Research Article

Numerical Simulation of Shell Model Single Particle Energy States using Matrix Numerov Method in Gnumeric Worksheet

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ABSTRACT:

Background: The Nuclear Shell Model single particle energy states have been successfully determined by solving time-independent Schrödinger equation (TISE) with the Woods-Saxon potential along with spin-orbit coupling terms. However for an under graduate or a post graduate student, solving this analytically is a difficult task. So in order to obtain single particle energy states, a simple numerical method is needed to solve the TISE, which can be easily implemented in a worksheet environment.

Purpose: Single particle energy states as described by nuclear shell model are obtained for doubly magic nuclei using Gnumeric worksheet environment. The time-independent Schrödinger equation (TISE) for a nucleus modeled using Woods-Saxon potential along with spin-orbit coupling term has been solved numerically by choosing Matrix Numerov method.

Methods: Numerov method rephrased in matrix form is utilised to solve time-independent Schrödinger equation (TISE) within mean-field approximation, described by Woods-Saxon (WS) potential along with spin-orbit term, to obtain the single particle energies for both neutron and proton states. Only the algorithm parameters, step size 'h' and matrix size 'N' are optimized to obtain the expected energy level sequence obtained using matrix methods.

Results: The energy level sequences for doubly magic nuclei up-to $Z = 82$, i.e $^{16}_{8}O$, $^{48}_{20}Ca$, $^{56}_{28}Ni$, $^{100}_{50}Sn$, $^{132}_{50}Sn$ and $^{208}_{82}Pb$.

Conclusions: Ground state configurations could be better predicted when energy level sequences are known for all nuclei as compared to what is usually obtained from that of $^{208}_{82}Pb$ alone. An attempt is made, by incorporating this tool within the framework of guided enquiry strategy (a constructivist approach to learning), to actively engage the students in assigning appropriate J^{π} configurations for ground states of nuclei neighboring the doubly magic ones.

Keywords: Nuclear Shell Model, Single Particle Energy States, Matrix Numerov Method, Gnumeric

1. Introduction

Shell model [1] has been one of the most successful models to have explained evidence for magic numbers, that has emerged from binding energy data. While harmonic oscillator potential along with inclusion of spin-orbit term has been very effective in obtaining shell closures at magic numbers, actual energy level sequencing as seen from experimental data is better deduced by utilizing a rounded square well potential as demonstrated by WS potential [2]. Even though square

well and harmonic oscillator potentials are included in both under-graduate(UG) and post-graduate(PG) nuclear physics courses [3], they are not dealt beyond establishing the fact that magic numbers result due to $\bar{L}.\bar{S}$ splitting that gives rise to levels with higher j-values corresponding to a particular N-oscillator getting clubbed with those of a lower (N-1) oscillator. There is no way to judge the magnitude of splitting due to this spin-orbit coupling and hence different textbooks [4, 5, 6] present varying energy level

sequences which could lead to difficulties while assigning the ground state total angular momentum J and spin-parities $(-1)^\ell$ for different nuclei. Another important lacuna in the pedagogy of topics in this subject is the lack of lab activities that enhance interaction with the content. Our physics education research (PER) group has been focusing on this much needed aspect and have developed various experimental [7, 8, 9] and simulation [10, 11, 12, 13] activities to supplement the classroom lectures. With regard to single particle energy level structure, we have solved the TISE for WS potential along with spin-orbit term, utilizing matrix methods technique employing sine wave basis in Scilab [10]. In spite of the simplicity of sine basis, the technique still requires determining integrals that appear in the matrix elements numerically. This makes it invariable to use a programming environment such as Scilab. So as to overcome this limitation and keep ease of simulating the problem using simple worksheet environment, matrix methods numerical technique has been replaced with Numerov method rephrased in matrix form [14].

In this paper, we utilize model parameters obtained through optimization, while solving TISE using matrix methods [10], with respect to available experimental single particle energies [15]. The nuclear shell model with interaction potentials based on these model parameters, which are rephrased in appropriate choice of units, is described in Section II. A brief discussion on numerical Numerov method and its algorithm are given in Section III. The implementation details, for a typical example of $^{40}_{20}Ca$ using Gnumeric worksheet environment have been presented in a step by step approach in Appendix. The algorithm parameters are optimized to obtain convergence of single particle energies with those obtained using matrix methods [10] and final results are discussed in Section IV along with our initial attempts at implementation of a pilot study, by incorporating this tool into guided inquiry strategy (GIS) framework. Finally, we draw our conclusions in Section V.

2. Method & Materials

2.1. Nuclear Shell Model using Woods-Saxon potential

The modeling methodology [16] has been described in great detail in our previous paper on Shell model simulation [10]. So, only a brief description of the potentials rephrased in MeV and fm units are given here. In shell model, a nucleus of mass number A, consisting of N neutrons and Z protons has been modeled by the assumption that each nucleon experiences a mean field of central potential type due to rest of the nucleons. Woods-Saxon (WS) potential, which has typically a rounded square well shape, is one of the successful mathematical formulations graphically represented in Figure 2 and is given by

$$V_{WS}(r) = \frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)} \qquad (1)$$

where V_0 is the depth of the well, given by [18]

$$V_0 = \begin{cases} -51 + 33((N-Z)/A) \quad MeV, \\ \qquad\qquad \text{for neutrons} \\ -51 - 33((N-Z)/A) \quad MeV, \\ \qquad\qquad \text{for protons} \end{cases} \qquad (2)$$

