B Nuclear shell model wave function - NEPTUNE

B.1 Generation of the nuclear shell model wave function

The program "NEPTUNE" calculates the bound state wave function. It consists of a main program, also called NEPTUNE, and subroutines BSAXON and UNCPST.

The main program reads in 7 data cards, containing control characters, the quantum numbers of the bound state, mass and charge of the orbiting particle, mass and charge of the nucleus, binding energy of the particle in the nucleus, accuracy parameters for the program's automatic search feature, and the parameters of the Woods-Saxon potential in which the particle moves. It outputs this data, and calls BSAXON.

BSAXON sets up the initial constants needed for numerical integration of the bound state Schrödinger equation and for automatic search on well depth of binding energy, and calls UNCPST.

BSAXON first calculates up the total potential, consisting of a real Woods-Saxon central potential plus a Thomas-type derivative Woods-Saxon spin-orbit potential and a Coulomb potential if the orbiting particle is charged.

UNCPST computes the radial wave function using the Störmer method to solve the radial Schrödinger equation. It tests input quantum numbers, well depth, and binding energy for consistency and ability to satisfy boundary conditions at this point, iterates either well depth or binding energy, and solve the Schrödinger equation again. This process is repeated until a solution is found satisfying the boundary conditions.

The Schrödinger equation solved is

$$[-\frac{\hbar^2}{2\mu}(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}) + \epsilon + V_j]u_{j\ell}(r) = 0$$

where $u_{j\ell}(r)$ is the radial state function times r, ϵ is the binding energy, j and ℓ are the total and orbital angular momentum quantum numbers, and $V_j(r)$ is the total potential energy function. $u_{j\ell}(r)$ is subject to the boundary condition $u_{j\ell}(0) = 0$. The potential $V_j(r)$ is of standard form,

$$\begin{aligned} V_j(r) &= \frac{-V_0}{1+\exp(\frac{r-R_0}{a_0})} + V_C(r) \\ &\quad +(\frac{\hbar}{m_\pi c})^2 \frac{V_{SO}}{r}(\vec{\sigma}\cdot\vec{\ell})\frac{d}{dr}[\frac{1}{1+\exp(\frac{r-R_{SO}}{a_{SO}})}] \end{aligned}$$

where

$$V_C(r) = \begin{cases} \frac{Ze^2}{2R_C}[3-(\frac{r}{R_C})^2] & r < R_C \\ \frac{Ze^2}{r} & r > R_C \end{cases}$$

$$< jm_j|(\vec{\sigma}\cdot\vec{\ell})|jm_j > = \begin{cases} \ell & j = \ell + \frac{1}{2} \\ -(\ell+1) & j = \ell - \frac{1}{2} \end{cases}$$

with $R_0 = r_0 A^{1/3}$, $R_C = r_C A^{1/3}$, and $R_{SO} = r_{SO} A^{1/3}$

The region of integration is divided into two parts at a distance of $R_m \approx r_0 A^{1/3}$, the *half-radius* of the central potential. The solution started from the origin is carried two points past R_m. A second solution is started at a large distance (generally 2 or 3 fermis beyond the greatest distance at which the function is needed) and carried inward two points inside R_m. Its logarithmic derivative at R_m is compared to the logarithmic derivative of the inner solution.

Let α_0 be the value of some parameter α (well-depth or binding energy), such that the logarithmic derivatives are the same to within some desired accuracy. The value actually used for α may be

$\alpha_1 = \alpha_0 + \Delta\alpha$. But the condition that the logarithmic derivatives agree can be put in the form $f(\alpha_0) = 0$. Thus

$$f(\alpha_0) = f(\alpha_1 - \Delta\alpha) = f(\alpha_1) - \frac{\partial f}{\partial \alpha}|_{\alpha_1} \Delta\alpha = 0,$$

or

$$\Delta\alpha = f(\alpha_1)/[\frac{\partial f}{\partial \alpha}|_{\alpha_1}]$$

This condition is used to iterate well depth or binding energy until $\Delta\alpha/\alpha$ is sufficiently small ($|\Delta\alpha/\alpha| \approx$ ACURCY). In practice, in NEPTUNE,

$$\frac{\partial f}{\partial \alpha}|_{\alpha_1} = [f(1.01\alpha_1) - f(0.99\alpha_1)]/(0.02\alpha_1)$$

is used to evaluate the derivative.

