

Numerical Study on Nuclear Shell Structure of ^{208}Pb

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Abstract

The shell structure of ^{208}Pb has been studied by solving Schrödinger equation numerically. The truncated Taylor's series for second order differential equation was applied. The energy levels of ^{208}Pb were studied by using Harmonic Oscillator potential and Wood-Saxon potential. When spin-orbit interaction was included, the energy levels splitting were clearly seen and could explain the magic numbers up to 82 correctly.

Keywords: Taylor series, Schrödinger equation

Introduction

Most of the undergraduate students have to study nuclear structures and models. Nuclear models have the property to help us to better understanding of nuclear structure which contains main physical properties of nuclei. Nuclear model that have been proposed over the years by scientists were known as liquid drop model was used to explain the nuclear fission, Fermi gas model was used to describe the level densities of nuclei, shell model or also known as independent particle model and collective model was based upon the deformation of nuclei. Obtaining the nuclear structure and energy levels of nuclei is one of the most criteria to improve investigations of nuclei properties. The shell model is partly analogous to atomic shell model which describes the arrangement of electrons in an atom.

Nuclear shell model has been found that the nuclei with proton number or neutron number equal to certain numbers 2,8,20,28,50,82 and 126 behave in a different manner when compared to other nuclei having neighboring values of Z or N. Hence these numbers are known as magic numbers. The shell model plays one of the most important and successful model because the shell model allows to know how the structure of nuclei changes and how the energy levels splitting which depends on potential.

In this work we intend to undergraduate students who have to study nuclear shell model and the shell model can easily be understood with our method. To study shell model, one must have to use Schrödinger equation which is second order differential equation. To solve the second order differential equation, we have applied Taylor's series which is very familiar with undergraduate students.

Numerical differentiation

The function to be differentiated or integrated will typically be a complicated continuous function that is difficult or impossible to differentiate or integrate

directly, in this situation we have to use numerical method. One of the numerical methods to differentiate a function is using Taylor's series expansion which is the easiest one.

Taylor's expansion is

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \frac{1}{4!}f''''(x)h^4 + \mathcal{O}(h^5) \quad (1)$$

By using Eq.(1) the truncated Taylor's expansion for first order forward and backward differences are as follows;

forward difference formula:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h^2) \quad (2)$$

backward difference formula:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h^2) \quad (3)$$

The second order forward and backward differences formula can also be deduced from Eq.(1).

Second order forward difference formula is

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \quad (4)$$

Second order backward difference formula is

$$f''(x) = \frac{f(x-2h) - 2f(x-h) + f(x)}{h^2} \quad (5)$$

Schrödinger equation

Erwin Schrödinger, who derived the equation in 1925, and published it in 1926, awarded the Nobel Prize in Physics in 1933 (Schrödinger, 1926). In quantum mechanics, the analogue of Newton's equation is Schrödinger equation for a quantum system. The equation is mathematically described as a linear partial differential equation, which describes the time evolution of the system's wave function.

The Schrödinger equation has two forms. One is that in which time explicitly appears and describes how the wave function of a particle will evolve in time. The other is the equation in which the time dependent has been removed and is known as the time independent Schrödinger equation. For non-relativistic quantum physics, the basic equation to be solved is the Schrödinger equation and which is of the following form;

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\psi(r) \quad (6)$$

We separate the Schrödinger equation into radial part and hence

$$-\frac{\hbar^2}{2mr} \frac{d^2u(r)}{dr^2} + \left(V(r) + \frac{\hbar^2 \ell(\ell+1)}{2m r^2} \right) u(r) = Eu(r) \quad (7)$$

where $u(r) = \frac{\psi(r)}{r}$.

For $r = 0, u(r \rightarrow 0) \rightarrow r^{l+1}$

For $r = \infty, u(r \rightarrow \infty) \rightarrow e^{-\alpha r}$, where α is constant.