Here, r is the distance between two interacting nucleons, R is the radius of the nucleus, empirically obtained as $R_0 A^{1/3}$, with value of R_0 being 1.28, a is surface diffuseness parameter and is found to be 0.66 [10].] Next, interaction of spin of nucleon with orbital angular momentum of nucleon, as confirmed in experiments [17], has been modeled by spin-orbit potential, as

$$V_{ls}(r) = V_1 \left(\frac{r_0}{\hbar}\right)^2 \frac{1}{r} \frac{d}{dr} \left[\frac{1}{1 + \exp\left(\frac{r-R}{a}\right)}\right] (\mathbf{L.S}) \quad (3)$$

Here, $\mathbf{L.S} = [j(j+1) - \ell(\ell+1) - 3/4]\hbar^2$, where ℓ is orbital angular momentum quantum number, $j = \ell + s$ is total angular momentum quantum number and s is spin angular momentum quantum number given by 1/2 for nucleons. The model parameters are $V_1 = -0.44V_0$ [18] and $r_0 = 0.90$, a proportionality constant optimised previously by our group [10] to obtain the right energy level sequence. In our earlier work [10], the parameters r_0 and a were adjusted for a fixed value of R_0 during simulation to better match

the experimental energy levels. It was found that for r_0 within range 0.86 - 0.95 and a within range 0.66 - 0.67, the χ^2 value comes out to be minimum.

In case of protons, Coulomb potential also needs to be considered and is given by

$$V_c(r) = \begin{cases} \frac{(Z-1)e^2}{4\pi\epsilon_0 r}, & \\ & \text{for; } r \geq R_c \\ \frac{(Z-1)e^2}{4\pi\epsilon_0 R_c}\left[\frac{3}{2} - \frac{r^2}{2R_c^2}\right], & \\ & \text{for; } r \leq R_c \end{cases} \quad (4)$$

Here R_c is the charge radius of the nucleus which in this case is considered to be equal to radius of nucleus R. The potential $V_c(r)$ is to be rephrased in MeV units. So, it is multiplied and divided by electron rest mass energy, [19] $m_e c^2 = 0.511$ MeV to obtain

$$V_c(r) = \begin{cases} \frac{(Z-1)*2.839*0.511}{r}, & \text{for } r \geq R_c \\ \frac{(Z-1)*2.839*0.511}{R_c}\left[\frac{3}{2} - \frac{r^2}{2R_c^2}\right], & \text{for } r \leq R_c \end{cases} \quad (5)$$

The radial TISE for central potentials is given by

$$\frac{d^2u(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left(V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right)u(r) = Eu(r) \quad (6)$$

where V(r) is net interaction potential experienced by a neutron or a proton and second term inside bracket, resulting from solution of θ-equation, is called as centrifugal potential $V_{cf}(r)$ and μ is the reduced mass given by:

$$\mu = \begin{cases} \frac{m_n*(Z*m_p+(N-1)*m_n)}{(Z*m_p+N*m_n)}, & \text{for neutron} \\ \frac{m_p*((Z-1)*m_p+N*m_n)}{(Z*m_p+N*m_n)}, & \text{for proton} \end{cases} \quad (7)$$

Here, $m_p = 938.272$ and $m_n = 939.565$ are masses of proton and neutron respectively, in units of MeV/c². The centrifugal potential $V_{cf}(r)$ is rephrased in MeV units, by multiplying and dividing it by c^2, so that

$$V_{cf}(r) = \frac{\ell(\ell+1)\hbar^2 c^2}{2\mu c^2 r^2} \quad (8)$$

The value of $\hbar c = 197.329$ MeV-fm.

3. Numerical Solution

3.1. Numerov technique in matrix form:

Consider TISE for a general potential V(r), given by

$$\frac{d^2u(r)}{dr^2} + k^2(r)u(r) = 0 \quad (9)$$

where

$$k^2(r) = \frac{2\mu}{\hbar^2}[E - V(r) - V_{cf}(r)] \quad (10)$$

The advantage of this Eq. (9) is that it is linear in 'u' having no first order derivative involved and is hence ideally suited for solving using Numerov method. The wave-function u(r) is expanded in Taylor series by explicitly retaining terms up-to $O(h^4)$ and is obtained to an accuracy of $O(h^6)$, [14]

$$u(r+h) = u(r) + hu'(r) + \frac{h^2}{2}u''(r)+$$
$$\frac{h^3}{6}u'''(r) + \frac{h^4}{24}u''''(r) + \dots \quad (11)$$

Discretizing x in steps of h as:

$r_1, r_2, \dots, r_{n-1}, r_n, r_{n+1}, \dots, r_N.$

Here, $r_n = r_1 + n \times h$

Now expressing $u(r_n + h)$ as u_{n+1}, so on and similarly, $k(r_n)$ as k_n, Eq. (11) can be written as

$$u_{n+1} = \frac{2(1 - \frac{5}{12}h^2 k_n^2)u_n - (1 + \frac{1}{12}h^2 k_{n-1}^2)u_{n-1}}{1 + \frac{1}{12}h^2 k_{n+1}^2}+$$
$$O(h^6) \quad (12)$$

Substituting from Eq. (10), $k_n^2 = \frac{2\mu}{\hbar^2}(E - V_n)$ into the above, clubbing the terms containing V_n and E, it can be recast into the following form:

$$-\frac{\hbar^2}{2\mu}\frac{(u_{n-1} - 2u_n + u_{n+1})}{h^2}+$$
$$\frac{(V_{n-1}u_{n-1} + 10V_n u_n + V_{n+1}u_{n+1})}{12} \quad (13)$$
$$= E\frac{(u_{n-1} + 10u_n + u_{n+1})}{12} \quad (14)$$