B.2 Meaning of key quantities.

XMES1 and XMES2 (recommended values are 0.0125 and 0.1 fm, respectively) are the minimum and maximum mesh sizes used in the Störmer method.

NXRM and NXCPL2 are defined by R_m = XMES2 *NXRM, R_c = XMES2*NXCPL2. Here R_c is the largest distance at which the state function is desired to be evaluated and R_m is the point at which the inner and outer solutions are matched. A third radius, R_a = XMES2*NXRA is used to extend the range of the inward integration that produces the outer solution, to ensure that it has the correct asymptotic form. Generally it is sufficient for R_a is to be 2 to 3 fermis greater than R_c.

NODER is the desired number of nodes. The actual number of nodes is counted in UNCPLB and stored in KEXCOM(42). If the two quantities differ, the quantity being searched is changed by 10 % in a direction determined to reduce the disagreement, and the calculation is repeated until the two agree or the number of iterations (Input data) is exceeded.

B.3 Input data of the program NEPTUNE

Line 1: READ(7,10) KTRL(1) - (14)
FORMAT(14I5)

KTRL(2)=0 causes the binding energy be searched for a given potential
KTRL(2)=1 causes the potential depth be searched for a given binding energy

Line 2: READ(7,10) KEXCOM(1) - (14)
FORMAT(14I5)

KEXCOM are all zero, unless one wants to input NXCPL2, NXRA
KEXCOM(2) = NXCPL2
KEXCOM(4) = NXRA-NXCPL2

Line 3: READ(7,10) KTLOUT(1) - (14)
FORMAT(14I5)

KTLOUT gives intermediate output, useful in case of suspicion
of numerical errors in the program.
KTLOUT(1) =1, Output of calculations
KTLOUT(2) =1, Detailed output (Potential etc.)

Line 4: READ(7,11) EXTCOM(1) - (14)
FORMAT(10F7.3)

EXTCOM(1) = XMES2 =0.10
EXTCOM(2) = XMES1 =0.0125
EXTCOM(3) = Desired normalization =1.0

Line 5: READ(7,10) ITBEMX,JBTRTW,LBTR,NODER
FORMAT(14I5)

ITBEMX	# of iterations
JBTRTW	$2j$
LBTR	ℓ
NODER	n, the desired # of nodes, not counting the zero at the origin.

Line 6: READ(7,11) TMAS,PMAS,ZZT,ZZP,
ACURCY, PERCNT, EGES
FORMAT(10F7.3)

TMAS	M_T, mass of the core nucleus.
PMAS	M_P, mass of the orbiting nucleus.
ZZT	Z_T, charge of the core nucleus.
ZZP	Z_P, charge of the orbiting nucleus.
ACURCY	"Accuracy" is the criterion for matching of interior and exterior solution. 0.003 is recommended.
PERCNT	"Percent" is the maximum allowed value of $\|\Delta\alpha/\alpha_1\|$ as discussed earlier. 0.2 is recommended. Should not exceed 1.0.
EGES	$\epsilon > 0$, the binding energy.

Line 7: READ(7,11) VSX,VSOR,DFNR,DFNSO,
RZR,RZSO,RZC,
FORMAT(10F7.3)

VSX	V_0, Potential depth parameter of the central potential.
VSOR	V_{SO}, Potential depth parameter of the spin-orbit potential.
DFNR	a_0, Diffuseness parameter of the central potential.
DFNSO	a_{SO}, Diffuseness parameter of the spin-orbit potential.
RZR	V_0, Radius parameter of the central potential.
RZSO	r_{SO}, Radius parameter of the spin-orbit potential.
RZC	r_C, Radius parameter of the Coulomb potential.