

A Numerical Calculation of the Nuclear Spin-Parity and Magnetic Moment Based on the Single-Particle Shell Model

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(Received 27 June 2019 : revised 08 August 2019 : accepted 30 August 2019)

Nuclear physics is an obligatory subject for the general physics program of undergraduates in most of the natural science universities worldwide. In nuclear physics, the shell model is one of the most important models, and is well used to determine the spin-parity and the magnetic moment of a nucleus. Over ten years of teaching general physics, we have realized that most undergraduate students find calculating these parameters by using this shell model to be difficult due to the classification of the subshells and the intrinsic spin of nucleons. With the hope to help these students, in the present study, we introduce a graphical-user-interface (GUI) program to execute our self-developed Shell Model Calculator (SMC) code written in the Visual Basic 6.0 (VB6) programming language. Our SMC validation results for the quantum quantities in a series of nuclei $Z = 1 - 20$ were compared with experimental data and found to be in good agreement. In general, we successfully developed an SMC program that can be used for teaching, learning, and researching nuclear physics in universities.

PACS numbers: 01.30.Kj, 01.30.-y, 21.10.Hw, 21.10.Ky, 21.10.-k

Keywords: Self-study, E-learning, Spin-parity, Ground state, Nuclear Physics

I. INTRODUCTION

Nuclear physics is a mandatory subject of the general physics program for undergraduates in universities. This subject covers fundamental principles in nuclear science and its engineering applications. Most of the stu-

dents found it is challenged to achieve the course due to complicated theory, a requirement of strong mathematics background, and lacking tools to calculate quantum parameters. To deal with these challenges, the computer has emerged as an essential tool in physics education during the last several decades. It provides an extensive environment for teaching and learning beyond the traditional educational methods [1]. Instead of using hard

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copies of books and listening in-class lectures, distance-learning students can study using online lectures through computers. On the other hand, together with software, computers are also widely used in physics study for data acquisition, simulation of phenomena, complicated numerical calculations, and data analysis in both fields of theoretical and experimental physics [1–5]. Therefore, varieties of software are in need to handle the data in a more sufficient way. Up to date, significant number of software has been designed to serve for teaching, learning, and researching purposes, which enhances the efficiency in physics education [6,7]. For instance, the software helps instructors and students overcome the difficulties in the solutions of the physics problems such as Schrodinger equation or nuclear reactions which are not available in the scope of a classroom. Therefore, computer codes are highly demanded in physics studies.

In nuclear physics, the shell model is one of the most important contents since it well describes the nuclear structure of stable isotopes. This model is a good candidate for predicting the quantum parameters of spin-parity and magnetic moment at the ground or low-excited state of nuclei. The numerical calculation of the parameters following the shell model is rather complicated for undergraduates. It takes time for students to manually check the shell of the nucleons and the other physical quantities and to repeat the calculation for various isotopes. In this scenario, a computer code is useful to solve these issues. There have been few computer codes developed based on shell model such as NuShellX [8], OXBASH [9,10], and so on. These codes, however, are not suitable for undergraduates since it requires extensive knowledge of the nuclear structure of the users and high capacity computers. Therefore, in the current study, we present an alternative code with a graphical user interface (GUI), named Shell Model Calculator (SMC), to compute the quantum parameters based on the shell model. This code was written in Visual Basic 6.0 programming language due to its advantages of simple graphical design, easy compilation, and the possibility of an execute output file. The program will be provided upon requests.

The present paper is organized as follows. The theoretical framework for the calculations of the spin-parity and magnetic moment based on the Single-particle Shell

Model is described in Section II. The algorithms, workflow and design of the SMC are detailed in Section III. The validation of the program, the spin-parity and magnetic-moment results of the odd nuclei with $Z = 1-20$ are analyzed and discussed in Section IV. The paper is summarized in Section V.

II. THEORETICAL FRAMEWORK

The shell model is proposed based on a series of experimental evidence related to the binding energy, the separation energy of nucleon (proton or neutron), the neutron absorption cross-section, the excited energies, and the large natural abundance of some extraordinary groups of isotopes [10,11]. These isotopes have a certain number of protons or neutrons, which are called "magic numbers". This phenomenon is similar to the electronic shell model of the noble gas in atomic physics. In which, the elements consisting of eight electrons in the outermost shell, so called closed shell, have a more stable state. Likewise, the magic numbers of nucleons (2, 8, 20, 28, 50, 82, 126), which function as the eight electrons in an atom of a noble gas, form the closed shells in more stable nuclei.