One has to keep in mind that whatever may be the potential, if wave-function were to be normalised, it should tend to 0 as x tends to ±∞. This implies, one has to choose the region of interest (RoI) large enough to ensure that the wave-function dies down to zero in

either direction. That is, x values are limited to an interval such as $[L_1, L_2]$, such that u goes to 0 at both ends of the interval. More specifically,

$$u_1 = u(r_1 = L_1) = 0 \qquad (15)$$

and

$$u(r_N = L_2) = 0 \qquad (16)$$

Expanding the above equation for all intermediate points $(j = 2, 3, \ldots, N-1)$, one will get a matrix equation as

$$\left(\frac{-\hbar^2}{2\mu} A + BV \right) u = EBu \qquad (17)$$

where in, u is a column vector $(u_2, \ldots, u_{n-1}, u_n, u_{n+1}, \ldots, u_{N-1})$,

Similarly, V is a column vector $(V_2, \ldots, V_{n-1}, V_n, V_{n+1}, \ldots, V_{N-1})$, but is converted into a diagonal matrix with these values along its central diagonal. Matrices A and B are given by

$$A = \frac{I_{-1} - 2I_0 + I_1}{h^2} \qquad (18)$$

and

$$B = \frac{I_{-1} + 10I_0 + I_1}{12} \qquad (19)$$

where I_p represents a matrix consisting of 1's along pth diagonal and zeros elsewhere, here p can be positive (above the main diagonal, i.e I_1), zero (the main diagonal, i.e I_0) or negative (below the main diagonal, i.e I_{-1}).

Multiplying Eq. (17) by B^{-1} on both sides, gives TISE as a matrix equation, utilising Numerov method,

$$\boxed{\left(\frac{-\hbar^2 c^2}{2\mu c^2} B^{-1} A + V \right) u = Eu} \qquad (20)$$

with an error of $O(h^6)$.

Notice that a factor of c^2 is introduced in both numerator and denominator to ensure the units are in MeV and fm as required in nuclear physics.

This is the final equation that needs to be solved numerically to get energy eigen-values and eigen-functions of a particle interacting with a given potential V(r). The imposition of boundary conditions as $u_1 = u_N = 0$ is equivalent to embedding the potential of interest, inside an infinite square well potential. Finally, $(N-2) \times (N-2)$ sub-matrices of A and B are utilised to solve for the energy eigen-values and their corresponding eigen-vectors.

4. Algorithm for implementation in Gnumeric:

A step by step approach to determining the single particle energies for protons of $^{40}_{20}Ca$ is presented.

a) **Initialisation of parameters:** There are two sets of parameters:

  i. *Physical system parameters*:
  Object and interaction variables constituting as inputs and state variables which we wish to determine, are outputs. Figure (1) show object variables, interaction variables, Algorithm variables, input variables and other variables required for the calculations.

  ii. *Algorithm parameters*:
  that arise from discretization of continuous variables and limiting the infinitely large quantities to finite values such as region of interest. The step size is chosen as $h = 0.1$ and is given in cell F17.

b) **Potential Definition:**
  First the values of 'r' are generated from 0.1 to $(3 \times R)$ with step-size $h = 0.1$ from A22 to A153, and to get the expected results, corresponding matrix size is 131×131. Then, four potentials are determined using the following formula for a particular ℓ and j values:

  i. Centrifugal potential V_{CF}, in cell B22 type the formula:

  `=($J$8*($J$8+1)*$J$14^2*`
  `($A22^(-2)))/(2*$J$13)`

  ii. Woods-Saxon potential V_{WS}, in cell D22 by typing the formula:

  `=$F$9*(1+$C22)^(-1)`

  iii. L.S potential V_{LS}, in cell F22 by typing formula:

	A	B	C	D	E	F	G	H	I	J	K
1	**Woods-Saxon potential with L.S coupling for proton**										
2	**(Ca40)**										
3											
4	**Initializing the parameters**										
5											
6	**Object variables-**				**Interaction variables-**				**Input variables-**		
7									(These are varied each time to obtain various bound states)		
8	**Mass of neutron *(mn)***	939.565	MeV/c^2		**Woods-Saxon potential:**				**Orbital ang mom qtm no. *(l)***	1.00	
9	**Mass of proton *(mp)***	938.272	MeV/c^2		**Well depth (V0)**	−51.00	MeV		**Total ang mom qtm no. *(j)***	0.50	
10	**Radius prop. Constt. (R0)**	1.28	fm		**Surface diffuse parameter (a)**	0.66					
11	**Mass of nucleus (A)**	40			**Range (R)**	4.378	fm		**Other variables-**		
12	**Charge of nucleus (Z)**	20			**Spin-orbit potential:**						
13	**Number of neutrons (N)**	20			**Dimensionality of distance (r0)**	0.90	fm		**Reduced mass (mu)**	914.831	MeV/c^2
14	**For Coulomb pot. (Z-1)**	19			**Dimensionality of energy (V1)**	22.44	MeV		**hbar*c**	197.329	MeV-fm
15	**Radius of nucleus (R)**	4.378	fm						**f (=(-hbar^2 c^2)/(2*mu c^2))**	−21.282	MeV-fm^2
16					**Algorithm parameter-**				**LS term**	−2.00	
17					**Step-size (h)**	0.1	fm		**Cut off distance (a0=3*R)**	13.133	fm

Figure 1: Initializing the parameters for the system

```
=-$F$14*$F$13^2*$J$16*$C22*
  $E22*($F$10*$A22)^(-1)
```

where, the L.S term in cell J16 is calculated by formula:

```
=$J$9*($J$9+1)-$J$8*
  ($J$8+1)-3/4
```

iv. Coulomb potential, for proton, is given by typing formula:

```
=$B$14*0.511*2.839*
  (3*$B$15^2-$A22^2)/(2*$B$15^3)
```

in cell G22 up-to radius 'R' of the nucleus. After that in cell G65, type the formula:

```
=0.511*2.839*$A65^(-1)*$B$14
```

which gives the Coulomb potential outside the range of nuclear radius.

