain pair force with $L^\pi = 0^+$. In following lines 5-9, the structural coefficient matrix of $A^{L\dagger}(y)$ is presented. Then, according to the same input convention, the second neutron multipole pair interaction is presented in lines 10-15. After the input of multipole pair interactions, in line 16, an integer "1" indicates that the Hamiltonian also includes one neutron-neutron multipole-multipole interaction, i.e., the $\sum_\kappa Q_\kappa^k(\boldsymbol{q})Q_\kappa^{k\dagger}(\boldsymbol{q})$ term in Eq. (4). The details of this 1 multipole interaction are described in lines 17-22, and the description convention is very similar to that of multipole pair interaction. Line 17 is also composed of one float and two integers as "-0.01 4 0", indicating that this neutron multipole interaction strength is -0.01 with angular momentum $k = 2\hbar$ and positive parity. The subsequent lines 18-22 present the structural coefficient matrix of the one-body operator, Q^k. After the input of neutron two-body interactions, in lines 23-30, the proton two-body interaction is inputted with the same convention. One sees the proton two-body interaction only includes one multipole-pairing interaction with angular momentum $L = 2\hbar$ and positive parity in the P.dat example we provide herein. After the input of like-nucleon interactions, lines 31-42 present the detail of neutron-proton interactions in form of $\sum_\kappa Q_{\kappa\nu}^k(\boldsymbol{q}_\nu)(-)^\kappa Q_{-\kappa\pi}^k(\boldsymbol{q}_\pi)$ as in Eq. (5). Line 31 presents one integer "1", indicating the Hamiltonian include one term of $\sum_\kappa Q_{\kappa\nu}^k(\boldsymbol{q}_\nu)(-)^\kappa Q_{-\kappa\pi}^k(\boldsymbol{q}_\pi)$ neutron-proton interaction. Then, one should input the detail of these neutron-proton multipole-multipole interaction (term by term, if more than one $\sum_\kappa Q_{\kappa\nu}^k(\boldsymbol{q}_\nu)(-)^\kappa Q_{-\kappa\pi}^k(\boldsymbol{q}_\pi)$s are required.) Line 32 contains one float and three integers as "0.07 4 0 1", corresponding to the interaction strength, angular momentum k, parity and conjugate property of the one-body operators Q_ν^k and Q_π^k. (Q_ν^k and Q_π^k in one multipole-multipole interaction should have the same angular momentum k, parity and Hermitian property to insure the full symmetry of nuclear Hamiltonian.) The conjugate property is presented as "1" or "-1", corresponding to two conjugate symmetries as $(Q_\kappa^k)^\dagger = (-)^{k-\kappa}Q_{-\kappa}$ or $(Q_\kappa^k)^\dagger = -(-)^{k-\kappa}Q_{-\kappa}$, respectively, which helps to optimize the AGPC-NPA. Lines 33-42 present the structure coefficient matrices of Q_ν^k and Q_π^k, respectively. The input order of neutron and proton here is interchangeable, but required to match sps.dat.

4.1.4 eig_input.dat

在eig_input.dat中，使用者应说明计算应给出的哪些本征态的信息，其具体描述格式示例如下：

eig_input.dat declares which low-lying states should be presented in final result. Its input convention is exemplified as

```
1 4
2 0  4  8  12
3 2  2  1  1
4 0
```

其中第1行输入1个整数（“4”）声明下一行所需输入的角动量的个数。然后在第2行中，我们依次输入4个整数，“0 4 8 12”，分别对应于角动量0$\hbar$、2$\hbar$、4$\hbar$、6$\hbar$。在最终结果中，只有那些携带了这些角动量的正宇称能量本征态的信息才会被输出。在第3行中我们用整数依次明确，对于每一种角动量来说，需要输出哪几个能量最低的本征态。在上述示例中，我们就要求输出能量最低的2个0^+态、最低的2个2^+态、最低的4^+态，以及最低的6^+态。其后从第4行始，按相同的规则说明需要输出的负宇称本征态信息。在上述示例中，我们没有要求输出负宇称能级，相应的角动量个数没为“0”（见第四行）。