In the present study, we focused on the simplest form of the shell model named Single-particle Shell Model. According to this model, a nucleus is described as a system of shells filled by nucleons. The model assumes that the interaction between nucleons can be ignored and each nucleon can travel independently in the nuclear potential well. The shells can be occupied by paired nucleons and an unpaired nucleon. The state of the unpaired nucleon decides the properties of the nucleus. The wave function associated with the travel of nucleons satisfies the Schrodinger equation [12]:

$$\left(-\frac{\hbar^2}{2\mu}\Delta + V(\vec{r}) - E\right)\psi(\vec{r}) = 0, \quad (1)$$

where \hbar and μ denote the reduced Planck constant and the nucleon mass; Δ , $V(\vec{r})$, and E are the Laplacian operator, nuclear potential, and the energy of the nucleon, respectively. Basically, the central part of nuclear mean field potential has a shape which is similar to that of the Wood-Saxon potential [13]. However, for most applications, this part is usually approximated within a simpler

shape such as a square well or harmonic oscillator, with which an analytical solution can be obtained. In the motion, the nucleon has an orbital momentum and an intrinsic spin characterized by vectors $\vec{\ell}$ and \vec{s} , respectively. These quantities are conserved by a total angular momentum j owing to the existing spin-orbit interaction [14] in the movement of the nucleon in the nuclear potential as following

$$\vec{j} = \vec{\ell} + \vec{s}. \quad (2)$$

Since the intrinsic spin of the proton or neutron has a magnitude of $s = 1/2$, the total angular momentum of the nucleon in Eq. (2) should have maximum and minimum values, $j = \ell + 1/2$ and $j = \ell - 1/2$, respectively, depending on the orients of the vectors. Accordingly, the nuclear potential must contain a spin-orbit term induced by two-body spin-orbit interaction [15–18]. Besides, protons also experience the repulsive electrostatic force due to other protons. Thus, the total potential of a nucleus takes the form of

$$V(\vec{r}) = V_0(\vec{r}) + V_{so}(\vec{r}) \langle \vec{\ell} \cdot \vec{s} \rangle + V_C(\vec{r}). \quad (3)$$

The spin-orbit term, $V_{so}(\vec{r})$, is usually assumed to be a constant [19] and the Coulomb term, $V_C(\vec{r})$, is constructed based on the assumption of the uniformed charge sphere [13]. The spin-orbit term controlling the splitting of subshells is responsible for predicting the nuclear magic numbers. Whilst, the Coulomb one stands for the difference between neutron and proton energy spectra.

Under conditions of the spherical symmetry potential, relevant for non-deformation nuclei, the wave function is described as

$$\begin{aligned} \psi_{n\ell jm}(r, \varphi, \theta) \\ = R_{n\ell}(r) \sum_{m_\ell m_s} \langle \ell \frac{1}{2} m_\ell m_s | jm \rangle Y_{\ell m_\ell}(\varphi, \theta) \chi_{1/2 m_s}(\vec{s}), \end{aligned} \quad (4)$$

where the closed bracket symbol represents the Clebsch-Gordan coefficients, $\chi_{1/2 m_s}(\vec{s})$ is spin dependent part of the wave function which is sometimes called "spinor", and \vec{s} is the spin variable.

The states of a nucleon can be deduced once the wave function in Eq. (1) is determined with the certain quantum parameters of the principle quantum number

n which characterizes the energy eigenvalue $E_{n\ell j}$, the orbital momentum ℓ , the total angular momentum (or spin) j , and its projection m on the z axis. Nucleons following the Pauli principle [19, 20] occupy shells and subshells of a nucleus. The shells are named after the principle number $n = 1, 2, 3 \dots$, similarly with the case of the electron shells. With a certain principle number n , there are various orbital momenta, ℓ . The names of the subshells, therefore, depends on the values of ℓ , which are $\ell = 0, 1, 2, 3, \dots$ corresponding to s, p, d, f, \dots . According to the Eqs. (1, 4), with the harmonic oscillator potential of $V(r)$ and the empirical scheme of nucleon arrangement studied by Klinkenberg [21–23], the states of protons and neutrons occupy the levels as [21]