Calculation of single particle energy levels of ²⁰⁸Pb

The Schrödinger radial Eq.(7) can be written as

$$\frac{d^2u(r)}{dr^2} + k(r)u(r) = 0 \quad (8)$$

where $k(r) = \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right]$ and it is known as kernel equation. By substituting second order forward difference formula Eq.(4) in Eq.(8) and after rearranging it becomes

$$u_{out}(r_{n+2}) = 2u_{out}(r_{n+1}) - u_{out}(r_n) - \{k(r)u_{out}(r_{n+1})\} \Delta r^2 \quad (9)$$

By substituting second order backward difference formula Eq.(5) in Eq.(8) and it becomes

$$u_{in}(r_{n+2}) = 2u_{in}(r_{n-1}) + u_{in}(r_n) - \{k(r)u_{in}(r_{n-1})\} \Delta r^2 \quad (10)$$

Both Eq.(9) and Eq.(10) are the solutions of Schrödinger equation.

The eigen-functions $u_{in}(r_c)$ and $u_{out}(r_c)$ and first derivatives $u'_{in}(r_c)$ and $u'_{out}(r_c)$ must be satisfied the continuity conditions.

$$u_{in}(r_c) = u_{out}(r_c) \text{ and } u'_{in}(r_c) = u'_{out}(r_c) \quad (11)$$

where r_c is arbitrary point and mostly taken in the inner region.

The physical $u_{in}(r_c)$ and $u_{out}(r_c)$ can be written as

$$u_{out}(r_c) = Au_{out}(r_c) \text{ and } u_{in}(r_c) = Bu_{in}(r_c) \quad (12)$$

where, A and B are constants. Their respective derivatives are

$$u'_{out}(r_c) = Au'_{out}(r_c) \text{ and } u'_{in}(r_c) = Bu'_{in}(r_c) \quad (13)$$

By substituting Eq.(12) and Eq.(13) into Eq.(11) then

$$A = \left[\frac{u_{in}(r_c) - u'_{in}(r_c)}{u_{out}(r_c) - u'_{out}(r_c)} \right] B = f_c B \quad (14)$$

where f_c will be a scaling factor to be applied to $u_{out}(r_c)$.

$$u_{out}(r_c) = Bf_c u_{out}(r_c) \text{ and } u_{in}(r_c) = Bu_{in}(r_c) \quad (15)$$

and B is a global factor that must be taken into account in the normalization process.

To determine energy eigen value E of Schrödinger equation we find the match point for a given E, satisfying the following condition

$$\text{Match}(E) = \left[\frac{u'_{out}(r_c)}{u_{out}(r_c)} \right] - \left[\frac{u'_{in}(r_c)}{u_{in}(r_c)} \right] = 0 \quad (16)$$

Harmonic oscillator potential

The harmonic oscillator potential is given by

$$V(r) = \frac{1}{2} m \omega^2 r^2 \quad (17)$$

where $\omega = \sqrt{k/m}$ is the angular frequency of the oscillator and m is nucleon mass. The energy levels of the harmonic oscillators are

$$E_n = \left(2(n-1) + l + \frac{3}{2} \right) \hbar \omega \quad (18)$$

where, $l=0,1,2,3,\dots$

Wood-saxon potential

Woods and Saxon introduced a potential to study elastic scattering of 20MeV proton by a heavy nuclei (Woods & Saxon, 1954). The Woods-saxon potential is a reasonable potential for nuclear shell model and hence attracts lots of attention in nuclear physics (Abe, K et al., 1996), (Garica, F et al., 1999) (Bespalova, Romanovsky, & Spasskaya, 2003). The Woods-Saxon potential plays an essential role in microscopic physics, since it can be used to describe the interaction of a nucleon with the heavy nucleus. The total potential is the sum of spin-independent Wood-Saxon potential central potential, a spin orbit potential and the Coulomb potential:

$$V(r) = V_o(r) + V_{so}(r) \vec{l} \cdot \vec{s} + V_c(r) \quad (19)$$

$V_o(r)$ is the spin-independent central potential which is given by

$$V_o(r) = \frac{V_o}{1 + \exp\left(\frac{r-R}{a}\right)} \quad (20)$$

where, R= nuclear radius; $R = r_o A^{\frac{1}{3}}$, $V_o = 53 + \frac{N-Z}{A} V_1$ for protons, $V_o = 53 - \frac{N-Z}{A} V_1$ for neutrons, $V_1 = -30MeV$, $r_o = 1.25fm$, $a = 0.65fm$. The

$V_{so}(r)$ is the spin orbit potential which can be written as

$$V_{so}(r) = V_{so} \frac{1}{ra} \frac{\exp\left(\frac{r-R}{a}\right)}{\left(1 + \exp\left(\frac{r-R}{a}\right)\right)^2} \quad (21)$$

where, $V_{so} = 22\text{MeV}$ (Brown, 2005).