The first line contains a integer, “4”, to declare how many angular momentums we are going to input in the next line, and then 4 integers, “0 4 8 12” are inputed in line 2, corresponding to 0$\hbar$, 2$\hbar$, 4$\hbar$, 6$\hbar$. Only the states with those angular momentums and positive parity will be displayed in the final result. In line 3, we specify how many lowest eigenstates for each angular momentum should be displayed. In the example above, we ask for the lowest 2 0^+, the lowest 2 2^+, the lowest 4^+, and the lowest 6^+ states. Then, starting with line 4, the display information for required negative-parity states is described with the same convention. In the example above, we do not require the negative-pairty states output, and thus the corresponding number of angular momentum is "0" in line 4.

4.2 spectra.out execution

在完成上述输入文件的准备工作后，通过输入“./spectra.out”启动计算：

After preparing above 4 input files for spectrum calculation, we can start the program by inputing “./spectra.out”, and the terminal would feedback as

```
1 $./spectra.out
2 Q_M mat index start from 1073741823
3 sp vector index start from 536870911
4 space 0 has 2 particle; space 1 has 2 particle.
5 input the M_tot(M_tot=0 disables some transition
    calculation)=
```

上述示例的第4行说明了在“sps.dat”中输入的价核子数信息，使用者都可以使用这一信息纠错。第5行要求使用者明确在M-scheme计算中角动量三

分量取值，对应计算中所能取到的最低角动量。角动量三分量的输入也需要乘以因子2。偶数核子体系此外的输入应为偶数，反之亦然。否则程序会报错自动终止。一般的，偶数核子体系可以设M_tot=0，奇数体系设M_tot=1（对应于1/2$\hbar$）。但是设M_tot=0时，将无法进行后继的磁矩或其它1秩单体算符矩阵元的计算。此处因为是偶数体系，我们输入0。终端回应：

The fourth line of the above example illustrates the number of valence nucleons specified in "sps.dat", which could help the user to verify the correction of input. Line 5 requires the user to specify angular momentum projection on principal axis in the M scheme, corresponding to the smallest angular momentum available in the calculation. The input of the angular momentum projection also needs to be multiplied by factor 2, following the AGPC-NPA input convention. Therefore, this input for the even-nucleon system should also be even, and vice versa. Otherwise, the program will report an error and terminate. In general, even-nucleon system could have M_tot=0, and odd one has M_tot=-1, corresponding to 1/2$\hbar$. However, when M_tot=0, it disables the calculations for magnetic moment or other 1-rank one-body operator matrix elements. Here because we specified an even-nucleon system in sps.dat, we input M_tot=0, and the terminal feedbacks as:

```
1 ...
2 input the M_tot(M_tot=0 disables some transition
    calculation)=0
3 are previous matrix files available?(y/n):
4 files available only under the modification of M_tot or
    Ham parameters.
5 by inputting n, the previous binary files will be
    erased no matter.
```

在第3行程序询问是否从当前路径中的二进制文件中读取此前已计算的矩阵元。如果输入"y"，就直接进入哈密顿量对角化。否则程序会删除当前路径中可能存在矩阵元数据，并开始矩阵元计算工作。程序在第4行也明确，只有在修改"M_tot"数值或是ham.dat中的单粒子能级与相互作用强度时，读取此前已计算的矩阵元才是有意义的。输入"y"的一个典型场景时，针对偶数核体系，首次计算可以使用"M_tot=0"，以包括所有可能的低激发态，同时再次计算输入"M_tot=2"，以方便后续的磁矩计算。作为示例，此处我们输入"n"。