$$\begin{aligned} 1s_{1/2} 1p_{3/2} 1p_{1/2} 1d_{5/2} 2s_{1/2} 1d_{3/2} 1f_{7/2} 2p_{3/2} 1f_{5/2} 2p_{1/2} \\ 1g_{9/2} 1g_{7/2} 2d_{5/2} 1h_{11/2} 2d_{3/2} 3s_{1/2} 1h_{9/2} 2f_{7/2} 2f_{5/2} 1i_{13/2} \\ 3p_{3/2} 3p_{1/2} 1i_{11/2} \text{ (proton)}, \end{aligned} \quad (5)$$

$$\begin{aligned} 1s_{1/2} 1p_{3/2} 1p_{1/2} 1d_{5/2} 2s_{1/2} 1d_{3/2} 1f_{7/2} 2p_{3/2} 1f_{5/2} 2p_{1/2} \\ 1g_{9/2} 2d_{5/2} 1g_{7/2} 1h_{11/2} 2d_{3/2} 3s_{1/2} 2f_{7/2} 1h_{9/2} 2f_{5/2} 3p_{3/2} \\ 1i_{13/2} 3p_{1/2} 2g_{9/2} 1i_{11/2} 3d_{5/2} 2g_{7/2} 3d_{3/2} \text{ (neutron)} \end{aligned} \quad (6)$$

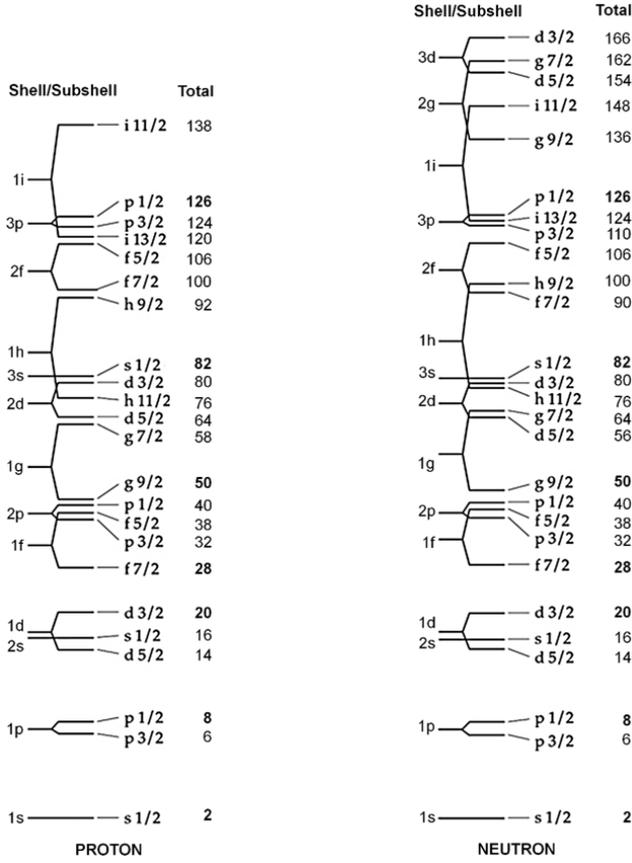
where the numbers in front of the letters denote the principle quantum numbers n and the subscript numbers (e. g. $1/2, 3/2$, etc ...) denote the total angular momentum j of the nucleus. The nucleon arrangement in subshells of a nucleus is illustrated in Fig. 1.

The behaviour, odd or even feature, of the wave function, is characterized by a parameter called parity. The parity, π , is defined based on the function as

$$\begin{aligned} \psi_{n\ell jm}(r, \pi + \varphi, \pi - \theta) &= \pi \psi_{n\ell jm}(r, \varphi, \theta) \\ &= (-1)^\ell \psi_{n\ell jm}(r, \varphi, \theta) \end{aligned} \quad (7)$$

because the space reflexion $\vec{r} \rightarrow -\vec{r}$ in cartesian coordinates is equivalent to the transformation $(r, \varphi, \theta) \rightarrow (r, \pi + \varphi, \pi - \theta)$ in spherical coordinates. If the spherical symmetry is conserved, it can be shown that the parity of single-particle wave functions is simply determined by the orbital momentum as expressed in Eq. (7). The parity is consequently a multiplicative quantum number determined by the product of all individual parities.