The Coulomb potential $V_c(r)$ is

$$V_c(r) = \frac{Ze^2}{r} \text{ for } r \geq R, \quad V_c(r) = \frac{Ze^2}{r} \left[\frac{3}{2} - \frac{r^2}{2R^2} \right] \text{ for } r \leq R \quad (22)$$

Numerical realization

In this section, we will present numerical accuracy and the results. This is very important in this research work because we have solved the second order differential Schrödinger equation directly with numerical difference method. The second order numerical differentiation can easily enter the numerical error (round off and/or truncation error). Therefore, we have to well understand the numerical precision. Firstly, we will study numerical accuracy of first order differential equation with forward and backward difference method. We consider arbitrary function $f(x) = x^3$, first order differentiation results $f'(x) = 3x^2$ and at $x = 2$ then $f'(2) = 12$. Here we have used Eq.(2) and Eq.(3) and compared this numerical results with analytical results which are shown in Table 1 and Table 2. Again the results of second order forward and backward formula of Eq.(4) and Eq.(5) are shown in Table 3 and Table 4. We have found that the numerical precisions are good in agreement with analytical result at $h=0.001$ for first order and $h=0.01$ for second order differential equation.

Energy levels of harmonic oscillator potential

After we have studied about the differential equation, we will continue to study the energy levels of protons and neutrons with Harmonic-oscillator potential, Woods-Saxon potential with spin independence central potential and Woods-Saxon with spin orbit potential. For the first we will study the energy levels of ^{208}Pb with Harmonic-oscillator potential. We have found 1s(11.41MeV), 2s(26.60MeV) and 3s(41.80MeV) energy levels respectively. For the “p” and “d” states, energy levels are 1p(19.99MeV), 2p(34.16MeV), 1d(26.58MeV) and 2d(41.76MeV) respectively. We have also found the energy levels of “f” and “g” states which are 1f(34.17MeV), 1g(41.76MeV) respectively.

In 1s state two nucleons can occupy and in 1p state 6 nucleons can occupy. The energy difference between these two states is 7.57MeV and then we can say that the magic number 2 and (2+6)8 can be

explained. The energy value of 2s and 1d are the same and the energy difference between 1p and these two state is about 7.61MeV so 2s and 1d can be considered as a shell, hence two nucleons stay in 2s state and 10 nucleons stay in 1d state, hence twelve nucleons can be occupied in these two levels. Therefore totally twenty nucleons can be filled up to this shell (1s up to 1d). Now the magic number 2, 8 and 20 are correctly predicted. Again, 2p and 1f are the same energy level and the energy gap between (2s, 1d) and (2p, 1f) is about 7.56MeV and so we can predict the level (2p, 1f) will be a shell twenty nucleons can occupy in this level (2p, 1f). The number of nucleons occupy up to this state (1s up to 1f) is 40, but this number does not include in magic number series. So Harmonic-oscillator model cannot be predicted magic number correctly.

Energy levels of Woods-saxon potential

The magic numbers cannot be correctly predicted with Harmonic Oscillator potential and hence we will continue to study the energy levels and magic numbers by using Woods-Saxon potential. In the following we will use the nucleon instead of neutron or proton. At first, we will use only central term. We have found three $s(\ell = 0)$ states such as 1s(42.45MeV), 2s(31.57MeV) and 3s(16.62MeV) respectively. For $\ell = 1$ and $\ell = 2$ we have also found the energy level states for each partial waves which are 1p(38.37MeV), 2p(24.97MeV), 3p(8.80MeV), 1d(33.41MeV), 2d(17.91MeV) and 3d(1.12MeV) respectively. For higher partial waves, we have found that 1f(27.73MeV), 2f(10.53MeV), 1g(21.38MeV), 2g(2.97MeV) and 1h(14.45MeV) respectively.

The energy difference between 1s and 1p is 4.08MeV, so it can be considered as two different shells and magic number 2 and 8 can be explained. The energy difference between 2s and 1d state is 1.84MeV so we can say that these two states to be formed a level and twelve nucleons can be occupied in this shell. So the magic number 20 (1s up to 1d) can be explained. Although the energy difference between 2p and 1f is 2.76MeV, we can regard as one level and twenty nucleons can stay in this level. The number of nucleons up to this level is forty nucleons but this number does not include in magic number.