In the third line in above box, the program asks the user if she/he wants to read the previously calculated matrix elements from the binary files in the current path. By typing "y", the program will directly perform the Hamiltonian diagonalization. Otherwise, the program erases the matrix-element files that may exist in the current path, and then begins to calculate matrix elements of Hamiltonian. In line 4, the program also declare that previous matrix-element files can be available only, only for two cases. The first one

is to change the "M_tot" value, and the second one is to change the single-particle energies or interaction strengths specified in ham.dat. A typical "y" scenario herein can be a magnetic transition calculation in an even-nucleon system. At first, a M_tot=0 calculation produces full energy spectrum in low-lying region, and then another M_tot=2 calculation enables the magnetic moment calculation. As an example, here we enter "n", and the program feedbacks:

```
1 ...
2 n
3 please specify which expectations are displayed in
     sequence of
4 pair(unpaired particle) num, sp occupation, PP, QQ_norp
    , QQ_np (y/n):
```

此处程序询问在完成对角化后，是否计算本征态的某些期望值，包括某种集体对（某个轨道上的未配对粒子）个数期望值、各轨道的单粒子占据数、同类核子的多极对力（无参数）期望值、同类核子的多极相互作用（无参数）期望值、中子-质子相互作用多极相互作用的（无参数）期望值。使用者需要用5个y/n输入来明确这些信息。此处，我们输入5个"n"，表明我们不会进行这些期望值计算。输入完成后，终端将给出低激态能量：

Here the program asks whether certain expectations of eigenstates are calculated after the diagonalization, including expectation of collective-pair number or unpaired-particle number in a certain orbit, the single-particle occupation number, and the expectation of some two-body terms in Hamiltonian without interaction strength, denoted by "PP, QQ_norp, QQ_np" in line 4. "PP" means like-nucleon multipole pairing interaction, "QQ_norp" for like-nucleon multipole-multiple interaction, and "QQ_np" for neutron-proton interaction. The user needs to input 5 "y/n" to clarify this information for expectation calculation. In the example presented above, 5 "n"s are inputted to indicate no expectation is required. When the above input is complete, the terminal will provide the low-lying spectrum:

```
1 ...
2 n n n n n
3 ...
4 J^pi=0_1^0 E= -1.51642 JpJm= 2.76001e-15
5 J^pi=4_1^0 E= -1.2502 JpJm= 6
6 J^pi=4_2^0 E= 4.0865 JpJm= 6
7 ...
8 t for mat cal=0s, for dig=0s
```

终端从上述示例中的第4行开始给出每一个本征态的角动量、宇称、本征能量以及J_+J_-算符的期望值（"JpJm"）。如果J_+J_-期望不能给出整数或半整数角动量，程序会提示此处可能有能量简并现象。此处的本征态只限于

在“eig_input.dat”明确需要输出的本征态。在第8行程序会总结矩阵元计算用时（mat cal=）与对角化用时(dig=)。计算完成后，程序会自动地将内存中已计算的重叠与算符矩阵元存入当前路径下的二进制文件中，供下次计算使用。程序也会将计算所得能谱与期望值存入名为“eig.dat”文本文件，将计算所得本征态的波函数存入当前路径的二进制文件供后续单体算符矩阵元计算用。

The terminal output (from line 4) in above box presents the angular momentum, parity, energy eigenvalue, and the J_+J_- expectation (denoted by “JpJm”). If the J_+J_- expectation cannot provide an integer or a half-integer angular momentum, the program will indicate that there may be an energy degeneracy. The eigenstates presented here are limited to the states that are specified in “eig_input.dat”. In line 8, the program summarizes the time used for the calculation of the matrix element (mat cal=) and the time used for diagonalization (dig=). When the calculation is complete, the program stores the calculated overlap and operator matrix elements into the binary files under the current path for the next calculation. The program will also store the calculated energy spectrum and expectations into a text file named “eig.dat”, and the calculated wave function of eigenstates will be stored in the binary file in the current path, for subsequent one-body-operator matrix-element calculation.