v. In cell H22, the net potential is determined by typing the formula as:

```
=$B22+$D22+$F22+$G22
```

Figure (2a) consists of the potential values for the few r values and Figure (2b) shows the plot of Woods-Saxon potential of $1s_{1/2}, 1p_{1/2}$ and $1p_{3/2}$ states for proton, showing that inclusion of angular momentum on L.S coupling affects the Woods-Saxon potential.

c) **Determination of single particle energies:**
   This step consists of generating the following matrices and the same steps can be easily applied to matrix of any size.

i. In Sheet 2, B-matrix is obtained as follows. Remember, B-matrix is constant for all problems. First generate index values for rows and columns as 1 to 5 from A43: A8 and B33: F3. In cell B4, the formula is given as

```
=if($A4=B$3,10/12,
  if($A4+1=B$3,1/12,
  if($A4-1=B$3,1/12,0)))
```

This is repeated by dragging across till EB4 and then downwards to EB134 to obtain the tridiagonal B-matrix as shown in Figure (3a).

ii. In Sheet 3, the inverse of B, is obtained by selecting cells B43: EB134 and giving the formula as

```
=minverse('Sheet 2'!B4:EB134)
```

press Ctrl+Shift+Enter keys together to obtain matrix-B^{-1} as in Figure (3b).

iii. In Sheet 4, A-matrix is generated similar to B-matrix, except that we need step size 'h' from Sheet 1 available in cell F17, say. Then, In cell D4, type $='Sheet1'!F17$.
In cell D3, insert the value of function $f = \frac{-\hbar^2 c^2}{2\mu c^2}$ from cell J15 of Sheet 1. Then, in cell B7, the formula is given as

```
=if($A7=B$6,(-2*$D$3/$D$4^2),
  if($A7+1=B$6,($D$3/$D$4^2),
  if($A7-1=B$6,($D$3/$D$4^2),0)))
```

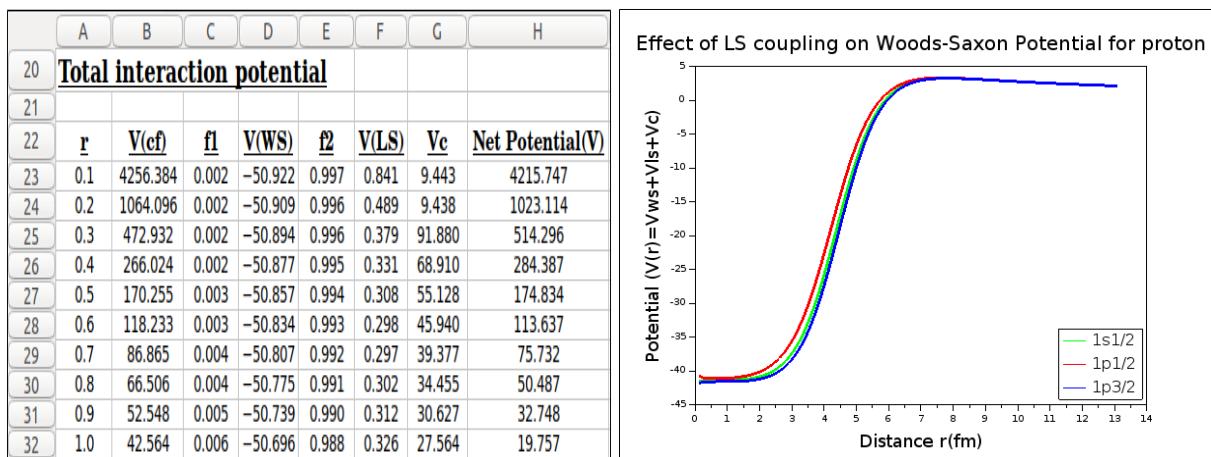|	r	V(cf)	f1	V(WS)	f2	V(LS)	Vc	Net Potential(V)
20	**Total interaction potential**							
22	r	V(cf)	f1	V(WS)	f2	V(LS)	Vc	Net Potential(V)
23	0.1	4256.384	0.002	−50.922	0.997	0.841	9.443	4215.747
24	0.2	1064.096	0.002	−50.909	0.996	0.489	9.438	1023.114
25	0.3	472.932	0.002	−50.894	0.996	0.379	91.880	514.296
26	0.4	266.024	0.002	−50.877	0.995	0.331	68.910	284.387
27	0.5	170.255	0.003	−50.857	0.994	0.308	55.128	174.834
28	0.6	118.233	0.003	−50.834	0.993	0.298	45.940	113.637
29	0.7	86.865	0.004	−50.807	0.992	0.297	39.377	75.732
30	0.8	66.506	0.004	−50.775	0.991	0.302	34.455	50.487
31	0.9	52.548	0.005	−50.739	0.990	0.312	30.627	32.748
32	1.0	42.564	0.006	−50.696	0.988	0.326	27.564	19.757