The single-particle shell model can successfully predict some properties such as spin (total angular momentum),



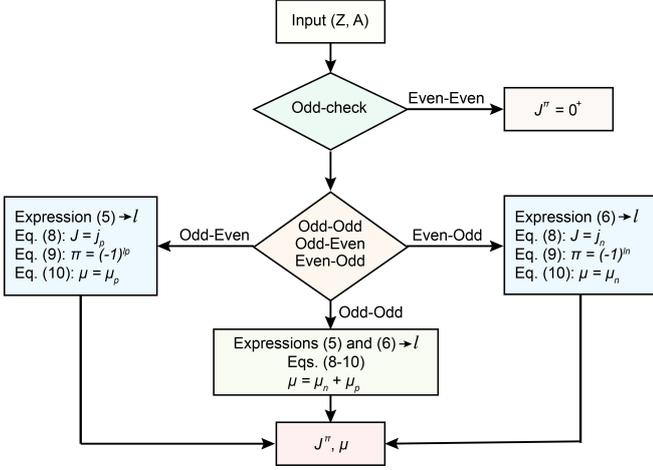


Fig. 2. (Color online) The workflow of the Shell Model Calculator (SMC) program for the calculation of the spin-parity and magnetic moment based on the shell model.

The plot of the magnetic moment in Eq. (10) against the nuclear spins will result in two lines corresponding to $j = \ell + 1/2$ and $j = \ell - 1/2$, called as the Schmidt lines [25]. Similar to the case of the atom, magnetic moments of nuclei attracted the attention of nuclear physicists since the early days. The nuclear magnetic moment is very difficult to be measured but it is important for physicists to understand deeply the structure of nuclei, especially of the odd ones which are discussed in this paper.

III. SHELL MODEL CALCULATOR PROGRAM

To calculate the spin-parity and magnetic moment of nuclei, we designed a Shell Model Calculator (SMC) by using the Visual Basic 6.0 programming language. This program is based on the theory that was mentioned in the previous section. The workflow of the SMC code is illustrated in Fig. 2.

The input parameters are only the atomic (Z) and mass (A) numbers of the interest nucleus. Initially, the program looks up the name of the element and the numbers of the nucleons (protons and neutrons) to determine which nucleon is unpaired. Notice that the number of neutrons, $N = A - Z$, is automatically calculated by the program. Since it is difficult to remember the atomic numbers and the associated elements of all the nuclei,

we integrated a list from hydrogen ($Z = 1$) to oganesson ($Z = 118$, the current heaviest element) that can be used to search for the interest information. In the *odd-check* step, the program checks if the number of protons/neutrons is divisible by 2 or not to confirm that the unpaired nucleon is a proton or a neutron. Once both of the numbers of protons and neutrons are even numbers (an even-even nucleus), the program generates the results of spin-parity of the nucleus as $J^\pi = 0^+$ based on the shell model theory. For the rest cases of the odd-odd, odd-even, and even-odd nucleus, the subshell occupied by the unpaired nucleon is used to determine the orbital momentum, ℓ , of the core-nucleon system.

The ℓ value is deduced based on the subshells s, p, d, f, \dots corresponding to $\ell = 0, 1, 2, 3, \dots$ of the nucleon. If the unpaired nucleon is a proton, the program determines the orbital momentum, ℓ , by using the configuration in Eq. (5), *vice versa* Eq. (6) is considered. The algorithm for determining ℓ and the total angular momentum, j , of the nucleon is based on the configuration of the shells as follows. The code searches for the last unpaired nucleon, x , if it is in the ranges of $x = (1-2); (2-6); (6-8); \dots; (154-162); (162-166)$ corresponding to the subshells of $1s_{1/2}; 1p_{3/2}; 1d_{5/2}; \dots; 2g_{7/2}; 3d_{3/2}$, respectively. This is the most important procedure in the computation of the spin-parity and magnetic moment, and it must be repeated for every isotope. Without the computer program, it takes lots of time for students to manually calculate these quantities. Obviously, the SMC program eliminates this inconvenience.

After determining the orbital and the total angular momenta of the unpaired nucleon, these quantities and the magnetic moment, μ , of the interest nucleus are calculated by using Eqs. (8) – (16). It should be noted that, for the odd-even (or even-odd) nuclei, the neutron terms (or proton terms) in these equations are omitted, and their full descriptions are applied for the odd-odd isotopes. Finally, the final results of the quantum parameters of the nucleus are monitored in the interface of the program. For example, the ${}^7\text{Li}$ nucleus consists of three protons and four neutrons. In the proton structure, two protons occupy the s -shell to make this shell becomes fully closed with two nucleons (a magic number), steering to the third proton occupies the p -shell.