To overcome this difficulty we add spin orbit interaction term to the Wood-Saxon potential. The 1p state splits into $1p_{\frac{3}{2}}$ (38.45MeV) and $1p_{\frac{1}{2}}$ (38.11MeV) respectively. Although the state $1p_{\frac{3}{2}}$ is lower than $1p_{\frac{1}{2}}$ by about 0.34MeV we can consider as a one level. So the first four nucleons occupy in $1p_{\frac{3}{2}}$ state and the rest two nucleons occupy in $1p_{\frac{1}{2}}$ state, it is still valid magic number 8 (1s up to $1p_{\frac{1}{2}}$).

The next level 1d is split into $1d_{\frac{5}{2}}$ (33.55MeV) and $1d_{\frac{3}{2}}$ (33.03MeV). The state $2s_{\frac{1}{2}}$ (31.57MeV) can

closely stay with $1d_{5/2}$ and $1d_{3/2}$ and therefore the third shell can be formed. In this shell, six nucleons stay in $1d_{5/2}$, four nucleons stay in $1d_{3/2}$ and two nucleons stay in $2s_{1/2}$ and hence twelve nucleons occupy in this level, so the magic number 20 can be explained ($1s_{1/2}$ up to $2s_{1/2}$). The energy difference between $2s_{1/2}$ (31.57MeV) and $1f_{7/2}$ (27.90MeV) is 3.67MeV therefore the state $1f_{7/2}$ (27.90MeV) can be considered as a shell and eight nucleons fill in $1f_{7/2}$ and found magic number 28. The states $1f_{5/2}$ (27.21MeV), $2p_{3/2}$ (25.14MeV) and $2p_{1/2}$ (24.45MeV) form a shell and the six nucleons fill in $1f_{5/2}$, four nucleons fill in $2p_{3/2}$ and two nucleons fill in $2p_{1/2}$ and ten nucleons fill in $1g_{9/2}$ (21.60MeV) hence twenty-two nucleons enter in this shell forming magic number 50. Eight nucleons fill in $1g_{7/2}$ (20.73MeV), six nucleons fill in $2d_{5/2}$ (18.12MeV), four nucleons fill in $2d_{3/2}$ (17.28MeV), two nucleons fill in $3s_{1/2}$ (16.64MeV) and twelve nucleons fill in $1h_{11/2}$ (14.72MeV), so thirty-two nucleons enter in this level and forming magic number 82. One can consider the level ordering for neutrons is the same as explained above. The proton level ordering is shown in Fig. 1. The left side in Figure 1 is the energy levels of harmonic oscillator, the middle is the energy levels of Wood-Saxon central potential only and the right side is Wood-Saxon central potential and spin orbit interaction. Here we have dropped neutron level ordering diagram to save the pages.

Conclusion

In this research work, we have calculated the energy levels of proton and neutron of ^{208}Pb with harmonic oscillator potential, Woods-Saxon spin independent central potential and Woods-Saxon spin-orbit potential. To find these energy levels, we have used Schrödinger equation and solved it numerically.

First of all, single particle energy levels of a nucleon moving in a potential well is determined by using forward and backward numerical differential equation. To solve forward and backward numerical differential equation, we have used FORTRAN90 code. Forward and backward numerical differential equation can easily handle and so we have applied this

method to the Schrödinger equation. After that, we have studied the energy levels and shell structure of ^{208}Pb . In this work we have considered for proton and neutron separately. After magic number 20 the energy gap for each sub-states are not too much different. To solve this problem we have to increase the potential strength of spin-orbit interaction term. In near future we will improve this potential strength and recalculate the shell structure of ^{208}Pb again.

Table 1. $f'(x) = 3x^2$ at $x = 2$ by using two point forward formula.

h	$f'(x)$	Total Error
0.1	12.60999	0.60999
0.01	12.06007	0.06007
0.001	12.00485	0.00485
0.0001	11.98769	0.01231

Table 2. $f'(x) = 3x^2$ at $x = 2$ by using two point backward formula.

h	$f'(x)$	Total Error
0.1	11.41000	0.59000
0.01	11.94010	0.05990
0.001	11.99436	0.00564
0.0001	12.00199	0.00199

Table 3. $f''(x) = 6x$ at $x = 2$ by using second order forward formula.

