组会

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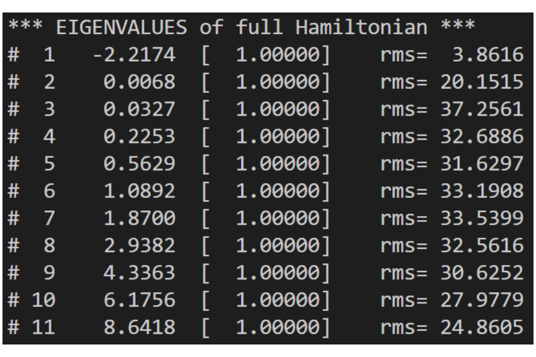
目录

1 用相同参数将 THO 和 THOx 进行 match

先看 np 的基态能量 E_{gs}
在 THOx 中, 得到的结果如下：



```
*** EIGENVALUES of full Hamiltonian ***
#  1   -2.2174  [  1.00000]    rms=  3.8616
#  2    0.0068  [  1.00000]    rms= 20.1515
#  3    0.0327  [  1.00000]    rms= 37.2561
#  4    0.2253  [  1.00000]    rms= 32.6886
#  5    0.5629  [  1.00000]    rms= 31.6297
#  6    1.0892  [  1.00000]    rms= 33.1908
#  7    1.8700  [  1.00000]    rms= 33.5399
#  8    2.9382  [  1.00000]    rms= 32.5616
#  9    4.3363  [  1.00000]    rms= 30.6252
# 10    6.1756  [  1.00000]    rms= 27.9779
# 11    8.6418  [  1.00000]    rms= 24.8605
```

图 1: THOx 中 np 的基态能量以及半径的方均根 rms

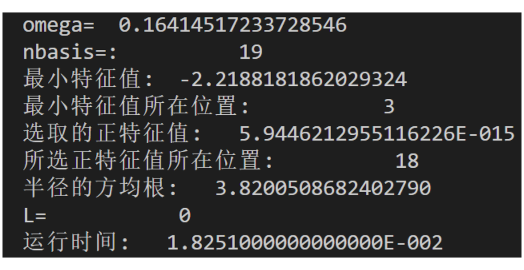
其中使用参数:

```
 &SYSTEM   Zv=0.  Av=1.0087      sn=0.0
           Zc=1.  Ac=1.0078    /

 &corestates  spin=0.0  parity=+1  ex=0.0  /
 &corestates  /

 &output  wfout(:)=1  5     xcdcc=F  verb=0  solapout(:)=0
cdccwf=F    /

 &GRID    rmin=0.0  rmax=60.0  dr=0.05  rlast=60  /

# p−n  potential
 &POTENTIAL  ptype=3  ap=1  at=0
    v10(0:2)=−72.150
    r0=0     a0=1.484    /

  &potential  ptype=0  /

 &pauli  n=0  /


  &JPSET  bastype=1  mlst=4  gamma=1.5  bosc=1.6  nho=20
/
```

还有一个要看的量是半径的方均根 rms:

$$\sqrt{<r^2>} = \sqrt{\int \varphi r^2 \varphi dr}$$

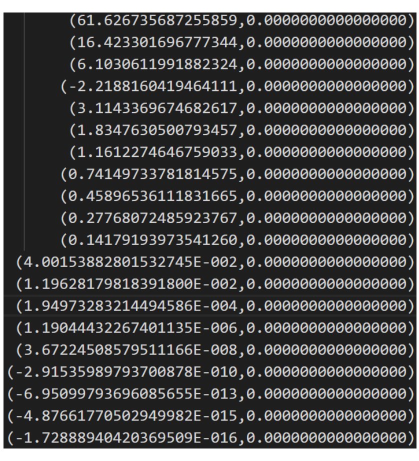
最后我们在 THO 中使用相同的参数, 得到的结果如下:



```
omega=  0.164145172337728546
nbasis=:            19
最小特征值:  -2.2188181862029324
最小特征值所在位置:            3
选取的正特征值:    5.9446212955116226E-015
所选正特征值所在位置:            18
半径的方均根:    3.8200508682402790
L=            0
运行时间:    1.8251000000000000E-002
```

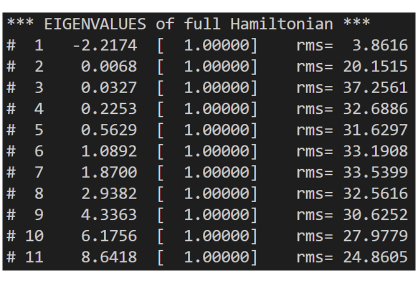
图 2: THO 中 np 的基态能量以及半径的方均根 rms

虽然 E_{gs} 的值和 THOx 的结果比较接近, 但是对角化得到的特征值, 即能级结构还是有差别, 我们给出 THO 的结果



```
(61.626735687255859,0.0000000000000000)
(16.423301696777344,0.0000000000000000)
(6.1030611991882324,0.0000000000000000)
(-2.2188160419464111,0.0000000000000000)
(3.1143369674682617,0.0000000000000000)
(1.8347630500793457,0.0000000000000000)
(1.1612274646759033,0.0000000000000000)
(0.74149733781814575,0.0000000000000000)
(0.45896536111831665,0.0000000000000000)
(0.27768072485923767,0.0000000000000000)
(0.14179193973541260,0.0000000000000000)
(4.0015388280153274SE-002,0.0000000000000000)
(1.1962817981839180E-002,0.0000000000000000)
(1.9497328321449458E-004,0.0000000000000000)
(1.1904443226740113E-006,0.0000000000000000)
(3.6722450857951116E-008,0.0000000000000000)
(-2.9153598979370087E-010,0.0000000000000000)
(-6.9509979369608565E-013,0.0000000000000000)
(-4.8766177050294998E-015,0.0000000000000000)
(-1.7288894042036950E-016,0.0000000000000000)
```