Figure 2: (a) Total Interaction potential $V(r) = V_{cf}(r) + V_{WS}(r) + V_{ls}(r) + V_c(r)$ for proton (b) Plots of $1s_{1/2}$, $1p_{1/2}$ and $1p_{3/2}$ states for proton, showing the effect of Spin-orbit interaction in Woods-Saxon potential.
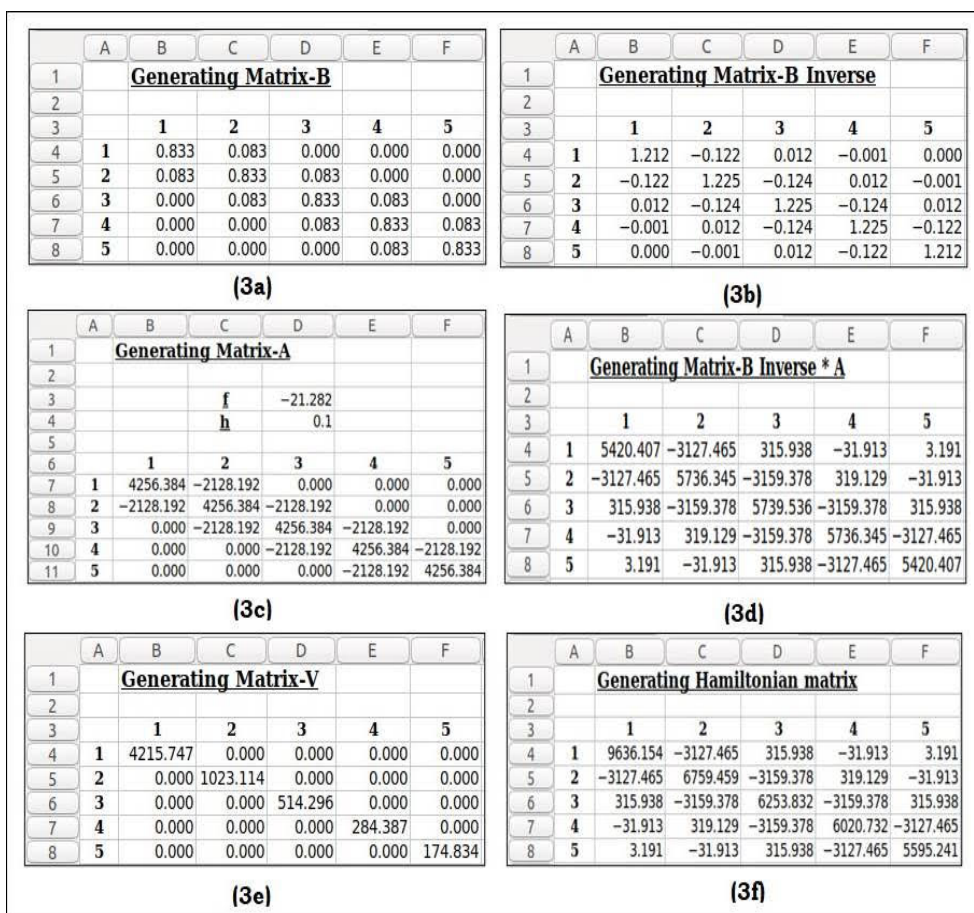

Figure 3: (a) Generating matrix-B (b) Generating matrix-B^{-1} (c) Generating matrix-A (d) Generating matrix-B^{-1}*A (e) Generating matrix-V (f) Generating Hamiltonian matrix

and dragged appropriately to generate the required values as shown in Figure (3c).

iv. To obtain matrix-$B^{-1} * A$, in Sheet 5, select cells B4 : F8 and give formula:

```
=mmult(Sheet3!B4:EB134,'Sheet 4'!
B7:EB137)
```

The obtained matrix is shown in Figure (3d).

v. Generate-V-matrix in Sheet 6, by giving the formula in cell B4 as

```
=if($A4=B$3,'Sheet 1'!$H22,0)
```

so that only diagonal elements get populated as those of net potential values from Sheet 1 and seen in Figure (3e).

vi. In Sheet 7, finally we generate the Hamiltonian matrix (i.e. matrix-$B^{-1} * A + V$) by simply giving the formula in B4 as

```
=(Sheet5!B4:EB134+'Sheet 6'
  !B4:EB134)
```

and dragging the formula to fill values from B4 : EB134 as seen in Figure (3f).

vii. The main feature of Gnumeric which makes it different from other worksheet environments such as MS-Excel or open Office Calc. is that, it has an eigen-value solver.

Now, the eigen-values and corresponding eigen-vectors are obtained in Sheet 8 by selecting cells B4 : EB135, a matrix of size 132×131, with an extra row to incorporate the eigen values. Each eigen vector of size 131×1 will be available below each of the eigen values in the first row. The formula is typed as

```
=eigen(Sheet7!B4:EB134)
```

and all the three keys Ctrl+Shift+Enter pressed together. The resultant values are shown in Figure (4a) and (4b).

d) **Generating the energies for different ℓ and j values:** Now, the bound state energies, those for which eigen values are negative, are tabulated for different values of ℓ and j.

- Starting from $\ell = 0$, s-states, in which case $j = 0.5$ alone exists
- for $\ell = 1$, p-states, we have two values of j: $j = 0.5$ and $j = 1.5$.
- Similarly for $\ell = 2$, d-states, j takes values 1.5 and 2.5 , and so on.

This is continued till no bound states are obtained for particular ℓ and j values.

5. Results and Discussions:

In this section, we will first validate our approach to obtain energy eigen-values and eigen-functions using Woods-Saxon potential with $\bar{L}.\bar{S}$ coupling for both neutron and proton for doubly magic nucleus $^{40}_{20}Ca$. This is done by comparing our results with available experimental results and those obtained numerically by using matrix method with Fourier basis [10] for different angular momentum values ℓ and j. The results are tabulated in Table 1.

The obtained energy eigen values are in good agreement with experimental energy values of different neutron and proton single particle states for step size of h=0.1 thus validating our approach. One can observe from the Table 1, that while the numerical or simulated values are below than those of experimental ones for lower proton and neutron states, the trend is opposite for higher states. This discrepancy arises because the optimization algorithm, in its attempt to minimize χ^2, tends to find values close to the expected ones.