h	$f''(x)$	Total error
0.1	11.99989	0.00011
0.01	11.99722	0.00278
0.001	11.44409	0.55591

Table 4. $f''(x) = 6x$ at $x = 2$ by using second order backward formula

h	$f''(x)$	Total Error
0.1	11.39998	0.60002
0.01	11.94000	0.06000
0.001	12.87460	0.87460

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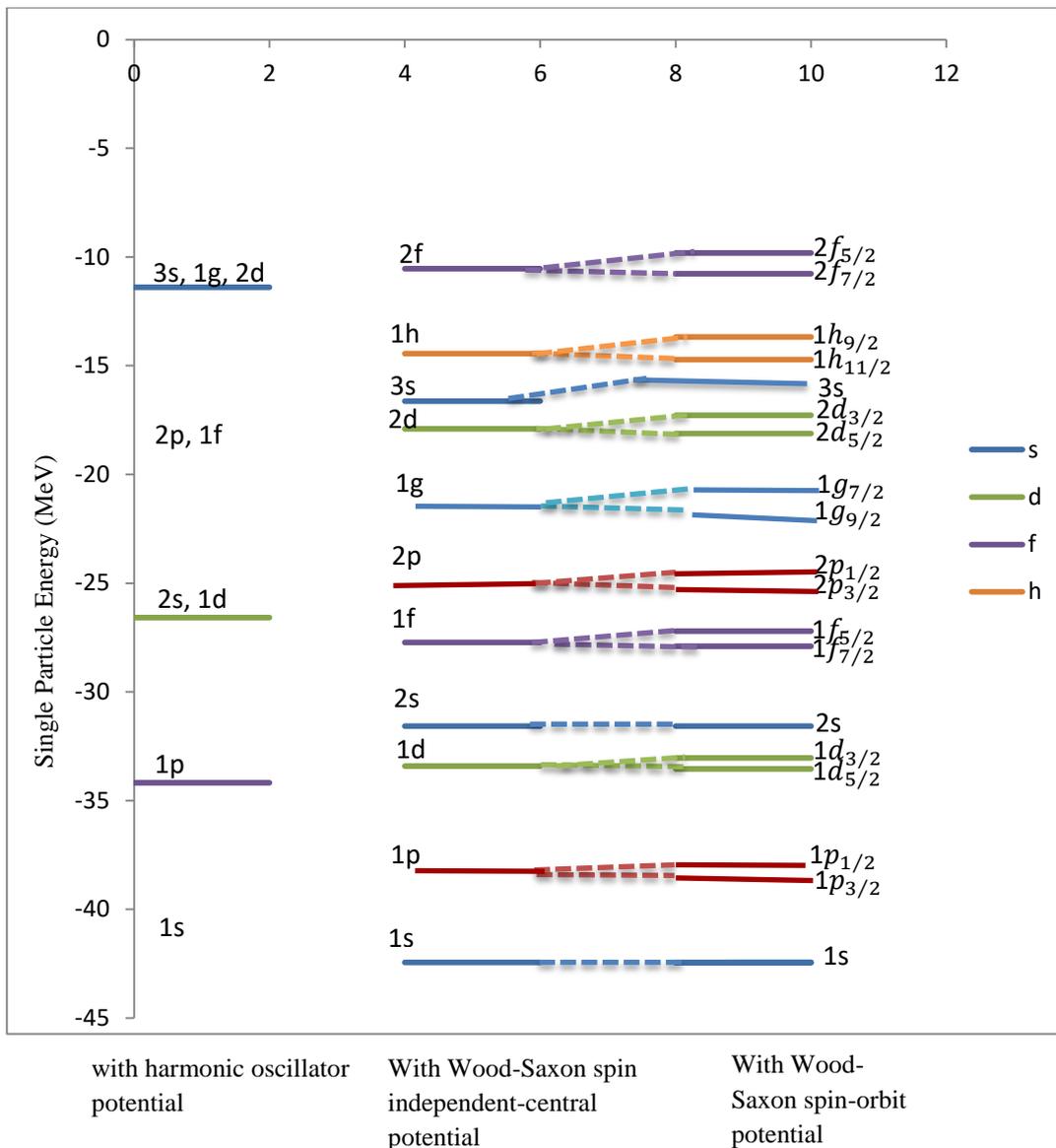


Figure 1. Neutron single- particle states in ²⁰⁸Pb

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