Since those neutrons are paired to each other, the property of the nucleus is thus defined by the leftover odd proton. On the other hand, the orbital momentum of the core-nucleon system is determined as $\ell = 1$ corresponding to the p -shell. The code for this sub-shell identification is provided upon requests. According to the rule of the arrangement as shown in Fig. 1 or in Eq. (5), the odd proton locates at the state with the spin of nucleon $j = 3/2 = \ell + 1/2$. Hence, the spin of the interest nucleus will be $J = j = 3/2$. Subsequently, the parity of the ${}^7\text{Li}$ nucleus is $\pi = (-1)^{\ell_p} = -1$, an odd parity. The magnetic moment is calculated by using Eqs. (10)–(16) without the neutron terms. With the intrinsic spin $s = 1/2$, the total angular momentum $j = 3/2$, and the orbital momentum $\ell = 1$ of the odd proton, the magnetic moment of the ${}^7\text{Li}$ isotope is $\mu = 3.79 \mu_N$. This result is consistent with the spin-parity and magnetic moment ($J^\pi = 3/2$ and $\mu = 3.25 \mu_N$) obtained in Ref. [19,23]. The discrepancy between the estimated value and the measured data of the magnetic moment can be understood by the reasons of the deviations from the Schmidt lines explained in Section IV.

Taking advantages of the graphic user interface (GUI), we designed a program to execute our SMC calculation to help users easily manipulate the code. It is unnecessary to re-compile the code when the input parameters are varied. The main graphical interface is designed by using a *form* in VB6 with eight *text boxes* and a *list box* for looking up elemental data, three *command buttons*, two *option buttons* of record/non-record mode to write the results in ASCII file and save that file in a storage hard disk. Three *menus* including sub-menus for exercises, nuclear mass database, and constants often used in nuclear physics, as shown in Fig. 3. All the components are divided into seven groups: (1) menus for data sheets; (2) the proton, neutron, mass numbers and the name of the interest isotope; (3) the shell configuration of the nucleons, and the results of spin-parity and the magnetic moment; (4) the list box that users use to search for the atomic numbers and names of the elements; (5) the information of stable, unstable, or unknown isotopes will be presented in this text box; (6) option buttons for recording results; (7) and the executing buttons of the program. Once Z and A are properly input, the program will automatically display the neutron number and the name of

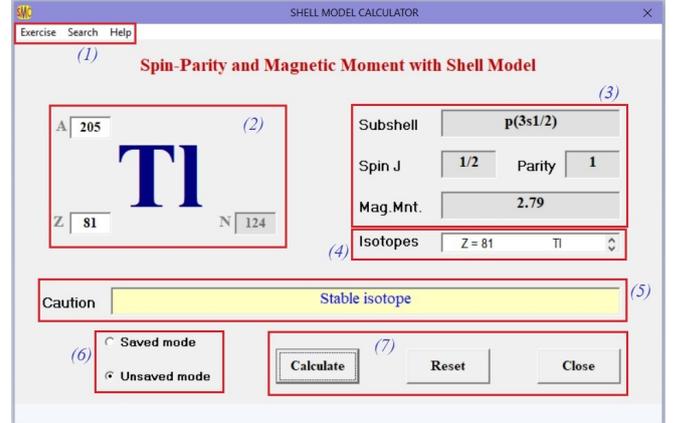


Fig. 3. (Colour online) The graphical interface user (GUI) of the Shell Model Calculator program.

the element of the nucleus after executing the calculation by pressing the *Calculate* button. The results including the nucleon configuration in subshells, the spin, the parity, and the magnetic moment are respectively presented in the text boxes named as *Shell*, *Spin*, *Parity*, and *Mag.Mnt* on the interface. Users also can compile both results in an ASCII file and save that file after the calculation by selecting the *Save mode* option. To refresh the program, users can press the *Reset* button. When users click on the menus, the related Microsoft–Word files will be shown in a new window. For examples, the *Exercise* menu generates the files of problems as homework for students; the *Search* provides data sheets of mass, mass excess, and binding energy of nuclei, or of the nuclear constants, which are very useful for users. From the list box (5), the atomic numbers of all the known elements will be shown.

The Shell Model Calculator executive file can also be exported without the requirement of the source code. This program is compatible with Windows-based computers and has a small storage capacity of about 200 kilobytes. These advantages have made this program more accessible to users with limited knowledge in nuclear physics and weak computers, for that, other mentioned shell-model based programs could not offer.