5 matrix-element calculation for eigenstates

5.1 tran_input.dat

本征态单体算符矩阵元的计算必需在能谱计算之后进行。同时计算之前必需准备名为“tran_input.dat”的文本文件，以说明所需计算的单位算符矩阵元信息。以下为这一文件文件的格式示例：

The one-body-operator matrix-element calculation for eigenstate has to be carried out after the spectrum calculation. A text file named “tran_input.dat” also needs to be prepared before the calculation, to specify the detail of matrix elements to be calculated. The following is an example of such text file:

```
1  4
2  4  0  1  2  1  4  0  1
3  4  0  1  1  1  4  0  1
4  0  0  1  2  1  4  0  1
5  0  0  1  1  1  4  0  1
6  2
7  4  0  1
8  -0.0  1.335  1.635  0.0  -0.0
9  -1.335  1.388  -0.908  1.717  -0.0
10 1.635  0.908  1.817  0.572  -0.0
```

```
0.0  1.717  −0.572  2.141  −0.0
−0.0  −0.0  −0.0  −0.0  3.142
2  0  1
0.0  0.0  −0.0  −0.0  −0.0
−0.0  −1.311  0.437  −0.0  −0.0
−0.0  −0.437  −1.635  0.0  −0.0
−0.0  −0.0  −0.0  −3.518  −0.0
−0.0  −0.0  −0.0  −0.0  −5.312
1
4  0  1
−0.0  1.335  1.635  0.0  −0.0
−1.335  1.388  −0.908  1.717  −0.0
1.635  0.908  1.817  0.572  −0.0
0.0  1.717  −0.572  2.141  −0.0
−0.0  −0.0  −0.0  −0.0  3.142
```

在该文件的第1行，应明确所需计算的单体算符矩阵元的个数。这里我们要求计算4个矩阵元。在其后的2-5行，依次通过整数输入明确这4个矩阵元的左矢、算符、右矢信息。比如说在第2行中，要求计算的矩阵元左矢表为“4 0 1”，说明左矢角动量为$2\hbar$，宇称为正，在能谱中为最低的第一个本征态，即2_1^+态。而后输入两个整数“2 1”表明该矩阵元所对应算符为本文件后续将要输入第2种核子空间中的第1个单位算符。这里，第2种核子即为在“sps.dat”中最后明确的核子空间（质子）。右矢也表为“4 0 1”，对应于2_1^+态。而后的三行均按相同规则进行输入。在6-25行，输入算符的具体信息。第6行明确此处所涉及的第1种核子的算符的个数。这里输入为“2”，说明要输入2个第1种核子的单体算符。接着在第7行开始输入第1个单体算符信息。3个整数“4 0 1”，分别对应于该算符的秩、宇称、以及轭密性质，输入约定与“ham.dat”中的中子-质子多体相互作用中的单极算符输入约定一致。而后在第8到12行，用浮点数输入该算符的结构系数矩阵。在13-18行按相同的输入规则输入第1种核子的第2个算符信息。在第1种核子的单体算符信息输入完成后，在第19-25行按相同规则输入“sps.dat”中明确的第2种核子（质子）的单体算符信息。这里我们的第1种核子与第2种核子的第1个算符实际上都是四极算符，那么在第2-5行中所计算的矩阵元分别对应着2_1^+态的电矩计算的中子贡献、质子贡献、$2_1^+ \to 0_1^+$的B(E2)计算的中子贡献与质子贡献。

