用现实核力求解np束缚态

验证程序的自洽性

计算T+V的期望值并于束缚能比较来验证程序的自洽性

$$\langle \phi | V + T | \phi \rangle$$

$\phi(p)$为束缚态波函数

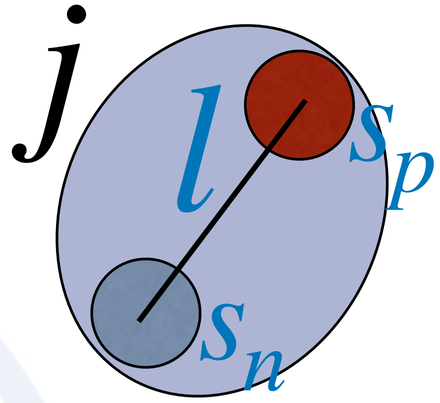
$$= \langle \phi | T | \phi \rangle + \langle \phi | V | \phi \rangle$$

$$= \sum_{\alpha} \int_0^{\infty} \langle \phi | k\alpha \rangle \frac{k^2}{2\mu} \langle k\alpha | \phi \rangle k^2 dk$$

$$+ \sum_{\alpha\alpha'} \int_0^{\infty} k^2 k'^2 \langle \phi | k\alpha \rangle \langle k\alpha | V | k'\alpha' \rangle \langle k'\alpha' | \phi \rangle dk dk'$$

角动量耦合

$|\alpha\rangle = |l(s_n s_p)s_{np}; j\rangle$　　j是好量子数



NNDC可查

Ground and isomeric state information for $^{2}_{1}\mathrm{H}$

E(level) (MeV)	Jπ	Δ(MeV)	$T_{1/2}$	Abundance	Decay Modes
0.0	1+	13.1357	STABLE	0.0115% *70*	

相对应的就是$j = 1,\quad l = 0,2$

因此

$|\alpha_1\rangle = |0\ (0.5\ 0.5)1.0\ ;\ 1.0\rangle$ ← s-wave

$|\alpha_2\rangle = |2\ (0.5\ 0.5)1.0\ ;\ 1.0\rangle$ ← d-wave

求解现实核力下的np束缚态

$$\langle k\alpha|\phi\rangle = \frac{1}{E-\frac{k^2}{2\mu}}\sum_{\alpha'}\int_0^\infty V(k\alpha,k'\alpha')\langle k'\alpha'|\phi\rangle k'^2\,dk'$$

积分运算在数值运算中为求和运算

$$\phi(k_i\alpha) = \sum_{j\alpha'} k_j^2\omega_j \frac{1}{E-\frac{k_i^2}{2\mu}} V_l(k_i\alpha,k_j\alpha')\phi(k_j\alpha')$$

A_{ij}

$$\begin{pmatrix}\phi_0\\ \phi_2\end{pmatrix} = \begin{pmatrix}A_{00} & A_{02}\\ A_{20} & A_{22}\end{pmatrix}\begin{pmatrix}\phi_0\\ \phi_2\end{pmatrix}$$

Krylov子空间方法简化矩阵

数值计算本征值问题中，计算速度与矩阵大小相关，矩阵越大求解速度越慢

对于

$$K(E)|\phi\rangle = \lambda(E)|\phi\rangle$$

我们假设本征态可以由一组正交基展开

$$|\phi\rangle = \sum_{i=0}^{\mathcal{N}} c_i \left|\bar{\varphi}_i\right\rangle$$

把上式代入本征值问题，可得

$$\sum_{j=0}^{\mathcal{N}} \left\langle \bar{\varphi}_i | K | \bar{\varphi}_j \right\rangle c_j = \lambda(E) c_i$$

即

N一般比较小

$$\sum_{j=0}^{\mathcal{N}} B_{ij} c_j = \lambda(E) c_i$$

$$B_{ij} = \left\langle \bar{\varphi}_i | K | \bar{\varphi}_j \right\rangle$$

建立Krylov子空间正交基

(a) Choose a normalized starting vector $|\bar{\varphi}_0\rangle$ and apply the kernel to generate the state $|\varphi_1\rangle$.

$$|\varphi_1\rangle = K|\bar{\varphi}_0\rangle \tag{1.8}$$

(b) Orthogonalize and normalize the state $|\varphi_1\rangle$ with respect to the state $|\varphi_0\rangle$.