IV. RESULTS AND DISCUSSION

To validate our SMC program, we compared the quantum parameters of a series of nuclei estimated by using

SMC and those obtained from the database of International Atomic Energy Agency in Ref. [26]. Tables 1, 2 show our calculations of the spin-parity and the magnetic moments of the odd isotopes with the medium atomic numbers in a range of $Z = 1 - 20$ computed by the SMC. For spins and parities, these results are in a good agreement with those from the database published in Ref. [26] with few exceptions of measurements of ^{19}F , ^{19}Ne and ^{21}Ne isotopes. This discrepancy between the theoretical and experimental values can be understood by limitations of the single-particle shell model for the unstable isotopes in Ref. [27, 28]. The nucleons in the isotopes may change their shells as an extraordinary arrangement due to the deformation. Considering ^{19}F as an example, this nucleus has a prolate shape [28], therefore the spin j of the single-particle state is no longer conserved. The $1d_{5/2}$ shell splits up with deformation into states with definite values of j_z along the axis of symmetry. At the same time, the lowest j_z sub-shell ($j_z = 1/2$) drops the fastest [29]. As a result, the spin and parity of the ground state of this nucleus would be $1/2^+$ instead of $5/2^+$.

In Tables 1, 2 we also compare our results with the other existing shell-model calculations using empirical effective interactions. For nuclei with masses in the range of $A = 7 - 13$, the calculations were done in the p -shell using the Cohen-Kurath [30] or the (6-16)TBME effective interaction [31]. For those in the $p - sd$ cross-shell region, namely ^{15}N , ^{15}O and ^{17}N , the calculations were done using the WBP effective interaction in the $p - sd$ model space [32]. Those with masses $A = 19 - 31$ were calculated in the sd model space using the USD [32] or the USDB interaction [33]. While the nuclei in the $sd - pf$ cross-shell region were computed in the model space that includes sd and pf orbits within modern interactions [15, 34, 35]. From Tables 1 and 2, it is obvious that, the spins and parities obtained by the shell-model calculations exactly match the experimental data, reflecting the fact that, in the shell-model framework the deformation effects can be taken into account indirectly via the configuration mixing mechanism [36]. On the other hand, the good agreement between the results calculated by SMC compared with the others show an advantage of our code in spin-parity prediction. Obviously, our code is simpler and easier to be used than existing codes but we can determine the same results.

Table 1. Comparison of the spin-parity and magnetic moment of the odd isotopes in the range of $Z = 1-20$ computed by the current SMC code and those from the existing shell-model calculations from Ref. [15, 30–35], as well as the measured values. Experimental data are taken from Ref. [26], if not specified. The magnetic moments are in the nuclear magneton unit.