The distance parameter 'r' is discretized as per step size 'h' and its values are varied from $r = 0.1$ to $r = 3R$, where $R = R_0 A^{(1/3)}$. Therefore, it is necessary to vary the size of matrix 'N' for different A values for a chosen step size 'h'. This simulation activity can be utilised as a tool to apply GIS[20] of constructivist approach to learning and has been done as follows:

5.1. GIS Implementation:

The students have been taken through following six step process of GIS. All steps were implemented on online Moodle platform [21] during COVID-19 lockdown of university.

- **Initiation:** The matrix Numerov technique was already introduced before, for solving the harmonic oscillator potential. Next, it has been applied to solve for single particle energies of both neutrons and protons, as dealt with in this paper, for Woods-Saxon potential with spin-orbit potential. This has been explained and also demonstrated in two successive lab sessions.

- **Selection:** The students were made to explore the binding energy and separation energies
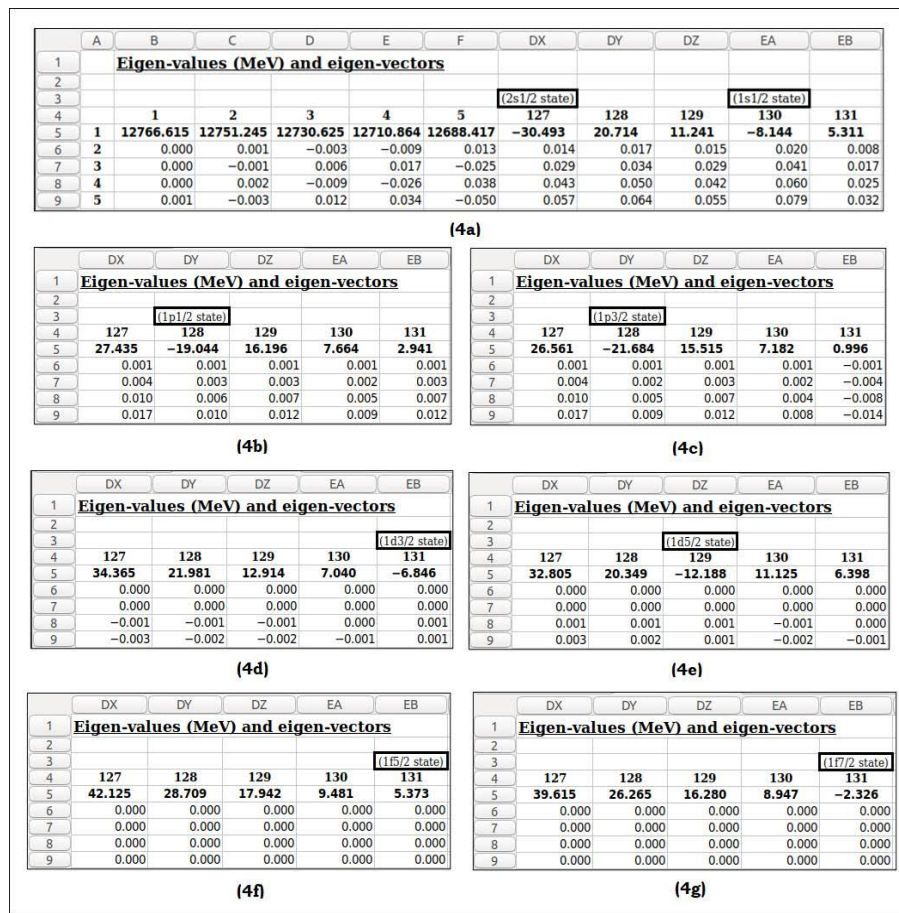
Figure 4: Calculation of eigen-values and eigen-functions

Table 1: Single particle shell model energy values for **Neutron states** and **Proton states** of doubly magic nucleus $^{40}_{20}Ca$ obtained by current work (*using Matrix Numerov method* [14]) with available experimental values [15] and numerical values previously obtained by our group [10], (*using Matrix method with Fourier basis*) for the highest occupied levels.

States	Proton states (MeV)			States	Neutron states (MeV)		
	Exp.	Numerical values			Exp.	Numerical values	
	Ref[15]	Ref[10]	Current		Ref[15]	Ref[10]	Current
$1s1/2$	...	−30.49	−30.49	$1s1/2$	...	−38.90	−38.90
$1p3/2$	...	−21.68	−21.68	$1p3/2$	...	−29.55	−29.55
$1p1/2$	...	−19.04	−19.04	$1p1/2$	...	−26.99	−26.99
$1d5/2$	−15.07	−12.19	−12.19	$1d5/2$	−22.39	−19.54	−19.54
$2s1/2$	−10.92	−8.14	−8.14	$2s1/2$	−18.19	−15.54	−15.54
$1d3/2$	−8.33	−6.85	−6.85	$1d3/2$	−15.64	−14.28	−14.28
$1f7/2$	−1.09	−2.33	−2.33	$1f7/2$	−8.36	−9.15	−9.15
$2p3/2$	0.69	1.00	1.00	$2p3/2$	−5.84	−5.42	−5.42
$2p1/2$	2.38	2.94	2.94	$2p1/2$	−4.20	−3.10	−3.10
$1f5/2$	4.96	5.37	5.37	$1f5/2$	−1.56	−1.19	−1.20

curves that they have plotted in previous sessions, to identify various double magic nuclei suitable for study. The doubly magic nuclei from $^{16}_{8}O$ to $^{208}_{82}Pb$ were selected. The determination of single particle proton and neutron energy

level sequences for six double magic nuclei, are assigned to students by dividing them into 12 groups. Each group is expected to obtain the energy level sequence of either neutrons or protons

for the assigned nuclei by carefully following the simulation procedure.