a: THO 算的各个特征值



```
*** EIGENVALUES of full Hamiltonian ***
#  1   -2.2174  [  1.00000]    rms=  3.8616
#  2    0.0068  [  1.00000]    rms= 20.1515
#  3    0.0327  [  1.00000]    rms= 37.2561
#  4    0.2253  [  1.00000]    rms= 32.6886
#  5    0.5629  [  1.00000]    rms= 31.6297
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#  9    4.3363  [  1.00000]    rms= 30.6252
# 10    6.1756  [  1.00000]    rms= 27.9779
# 11    8.6418  [  1.00000]    rms= 24.8605
```

b: THOx 的能级结构

图 3: THO 和 THOx 能级结构对比 (其中 THOx 只列出了 $-5MeV-10MeV$ 的特征值)

2 用 THO 给相移

在 reference:https://journals.aps.org/prc/pdf/10.1103/PhysRevC.82.024605以及https://journals.aps.org/pra/pdf/10.1103/PhysRevA.1.1109中给出了计算相移的方法:
从 Schwinger 的 Green 函数形式的相移公式出发:

$$tan\eta = \frac{[\int_0^\infty \Psi(x)V(x)sinkxdx]^2}{\int_0^\infty \int_0^\infty \Psi(x)V(x)G(x,x')V(x')\Psi(x')dxdx'}$$

其中 $G(x,x')$ 是自由粒子 Green 函数：

$$G(x,x') = \frac{1}{k}sinkx'coskx, x' < x$$

$$G(x,x') = \frac{1}{k}sinkxcoskx', x < x'$$

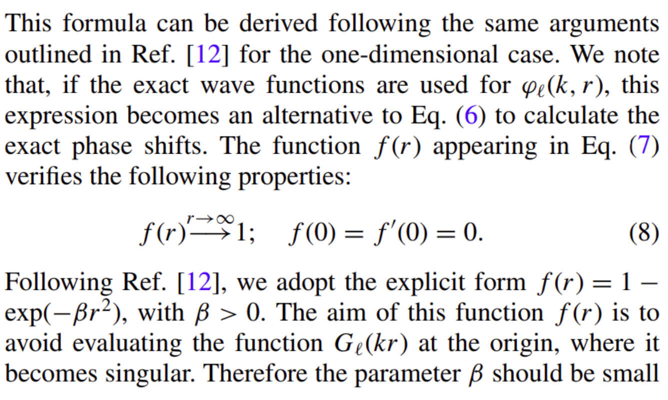
reference 的作者用 Schrodinger 方程将 $tan\eta$ 化简得:

$$tan\eta = -\frac{\int_0^\infty \Psi_E^*[E-H(x)]f(x)sinkxdx}{\int_0^\infty \Psi_E^*[E-H(x)]f(x)coskxdx}$$

其中 f 是一个具有规定的好的性质的函数, 这里选为:

$$f(r) = 1 - e^{-\beta r^2}$$

β 是一个可调参数, 先取 $0.01fm^{-1}$
上述公式的优点是: 不依赖本征函数 Ψ_E 的模, 因为动量算符作用在了 $f(x)$ 上面, 在做除法的时候, 模的影响被消除了, 所以即使是收敛的 basis 也可以用。
THO 用特定的方法给相移算是它和严格的解散射流程为数不多的相关联之处。(说为数不多的原因是 THO 不能严格给远处的波函数的渐近行为，却能在一定程度上给出本该需要用渐近行为才能定出来的相移)



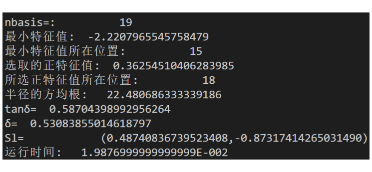
This formula can be derived following the same arguments outlined in Ref. [12] for the one-dimensional case. We note that, if the exact wave functions are used for $\varphi_\ell(k,r)$, this expression becomes an alternative to Eq. (6) to calculate the exact phase shifts. The function $f(r)$ appearing in Eq. (7) verifies the following properties:

$$f(r) \xrightarrow{r\to\infty} 1; \quad f(0) = f'(0) = 0. \tag{8}$$

Following Ref. [12], we adopt the explicit form $f(r) = 1 - \exp(-\beta r^2)$, with $\beta > 0$. The aim of this function $f(r)$ is to avoid evaluating the function $G_\ell(kr)$ at the origin, where it becomes singular. Therefore the parameter β should be small

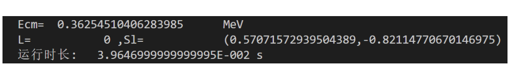
图 4: 参考地址:https://journals.aps.org/prc/pdf/10.1103/PhysRevC.82.024605

但结果是: 用这个方法算下来有明显的误差



```
nbasis=:            19
最小特征值:  -2.2207965545758479
最小特征值所在位置:            15
选取的正特征值:  0.36254510406283985
所选正特征值所在位置:            18
半径的方均根:   22.480686333339186
tanδ=  0.58704398992956264
δ=  0.53083855014618797
Sl=            (0.48740836739523408,-0.87317414265031490)
运行时间:   1.9876999999999999E-002
```

a: THO 给的相移



```
Ecm=  0.36254510406283985       MeV
L=            0 ,Sl=            (0.57071572939504389,-0.82114770670146975)
运行时长:   3.9646999999999995E-002 s
```

b: 精确相移