In the first line of the file, one should specify the number of matrix elements to be calculated. Here we require to calculate 4 matrix elements. In the next 2-5 lines, each of these 4 matrix elements is presented with 8 integers, which represent the bra, the operator and the ket. For example, in line 2, the first matrix element is represented with “4 0 1 1 1 4 0 1”, where the first three integers “4 0 1” indicates that the bra is the first lowest (1) eigenstates with angular momentum $2\hbar$ (4) and positive parity (0), i.e., the 2_1^+ state from previous spectrum calculation, the last three integers “4 0 1” indicates that the ket is also the 2_1^+ state by the same convention. The two

integers “2 1” in the middle correspond to the first (1) one-body operator (specified later) in the second (2) single-particle space specified in sps.dat. Here the second single-particle space is proton space as described previously. The next three lines are organized according to the same input convention. In lines 6-25, the detail of the one-body operators are specified. Line 6 includes a integer “2”, corresponding to the number of one-body operators for the first valence nucleon, i.e., neutron here according to sps.dat. From line 7 to line 12, the first neutron one-body operator should be specified. In line 7, 3 integers "4 0 1" are presented, corresponding to the angular momentum, parity, and conjugate property of the first operator, following the similar input convention for Q^k_ν or Q^k_π one-body operator in ham.dat. Then, from line 8 to line 12, the structure coefficient matrix of this operator is presented with floats. From line 13 to line 18, the second neutron one-body operator is presented according to the same input convention for lines 7-12. After the input for neutron, the proton operator(s) will be specified in line 19-25 according to the same input convention as for neutron. One sees that both first operators for neutron and proton are actually quadrupole operators, so that the matrix elements specified in line 2-5 correspond to neutron and contributions of electric quadrupole moment and B(E2, $2^+_1 \rightarrow 0^+_1$), respectively.

5.2 tran.out execution

准备好上述输入文件之后，可以运行“tran.out”，如下：

After preparing the “tran_input.dat” file, one can perform the one-body matrix-element calculation via typing “./tran.out” as

```
1 $./tran.out
2 ...
3 are transition Q matrix files available?(y/n):
4 files available only under modification of interesting
    tran_mat elements (modification of interesting tran
    Q operator is not the case), or the M_tot
    modification in previous spectra.out operation
```

此时程序询问当前文件夹下是否存有可用的矩阵元二进制文件，并且说明这些二进制文件只有在改变所需计算的矩阵元，而非单体算符，或者是在前期“spectra.out”执行中改变M_tot输入时才是可用的。如果输入“n”，程序删除当前路径中的矩阵元二进制文件，并重新针对上述单体算符进行矩阵元计算。如果输入“y”，程序将直接使用此前计算所得矩阵元计算结果，结合能谱计算所得波函数，给出在本征态下的矩阵元。作为示例，此处我们输入“n”，进而得到以下输出：

At this point, the program asks if there are available matrix-element binary files from previous calculations under the current folder, and explains that these binaries are available only if the user changes the matrix elements

(not the one-body operators) specified in “tran_input.dat”, or changes the M_tot input in previous spectrum calculation. If one inputs “n", the program deletes the matrix-element binary files in the current path, and then perform the AGPC calculations for each one-body operator. If “y” is inputed, the program will adopt previous calculated matrix elements and the wave-functions from previous spectrum calculation, and provide the matrix elements of eigenstates. Here, as an example, we input “n” and obtain the following output:

```
1 n
2 ...
3 <4_1^0,M=4,e=-1.2502|Q_0^1|>: <||~||>= 0.0201021 CG
    *<||~||>= 0.010745
4 <4_1^0,M=4,e=-1.2502|Q_0^0|>: <||~||>= -1.01017 CG
    *<||~||>= -0.539961
5 <0_1^0,e_l=-1.51642||Q_0^1||4_1^0,e_r=-1.2502>:
    <||~||>= -0.106476 (hat J_l/ hat J_r)*<||~||>=
    -0.0476175 D E= 0.266221
6 <0_1^0,e_l=-1.51642||Q_0^0||4_1^0,e_r=-1.2502>:
    <||~||>= 4.94195 (hat J_l/ hat J_r)*<||~||>= 2.21011
     D E= 0.266221
7 t_mat=0 t_tran=0
```