- **Presentation:** The students in each group could be asked to present their findings to the rest of the class so that everyone gets to know each other's experience. Even though all the groups could get to expected level sequence by following the steps correctly, some of the students have not ensured reduction of step-size systematically. Hence, they have come up with lower accuracy for energies even though they obtained correct level sequence. They have been guided accordingly.

- **Exploration:** The collective findings were shared with entire class and they were asked to explore nuclei adjacent to the magic numbers with one neutron or proton more and find out ground state J^π configuration for each of them.

- **Formulation:** They were expected to formulate their findings based on right choice of level sequence and also figure out what they would get if they followed the level sequence given in their prescribed textbook [4].

- **Collection:** To understand variation of energy level structure with mass number, students were asked to plot the compiled energy data for protons and neutrons as a function of mass number A. They were able to obtain plots similar to what have been presented in [10].

- **Assessment:** They have assessed their formulated ground state angular momentum and spin configurations based on the experimental findings and thus validated their outcomes. They could be further asked to obtain the ground state configurations of nuclei slightly away from magic nuclei till the results obtained are in variance with those from experiments as an excercise.

5.2. *Outcomes from GIS:*

The results matching with experimentally available values [15] were obtained for step-size 'h = 0.1' for

doubly magic nuclei from $^{16}_{8}O$ to $^{208}_{82}Pb$. The value of N (to solve N × N matrix) for each of these nuclei are obtained as 96, 131, 138, 145, 177, 194 and 229 respectively. The obtained energy level sequences for neutrons and protons of these nuclei are given separately in tabular form in Tables 2 and 3. The first four levels, $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$ ad $1d_{5/2}$ are not shown, as there are no discrepancies found in the ordering of these levels across the periodic table due to our simulation. The numerically obtained energy values are found to match to two decimal places with those obtained using the matrix method approach [10]. The χ^2-value defined as relative mean-squared error

$$\chi^2 = \frac{1}{N} \sum_{i=1}^{N} \frac{(E_i^{expt} - E_i^{sim})^2}{|E_i^{expt}|} \qquad (21)$$

These are determined w.r.t experimental [15] and are shown in Tables. In Tables 2 and 3, energy level sequence obtained for lighter nuclei ^{16}O to ^{56}Ni are shown in first column and that for ^{100}Sn to $^{208}_{82}Pb$ in last column. It can be observed that the energy level sequence for lighter nuclei is different than that for heavier ones. This might be because the effect of spin-orbit coupling is different for light nuclei and heavy nuclei which results into the change in internal structure. Also, the amount of splitting in the energy levels is different for different mass numbers. The observed discrepancies in energy sequence are highlighted in red colour.

The discrepancy in level sequence for lighter nuclei w.r.t heavy nuclei is highlighted in blue colour in both tables; i.e for neutron and proton states. Further, it is found that in most of the textbooks at UG and PG level [4, 5, 6, 18, 22, 23], energy level sequence given is different. Also, there is only single energy level sequence given for both neutrons and protons, and that too common for all mass ranges. But according to our calculations as well as Bohr and Mottelson book, there should be different energy level sequences for nuclei across the periodic table.

Next, J^π assignments for nuclei near to doubly magic nuclei in mass range equal to and less than $^{208}_{82}Pb$ based on our simulation, which match with

Table 2: Single particle shell model energy states for **Neutron** of doubly magic nuclei $^{16}_{8}O$, $^{48}_{20}Ca$, $^{56}_{28}Ni$, $^{100}_{50}Sn$, $^{132}_{50}Sn$ and $^{208}_{82}Pb$ obtained by using Matrix Numerov method

States	Numerical energy values(MeV)						States
	$^{16}_{8}O$	$^{48}_{20}Ca$	$^{56}_{28}Ni$	$^{100}_{50}Sn$	$^{132}_{50}Sn$	$^{208}_{82}Pb$	
$2s1/2$	−3.03	−14.19	−20.51	−29.27	−25.57	−30.90	$1d3/2$
$1d3/2$	2.11	−13.58	−20.35	−28.34	−24.46	−29.67	$2s1/2$
$1f7/2$	...	−8.33	−14.96	−24.04	−20.78	−26.74	$1f7/2$
$2p3/2$	...	−4.90	−10.56	−20.08	−18.07	−25.07	$1f5/2$
$1f5/2$	...	−1.87	−8.41	−19.75	−17.15	−23.59	$2p3/2$
$2p1/2$	...	−3.00	−8.32	−18.19	−16.06	−22.87	$2p1/2$
$1g9/2$	...	1.16	−5.25	−16.07	−14.01	−21.20	$1g9/2$
$2d5/2$	...	...	−1.70	−10.01	−9.79	−18.50	$1g7/2$
$3s1/2$	...	...	−0.94	−11.17	−9.76	−17.20	$2d5/2$
$1g7/2$	...	...	3.52	−8.36	−7.99	−15.76	$2d3/2$
$2d3/2$	...	...	...	−9.05	−7.74	−15.44	$3s1/2$
$1h11/2$	...	...	...	−7.69	−6.83	−15.24	$1h11/2$
$2f7/2$	...	...	...	−2.95	−0.94	−11.28	$1h9/2$
$3p3/2$	...	...	...	−1.53	−2.61	−10.64	$2f7/2$
$3p1/2$	...	...	...	−0.53	−0.57	−8.90	$1i13/2$
$1h9/2$	...	...	...	0.59	−1.34	−8.45	$3p3/2$
...	...	...	...	...	0.03	−8.36	$2f5/2$
...	...	...	...	...	...	−7.55	$3p1/2$
...	...	...	...	...	...	−4.04	$2g9/2$
...	...	...	...	...	...	−3.49	$1i11/2$
...	...	...	...	...	...	−2.24	$1j15/2$
...	...	...	...	...	...	−2.07	$3d5/2$
...	...	...	...	...	...	−1.41	$4s1/2$
...	...	...	...	...	...	−1.01	$2g7/2$
...	...	...	...	...	...	−0.82	$3d3/2$
χ^2	0.24	1.18	0.09	0.06	0.03	0.06	...

experimentally[15] available energy sequence, are tabulated. These assignments are compared with those calculated using energy level sequence given in usually referred textbook *Introductory Nuclear Physics* by Kenneth Krane[4] by considering only the energy level sequence of lighter nuclei, and are shown in Table 4. The discrepancies in spin assignments are highlighted in blue colour. These discrepancies are also observed in other textbooks [5, 6, 17, 22, 23] as well.

