Numerical Simulations of ^{208}Pb Neutron Single Particle States using Fourier Basis Functions in Scilab

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Introduction

In this work, we obtained the shell model neutron levels of ^{208}Pb utilizing numerical matrix diagonalization method as proposed by Marsiglio's et al.[1] by implementing the algorithm using free open source software(FOSS) Scilab. The central idea of this method is to embed the nuclear potentials inside the infinite square well potential ranging from r=0 to r=a_0, where a_0 is equivalent to choosing some cut-off radius. The eigen functions of infinite square well given by sine functions form the basis functions and hence the numerical solution is alike to Fourier analysis, which is within the reach of UG students. This technique is currently being implemented as a part of Nuclear Physics Simulation Lab for PG students.

Methodology

Following Marsiglio's paper[1], starting with Schrodinger equation for potential embedded in an infinite square well, in Dirac notation, as

$$(H_0 + V)\,|u\rangle = E\,|u\rangle \tag{1}$$

where

$$V = V_{inf}(r) + V_{eff}(r)$$

Here, $V_{inf}(r)$ is infinite square well potential and $V_{eff}(r)$ is effective nuclear potential. For calculating single particle neutron states

$$V_{eff}(r) = V_{WS}(r) + V_{ls}(r) + V_{c.f}(r)$$

having analytical expressions as

$$V_{WS} = \frac{-V_0}{1 + exp(\frac{r-R_0}{a})}$$

$$V_{ls}(r) = V_1 \left(\frac{r_o}{\hbar}\right)^2 \frac{1}{r}\left[\frac{d}{dr}\frac{1}{1+exp(\frac{r-R_0}{a})}\right](L\cdot S)$$

$$V_{c.f}(r) = \frac{l(l+1)\hbar^2}{2\mu r^2}$$

We have chosen the parameterization suggested by Bohr & Mottelson[2]. Here, all distances and energies are in fm and Mev respectively. Now, on expanding the wavefunction $u(r)$ in terms of infinite square well basis, $|u\rangle = \sum_{m=1}^{\infty} c_m\,|m\rangle$ followed by inner product with $\langle n|$ and then substituting in eqn.(1) and using orthonormality condition we get eigen value matrix equation in dimensionless form as

$$\sum_{m=1}^{n_{max}} h_{nm}c_m = ec_n \tag{2}$$

where $h_{nm} = \delta_{nm}\Big[n^2 - \frac{V_o}{c1} * L1 + \frac{l(l+1)}{\pi^2} * L3 - (\frac{V_{ls}r_0^2}{a_o ac1}(J - L - 3/4)) * L5\Big]$
$+ (1-\delta_{nm})\Big[\frac{V_o}{c1} * L2 + \frac{l(l+1)}{\pi^2} * L4 - (V_{ls}\frac{r_0^2}{a_o ac1}(J - L - 3/4)) * L6\Big]$
and L1-L6 are the integrals corresponding to different potentials as given below.

For V_{WS}
$\begin{cases} L1 = \int_0^1 dx \frac{(1-cos(2n\pi x))}{1+exp(\frac{ax-R_o}{a})} \\ L2 = \int_0^1 dx \frac{cos(n-m)\pi x - cos(n+m)\pi x}{1+exp(\frac{ax-R_o}{a})} \end{cases}$
For $V_{c.f}$
$\begin{cases} L3 = \int_0^1 dx \frac{(1-cos(2n\pi x))}{x^2} \\ L4 = \int_0^1 dx \frac{cos(n-m)\pi x - cos(n+m)\pi x}{x^2} \end{cases}$
For V_{ls}

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$$\begin{cases} L5 = \int_0^1 dx \frac{(1-cos(2n\pi x))exp(\frac{ax-R_o}{a_{so}})}{x(1+(exp(\frac{ax-R_{so}}{a_{so}}))^2)} \\ L6 = \int_0^1 dx \frac{(cos((n-m)\pi x - cos((n+m)\pi x))exp(\frac{ax-R_o}{a_{so}})}{x(1+(exp(\frac{ax-R_{so}}{a_{so}}))^2)} \end{cases}$$

The integrals and the eigen solver can be easily computed with in-built functions in Scilab and the implemented code is available on request from the authors.

Results and Discussion

A. Single particle energy spectra: For obtaining energy spectra, the algorithm parameters: infinite potential well width 'a' and number of basis functions'N' have been optimized and the value of a=2R, where R=R_0 $A^{\frac{1}{3}}$ has resulted in the right sequence of expected energy levels and N=30 basis function was enough to obtain the energy values to a two decimal accuracy. The shell model neutron single particle states in ^{208}Pb computed by using Woods-Saxon potential with spin-orbit coupling term are shown in FIG.1

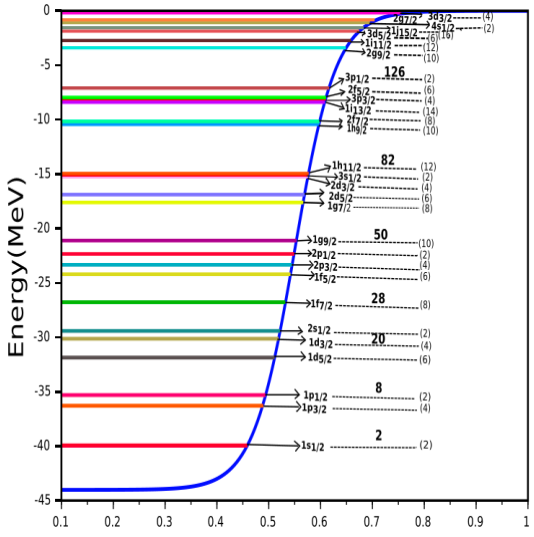

FIG. 1: `Neutrons single particle states in` ^{208}Pb `with two potential models.`

Here, the potential function is plotted for $l = 0$ state and the level scheme so obtained is well matched with those of [2] and [3].

B. Comparison of Single particle energies of ^{208}Pb with experimental results[4]: The single particle neutron energies calculated by using the current simulation are compared with experimental values and the obtained energy spectra is presented in FIG. 2. The

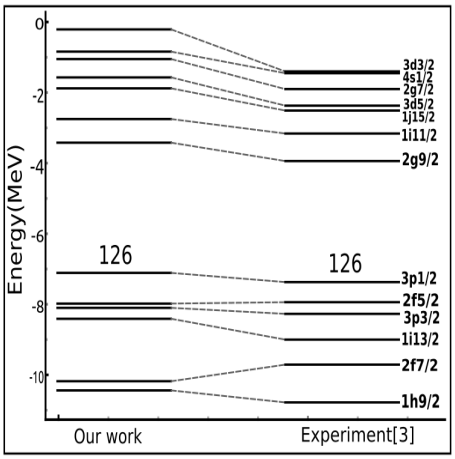

FIG. 2: `Comparison of single particle neutron energy levels with experimental results for` ^{208}Pb `nuclei`

numerical and experimental results[3] shows good agreement with chi square value of 0.09 for the levels presented in FIG.2.

Conclusion

In this paper, we have presented the neutron single particle energy levels for ^{208}Pb only, while the algorithm has also been implemented for proton energy levels and the level structures have been verified for other magic nuclei as well.

References

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