$$|\tilde{\varphi}_1\rangle = |\varphi_1\rangle - |\bar{\varphi}_0\rangle\langle\bar{\varphi}_0|\varphi_1\rangle, \tag{1.9}$$

and

$$|\bar{\varphi}_1\rangle = \frac{|\tilde{\varphi}_1\rangle}{\||\tilde{\varphi}_1\|}. \tag{1.10}$$

(c) Repeat steps (a) and (b) $(i+1)$-times to generate $|\varphi_{i+1}\rangle$. Orthogonalize with respect to **all** vectors $\{|\bar{\varphi}_i\rangle, |\bar{\varphi}_{i-2}\rangle, ..., |\bar{\varphi}_0\rangle\}$ and normalize.

$$|\tilde{\varphi}_{i+1}\rangle = |\varphi_{i+1}\rangle - \sum_{n=1}^{i} |\bar{\varphi}_n\rangle\langle\bar{\varphi}_n|\varphi_{i+1}\rangle. \tag{1.11}$$

and

$$|\bar{\varphi}_{i+1}\rangle = \frac{|\tilde{\varphi}_{i+1}\rangle}{\||\tilde{\varphi}_{i+1}\|}. \tag{1.12}$$

建立Krylov子空间正交基

(d) Compute the matrix elements B_{ij}:

$$
\begin{aligned}
B_{ij} &= 0 && \text{for} \quad i > j+1 \\
&= \|\tilde{\varphi}_{j+1}\| && \text{for} \quad i = j+1 \\
&= \langle \bar{\varphi}_i | \varphi_{j+1} \rangle && \text{for} \quad i < j+1.
\end{aligned} \tag{1.13}
$$

(e) Use linear algebra techniques to obtain the eigenstates and eigenvalues of B, e.g. *dgeev.f* from LAPACK.

$$
B \cdot c = \lambda \cdot c \tag{1.14}
$$

建立Krylov子空间正交基

1. Choose a normalized starting vector $|\bar{\varphi}_0\rangle$ and a starting energy E_0.
2. Set the basis size $\mathcal{N} = 1$ and apply steps (a) to (e) and store the eigenvalue λ_1
3. Increase the basis size $\mathcal{N}$ by one and repeat steps (a) and (e). Iterate until the eigenvalues λ_n reach a constant value (upto a chosen precision, e.g., $|\lambda_n - \lambda_{n-1}| < 1e - 6$).
4. Choose the eigenstates corresponding to the eigenvalue closest to one and compute the wavefunction $|\phi\rangle$ from Eq. (1.5).
5. Change to a new energy E_1 and set $|\bar{\varphi}_0\rangle = |\phi\rangle$. Here a search routine, e.g. Newton-Raphson Secant, should be used to determine the value of the new energy E_1.
6. Repeat steps 2-4 until the variation in the energy falls below a chosen tolerance, e.g., $|E_n - E_{n-1}| < 1e - 6$

$$|\phi\rangle = \sum_{i=0}^{\mathcal{N}} c_i \left|\bar{\varphi}_i\right\rangle$$

程序说明

先编译NNpotentiale文件夹下的程序来获得现实核力

```
! list of potnr  implemented here
!       potnr=3      =>    Nijm93
!       potnr=7      =>    Nijm I
!       potnr=8      =>    Nijm II
!       potnr=11     =>    AV18  (needs input file!)
!       potnr=12     =>    separable (needs input file!) (for testing)
!       potnr=31     =>    CDB 2000
!       potnr=63     =>    Idaho N3LO
!       potnr=67     =>    Idaho N3LO 600

#define POTNR 31
```

选取现实核力的类型

计算A矩阵

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程序说明

计算D波的概率 $|\Phi\rangle = |\phi_0\rangle + |\phi_2\rangle$

$$D\% = \langle \phi_2 | \Phi \rangle$$

```
c     calculate d-state probability
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccc计算D-wave的概率ccccccccccccccccccccccccccccccc
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计算 $\langle \Phi | V + T | \Phi \rangle$

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cccccccccccccccccccc计算<\phi|T+V|\phi>cccccccccccccccccccccccccccccccc
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程序说明

挑战：使用Krylov子空间方法简化矩阵求解本征值问题