  Hence, from our observations, the level sequence for lighter mass range and heavy mass range nuclei can be modified accordingly so as to provide students with data consistent with experiments.

6. Conclusion:

The time-independent Schrödinger equation (TISE) for a nucleus modeled using Woods-Saxon potential along with spin-orbit coupling term has been solved numerically by choosing Matrix Numerov method. The main advantage of matrix Numerov method is that it can be easily extended to any arbitrary potential of interest. It is implemented in Gnumeric worksheet environment to obtain numerical solutions of single-particle neutron and proton states for doubly magic nuclei $^{40}_{20}Ca$. Then, using guided enquiry strategy, a Constructivist approach, students were grouped and encouraged to obtain energy level sequences for other doubly magic nuclei up-to Z = 82, i.e $^{16}_{8}O$, $^{48}_{20}Ca$, $^{56}_{28}Ni$, $^{100}_{50}Sn$, $^{132}_{50}Sn$ and $^{208}_{82}Pb$. Based on these obtained level structures, students obtained

Table 3: Single particle shell model energy states for **Proton** of doubly magic nuclei $^{16}_{8}O$, $^{48}_{20}Ca$, $^{56}_{28}Ni$, $^{100}_{50}Sn$, $^{132}_{50}Sn$ and $^{208}_{82}Pb$ obtained by our calculations using Matrix Numerov method

States	Numerical energy values(MeV)						States
	$^{16}_{8}O$	$^{48}_{20}Ca$	$^{56}_{28}Ni$	$^{100}_{50}Sn$	$^{132}_{50}Sn$	$^{208}_{82}Pb$	
$2s1/2$	−0.21	−15.18	−10.71	−14.25	−26.11	−24.16	$1d3/2$
$1d3/2$	4.82	−14.55	−10.60	−13.05	−24.61	−22.26	$2s1/2$
$1f7/2$	. . .	−9.75	−5.89	−9.83	−21.70	−20.56	$1f7/2$
$2p3/2$	. . .	−4.98	−1.56	−5.58	−18.24	−18.37	$1f5/2$
$2p1/2$	. . .	−2.38	0.54	−5.14	−16.97	−16.25	$2p3/2$
$1f5/2$	. . .	−1.71	. . .	−3.56	−15.58	−15.36	$2p1/2$
$1g9/2$	. . .	0.40	. . .	−2.43	−14.77	−15.18	$1g9/2$
$2d5/2$	. . .	. . .	. . .	3.92	−9.37	−11.71	$1g7/2$
$1g7/2$	. . .	. . .	. . .	2.55	−9.10	−9.89	$2d5/2$
$1h11/2$	. . .	. . .	. . .	. . .	−7.32	−9.29	$1h11/2$
$3s1/2$	. . .	. . .	. . .	. . .	−6.56	−8.09	$2d3/2$
$2d3/2$	. . .	. . .	. . .	. . .	−6.43	−7.57	$3s1/2$
$2f7/2$	. . .	. . .	. . .	. . .	−1.18	−4.26	$1h9/2$
$1h9/2$	. . .	. . .	. . .	. . .	0.330	−3.26	$2f7/2$
. . .	. . .	. . .	. . .	. . .	. . .	−2.95	$1i13/2$
. . .	. . .	. . .	. . .	. . .	. . .	−0.37	$2f5/2$
. . .	. . .	. . .	. . .	. . .	. . .	−0.28	$3p3/2$
χ^2	1.53	0.31	0.48	0.25	0.03	0.11	. . .

Table 4: Nuclear single particle shell model states for **Neutron** and **Proton** of nuclei near to closed shell nuclei, according to Ref.[4] and Current work.

Nuclei	Neutron states		Nuclei	Proton states	
	Ref.[4]	Current work		Ref.[4]	Current work
$^{17}_{8}O$	$1d5/2$	$1d5/2$	$^{16}_{9}F$	$1d5/2$	$1d5/2$
$^{41}_{20}Ca$	$1f7/2$	$1f7/2$	$^{40}_{21}Sc$	$1d3/2$	$1d3/2$
$^{49}_{20}Ca$	$2p3/2$	$2p3/2$	$^{48}_{21}Sc$	$1f7/2$	$1f7/2$
$^{57}_{28}Ni$	$2p3/2$	$2p3/2$	$^{56}_{29}Cu$	$1f7/2$	$2p3/2$
$^{101}_{50}Sn$	$1g7/2$	$2d5/2$	$^{100}_{51}Sb$	$1g9/2$	$2d5/2$
$^{133}_{50}Sn$	$1h9/2$	$2f7/2$	$^{132}_{51}Sb$	$1h11/2$	$2d3/2$
$^{209}_{82}Pb$	$2g9/2$	$1i11/2$	$^{208}_{83}Bi$	$1h9/2$	$2f7/2$

ground state total angular momentum and spin assignment for various nuclei close to doubly magic nuclei successfully and it could easily be extended to test the limits of validity.

whatsoever.

Declaration: This is an original data and has neither been sent elsewhere nor published anywhere.

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