2023.9.26 组会

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Pseudo-state

使用THO basis对哈密顿量进行对角化，得到一系列特征向量：

$$\psi_{i,l} = \sum_i c_{i,n} R_{n,l}^{\text{THO}}$$

我们希望这些特征向量能近似地组成完备性关系：

$$\sum_i |\psi_{i,l}\rangle\langle\psi_{i,l}| = I$$

在source term中插入一个完备基

$$\sum_i \langle\chi_b(k)|\chi_i^{\text{pseu}}\rangle\langle\chi_i^{\text{pseu}}|V_{\text{post}}|\chi_a(k)\phi_a(r_a)\rangle$$

定义变换的系数 $\langle\chi_b(k)|\chi_i^{\text{pseu}}\rangle = A_i$

生成的 THO basis 的归一化

```
do l=0,lmax
    do i=1, nho
       norm=0.0_dpreal
       do ir=1, nr
         norm = norm +  rr(ir)**2 *  rrw(ir) * thowf(ir,i,l)**2
         write(499,*) rr(ir), thowf(ir,i,l)*rr(ir)
       end do
       write(499,*) "&"
       write(*,*) "l=",l, "iho=",i, "norm=",norm
    end do
end do
```

归一化条件 $\int \mathrm{d}r r^2 |R^{\mathrm{THO}}(r)|^2 = 1$

&tho mtho=4.0 gamma=1.5 bosc=1.6 nho=15 /

norm

1	0.999999986279837
2	0.9999999302349100
3	0.9999998791871200
4	0.9999997760105100
5	0.9999997439610400
6	0.9999995900079800
7	0.9999996607663300
8	0.9999994435957000
9	0.9999996588842500
10	0.9999992374128100
11	0.9999997131553200
12	0.9999987363891500
13	0.9999997615806200
14	0.9999970171152100
15	0.99999412608102 8