第3-6行中，分别给出了“tran_input.dat”中所明确要计算的4个矩阵元结果。如果左右矢相同，如第3与第4行，程序默认这是一个多极矩计算。其中的“$<||\sim||>$=”对应于Rose约定下的约化矩阵元数值，而“CG$*<||\sim||>$”则对应着约化矩阵元乘以$\langle JJk\kappa|JJ\rangle$ Clebsch-Gordan系数，以方便后续多极矩计算。如果左右矢不同，如第5与第6行，程序默认这是跃迁矩阵元计算，还将给出“(hat J_l/ hat J_r)$*<||\sim||>$”数值，对应于约化矩阵元乘以$\frac{2J_f+1}{2J_i+1}$因子（左矢为末态，右矢为初态）；以及“D E”对应于跃迁能量。这些数值将可用于计算约化的约迁几率与初态寿命。在第7行，程序总结出“t_mat”与“t_tran”时间，分别对应于非正交归一基矢空间下的矩阵元计算时间与后续的本征态矩阵元计算时间。计算完成后，程序会自动地将内存中已计算的非正交归一基矢空间下的算符矩阵元存入当前路径下的二进制文件中，供下次计算使用。

In lines 3-6, the four matrix elements specified in “tran_input.dat” are displayed. If the bra and ket are the same, such as lines 3 and 4, the program supposes to corresponding matrix element is for a multipole moment calculation by default. The $<||\sim||>=$ value corresponds to the reduced matrix element under the Rose convention, while CG$*<||\sim||>$ to the product of such reduced matrix element and the Clebsch-Gordan coeffecient, $\langle JJk\kappa|JJ\rangle$ for further multipole moment calculation. If the bra and ket are different, such as lines 5 and 6, the program defaults that this is a transition matrix-element calculation, and will additionally provide a value represented

by "(hat J_l/ hat J_r)$*<||\sim||>$", corresponding the the reduced matrix element multiplied by $\frac{2J_f+1}{2J_i+1}$, where J_f is the angular momentum of final state (bra), and J_i is for initial state ket. Such a value, as well as the "D E" value (transition energy), could help to calculate the reduced transition rate and lifetime of initial state. In line 7, the program summarizes the times represented by "t_mat" and "t_tran", corresponding to computational times for the matrix elements between NPA bases and eigenstates, respectively. When the calculation is complete, the program stores the calculated matrix elements between NPA non-orthogonal bases into the binary file under the current path, to potentially boost the next matrix-element calculation.

6 epilogue

In this manual, we briefly introduce the AGPC-NPA usage. We believe there still exists a lot of room to make AGPC-NPA more user friendly and more functional. The users are welcome to bring up their problems and issues according to their AGPC-NPA using.

Acknowledgements

We thank B. C. He for the inspiration of M-scheme NPA. We are grateful for the financial support of the Sichuan Science and Technology Program (Grant No. 2019JDRC0017), the Doctoral Program of Southwest University of Science and Technology (Grant No. 18zx7147), and the National Natural Science Foundation of China (Grant No. 11875188).

References

[1] Y. M. Zhao, A. Arima, Nucleon-pair approximation to the nuclear shell model, Physics Reports 545 (1) (2014) 1 – 45, nucleon-pair approximation to the nuclear shell model. doi:https://doi.org/10.1016/j.physrep.2014.07.002.
URL http://www.sciencedirect.com/science/article/pii/S0370157314002117

[2] B. He, Y. Zhang, L. Li, Y. Luo, F. Pan, J. P. Draayer, Nucleons pair shell model in m-scheme (2020). arXiv:2004.09945.

[3] intel, Math kernel library, https://software.intel.com/content/www/us/en/develop/tools/m

[4] D. C. Sorensen, R. B. Lehoucq, C. Yang, M. K., Arpack, https://www.caam.rice.edu/software/ARPACK/.