ID	Z	A	SMC		Shell Model		Experimental Values	
			J^π	μ	J^π	μ	J^π	μ
H	1	1	1/2+	2.79			1/2+	2.79
		3	1/2+	2.79			1/2+	2.98
He	2	3	1/2+	-1.91			1/2+	-2.13
		7	3/2-	3.79	3/2-	3.171 [31]	3/2-	3.26
Li	3	9	3/2-	3.79	3/2-	3.488 [30]	3/2-	3.44
		9	3/2-	-1.91	3/2-	-1.288 [31]	3/2-	-1.40
Be	4	9	3/2-	-1.91	3/2-	-1.229 [30]	3/2-	-1.18
		11	3/2-	3.79	3/2-	3.509 [31]	3/2-	2.69
B	5	13	3/2-	3.79	3/2-	3.147 [30]	3/2-	3.18
		11	3/2-	-1.91	3/2-	-0.783 [31]	3/2-	-0.96
C	6	13	1/2-	0.64	1/2-	0.748 [30]	1/2-	0.70
		15	5/2+	-1.91			5/2+	-1.92
		13	1/2-	-0.26	1/2-	-0.38 [30]	1/2-	0.32
N	7	15	1/2-	-0.26	1/2-	-0.264 [32]	1/2-	-0.28
		17	1/2-	-0.26	1/2-	-0.333 [32]	1/2-	-0.35 [32]
		13	3/2-	-1.91	3/2-	-1.378 [30]	3/2-	-1.39
O	8	15	1/2-	0.64	1/2-	0.638 [32]	1/2-	0.72
		17	5/2+	-1.91	5/2+	-1.913 [33]	5/2+	-1.89
		17	5/2+	4.79	5/2+	4.793 [33]	5/2+	4.72
F	9	19	5/2+	4.79	1/2+	2.898 [33]	1/2+	2.63
		21	5/2+	4.79	5/2+	3.779 [33]	5/2+	3.92
		19	5/2+	-1.91	1/2+	-2.038 [32]	1/2+	-1.88 [32]
Ne	10	21	5/2+	-1.91	3/2+	-0.774 [32]	3/2+	-0.66 [32]
		23	5/2+	-1.91	5/2+	-1.05 [33]	5/2+	-1.08
		21	5/2+	4.79	3/2+	2.489 [33]	5/2+	3.70
Na	11	25	5/2+	4.79	5/2+	3.367 [33]	5/2+	3.68
		25	5/2+	-1.91	5/2+	-0.849 [33]	5/2+	-0.86
		27	1/2+	-1.91	1/2+	-0.412 [33]	1/2+	-0.41
Mg	12	29	3/2+	1.15	3/2+	1.071 [33]	3/2+	0.98
		25	5/2+	4.79	5/2+	3.655 [33]	5/2+	3.65
		27	5/2+	4.79	5/2+	3.455 [33]	5/2+	3.64
Si	14	27	5/2+	-1.91	5/2+	-0.678 [33]	5/2+	-0.86
		29	1/2+	-1.91	1/2+	-0.503 [33]	1/2+	-0.56
		33	3/2+	1.15	3/2+	1.206 [33]	3/2+	1.21
P	15	29	1/2+	2.79	1/2+	1.133 [33]	1/2+	1.23
		31	1/2+	2.79	1/2+	1.087 [33]	1/2+	1.13
		31	1/2+	-1.91	1/2+	-0.441 [33]	1/2+	0.48
S	16	33	3/2+	1.15			3/2+	0.64
		35	3/2+	1.15			3/2+	1.07
		33	3/2+	0.12			3/2+	0.75
Cl	17	35	3/2+	0.12			3/2+	0.82
		37	3/2+	0.12			3/2+	0.68
		35	3/2+	1.15	3/2+	0.688 [35]	3/2+	0.64
Ar	18	37	3/2+	1.15	3/2+	1.155 [35]	3/2+	1.15

Table 2. Same as Table 1.

ID	Z	A	SMC		Shell Model		Experimental Values	
			J^π	μ	J^π	μ	J^π	μ
K	19	39	7/2-	-1.91	7/2-	-1.436 [35]	7/2-	-1.56
		41	7/2-	-1.91			7/2-	-1.30
		37	3/2+	0.12			3/2+	0.20
		39	3/2+	0.12	3/2+	0.65 [15]	3/2+	0.39
Ca	20	41	3/2+	0.12	3/2+	0.33 [15]	3/2+	0.21
		39	3/2+	1.15			3/2+	1.02
		41	7/2-	-1.91	7/2-	-1.913 [34]	7/2-	-1.59
		43	7/2-	-1.91	7/2-	-1.712 [34]	7/2-	-1.31

In contrast to spin and parity, the magnetic moment is very sensitive to details of nuclear structure. The single-particle shell model is very simple, only the unpaired nucleon is responsible for the total spin and the magnetic properties of the whole nucleus while the paired

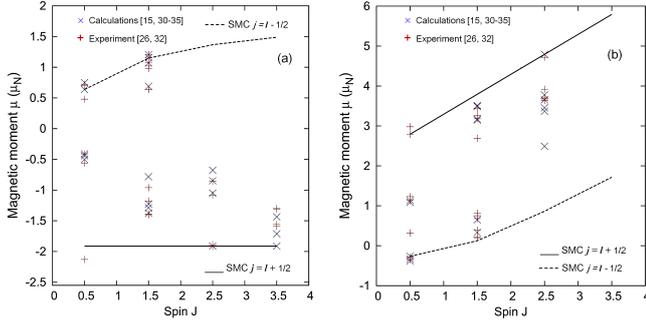


Fig. 4. (Colour online) Magnetic moments (in nuclear magnetons) of the odd isotopes in the range of $Z = 1-20$ plotted against nuclear spin. Panel (a) shows the values for odd- N nuclei and panel (b) for odd- Z nuclei. Full lines are the Schmidt limits (the values obtained from the SMC calculations), cross signs are the values from existing shell-model calculations [15,30–35], and plus signs are experimental data [26,32].