THO basis 下的特征向量的归一化与正交性

&tho mtho=4.0 gamma=1.5 bosc=1.6 nho=20 /

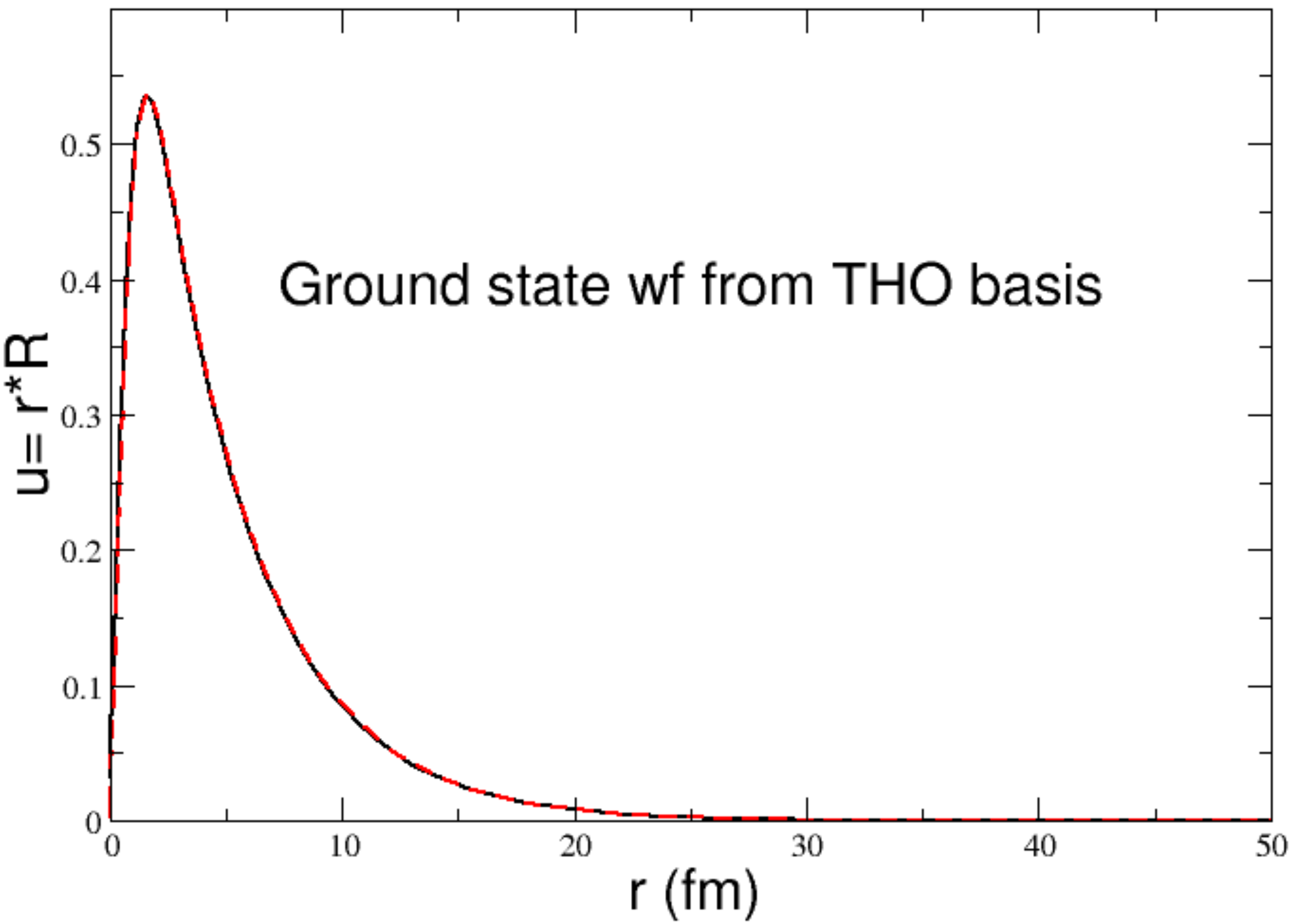
Overlap

1	**1**	(0.99999998627983677,0.0000000000000000)
1	2	(8.19460213894509077E-006,0.0000000000000000)
1	3	(-1.55006621133873420E-005,0.0000000000000000)
1	4	(-2.13718165868098752E-005,0.0000000000000000)
1	5	(-2.56104956276740072E-005,0.0000000000000000)
1	6	(2.84284904887762252E-005,0.0000000000000000)
1	7	(3.00573521046013082E-005,0.0000000000000000)
1	8	(-3.08996218260130341E-005,0.0000000000000000)
1	9	(-3.11277058097415802E-005,0.0000000000000000)
1	10	(-3.10629896856354749E-005,0.0000000000000000)
1	11	(3.07193056387805962E-005,0.0000000000000000)
1	12	(-3.03511463680112625E-005,0.0000000000000000)
1	13	(2.98301384970397176E-005,0.0000000000000000)
1	14	(-2.94087912868802649E-005,0.0000000000000000)
1	15	(2.87440557586595960E-005,0.0000000000000000)
1	16	(-2.81028860523739410E-005,0.0000000000000000)
1	17	(2.64625576043194564E-005,0.0000000000000000)
1	18	(-2.43999273581021999E-005,0.0000000000000000)
1	19	(2.18257262298510278E-005,0.0000000000000000)
1	20	(-2.99701089402602477E-005,0.0000000000000000)

波函数的Benchmark

&tho mtho=4.0 gamma=1.5 bosc=1.6 nho=15 /

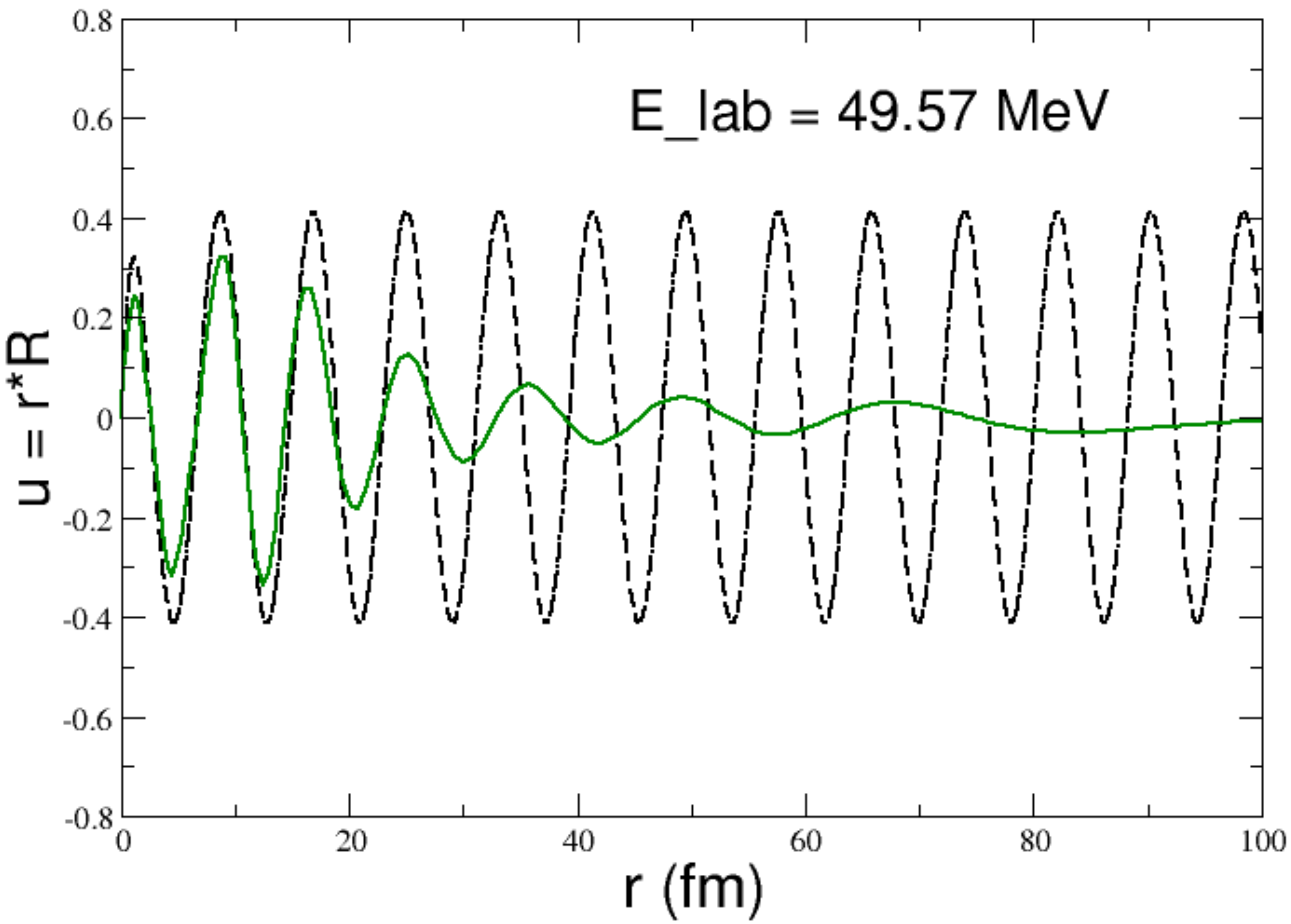
基态波函数的比较:



pseudo-state波函数是否内部一致?

&tho mtho=4.0 gamma=1.5 bosc=1.6 nho=15 /

得到15个特征值，我们人为设定我们的入射能量对应某个特定的特征值，考察在内部，pseudo-state波函数是否与求解微分方程的结果一致



Eigenvalue

1	-2.2208
2	0.0544
3	0.2202
4	0.5058
5	0.9263
6	1.5059
7	2.2811
8	3.3061
9	4.6628
10	6.4749
11	8.9390
12	12.3724
13	17.3251
14	24.7832
15	36.6824
16	56.9579
17	94.2530
18	166.5700
19	313.2220
20	640.8328

pseudo-state波函数是否内部一致?

Coefficient

	Real	Im
1	2.3885927015995E-03	5.28089177424181E-03
2	1.8439007525951E-04	4.0766432512264E-04
3	-7.46149848432516E-04	-1.64964775882496E-03
4	-6.16608531160967E-04	-1.36324745443413E-03
5	-1.60049006078317E-03	-3.53849142680788E-03
6	1.25509791358958E-03	2.77487084478857E-03
7	2.77308445580166E-03	6.1309568944569E-03
8	-2.35251070122238E-03	-5.20111880212216E-03
9	-4.7869095730166E-03	-1.0583282520814E-02
10	-4.64821233827045E-03	-1.02766395818193E-02
11	9.53225229794034E-03	2.10746657295242E-02
12	-1.19300020359593E-02	-2.63758026122237E-02
13	3.43668630733477E-02	7.59810093989675E-02
14	1.3668580372784700	3.0219590643421900
15	-3.91580780641105E-02	-8.65738106816642E-02
16	1.85482594474814E-02	4.10079753978633E-02
17	-1.47482459292769E-02	-3.26066016028015E-02
18	8.94895406448388E-03	1.97850633452723E-02
19	-4.0883807717929E-03	-9.03891918168892E-03
20	-9.92822075423406E-04	-2.19501044605817E-03

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系数再计算

令E_lab = 60 MeV

Coefficient

1	2.31427026809873E-03	4.22851210403192E-03
2	-3.74266673080133E-03	-6.83840249373828E-03
3	7.29253603381996E-03	1.33245357351581E-02
4	1.18576867087333E-02	2.16657373448818E-02
5	1.59649469758367E-02	2.91703058446207E-02
6	-2.22626878830596E-02	-4.06772045942319E-02
7	-2.82321301369098E-02	-5.15842534262863E-02
8	3.82236093261335E-02	6.98401551985211E-02
9	4.91359155189706E-02	8.97785433182551E-02
10	6.85170951765909E-02	0.12519080864541200
11	-9.51221091511173E-02	-0.17380208156801800
12	0.15019206153051000	0.27442298285800700
13	-0.27214342466679600	-0.49724605682361300
14	0.94144202716869300	1.72015302706954000
15	0.94473226721487200	1.72616477947902000
16	-0.36328621472555400	-0.66377733723249400
17	0.24018856898092400	0.43885983637525200
18	-0.18918301809666900	-0.34566519430603800
19	0.15710714861519400	0.28705786385746900
20	-0.13247647718876100	-0.24205400510649200

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