nucleons create a zero-spin core as evidence for even-even nuclei. However, it is well known that the magnetic moment obtained in this model is only an approximation to the experimental data, or the Schmidt limits. It can be seen from our results in Fig. 4 that, nearly all magnetic moments deviate from the Schmidt lines and quite considerably in some cases. Most important is the fact that, with very few exceptions among the lightest nuclei, all magnetic moments lie between the Schmidt lines, but do not coincide with them exactly. It is one of the successes of the single-particle shell model that it can account for the general dependence of the moments on the spin. However, it fails to explain why the observed values of moments do not coincide with those obtained by the single-particle shell model.

The deviations from the Schmidt lines have two reasons. First, in a real nucleus, the magnetic moment of a nucleon is influenced by the presence of the other nucleon, the single-nucleon g factors are reduced to typically about 70% of their free-nucleon value in heavy nuclei. However, for light nuclei, the experimental numbers are generally rather well reproduced with free-nucleon g factors. More detailed discussions can be found in Ref. [37]. The second reason is configuration admixtures due to the presence of residual interaction configuration mixing effects due to correlations among valence nucleons in opened-shell nuclei. In other words, the unpaired nucleons are not exactly independent as the single-particle shell model assumed. It is generally

not possible to reasonably reproduce the experimental data of magnetic moment within the single-particle shell model alone, even though the most precise effective g factors are used. Figure 4 shows that the SMC results are in better agreement with the measured values for the doubly-magic closed-shell ± 1 nuclei, such as ^{15}O , ^{17}O , ^{17}F , ^{39}K , ^{41}K , ^{39}Ca , ^{41}Ca due to smaller configuration-mixing effects. Furthermore, in most cases, the magnetic moment values from the shell-model calculations are in excellent agreement with the measured values because the interaction between the unpaired nucleon/hole and the closed-shell core is almost negligible. For some cases, the shell-model calculations are consistent with the experimental data, even they used the free-nucleon g factors. This phenomenon can be understood by the reason that all residual interactions beyond the single-particle model are properly treated leading to realistic wave functions in the form of admixtures of many single-particle configurations.

Our results indicate that the SMC program works well to determine the quantum parameters of the nuclei, especially for the spin and parity of the medium stable isotopes. In addition, SMC is also a tool to calculate the upper-, and lower-limits of the magnetic moments of nuclei. Subsequently, this validation encourages students to use this SMC program to predict quantum parameters of the isotopes far from the stability island of the nuclear chart. In principle, the SMC computer code can calculate the quantum parameters for isotopes with the atomic numbers of $Z < 139$ and the neutron numbers of $N < 185$. However, because of the limitations of the single-particle shell model as mentioned above [19,27], the calculated results have larger uncertainty compared with the experimental data when we apply the code to the deformed nuclei such as heavy or super-heavy isotopes due to their deformed structure.

V. CONCLUSION

In this study, we present an alternative code based on the single-particle shell model to execute the numerical calculation of the spin-parity and magnetic moment of non-deformed nuclei. Our computer code, named as Shell Model Calculator (SMC), was written in Visual Basic 6.0 language and possibly executed by SMC

GUI-program. The SMC program is portable and compatible with the Windows Operation System. The friendly graphical-user-interface of SMC and the nuclear database of the mass, mass excess, binding energy, and the searching tool for elements are also advantages of the program.

The nuclear quantities that were estimated by the SMC code are consistent with those obtained from the published database even it is simpler than the other codes in use. The test results indicate that SMC is appropriate to predict the concerned nuclear properties of non-deformed nuclei. The program is also a good tool for testing the manual calculations and extracting the Schmidt limits. Given the newly developed SMC program, we hope to help physics students save their time on checking manual calculations and searching for the values of the nuclear parameters of interest. Using the SMC program is expected to improve the efficiency in self-study of undergraduates in learning fundamental nuclear physics.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) under number of Nos. NRF-2017R1D1A1B03030019, NRF-2019R1F1A1058370, and the Vietnam Government under the Program of Development in Physics toward 2020 (Grant No. DT-DLCN.02/19). This work is also funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant Number of No. 103.04-2018.303. T. V. Nhan Hao (tvnhao@hueuni.edu.vn) thanks the financial support of the Nuclear Physics Research Group (NP@HU) at Hue University through the Hue University Grant 43/HD-DHH.

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