

Nice things about mean fields: Mean field potentials for the classroom

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We present two examples which use a mean field potential to determine valence electron and nucleon energy levels in atoms and nuclei, respectively. In atoms, we compute the energy levels of the alkali elements, and in nuclei the binding energy of valence nucleons in mirror nuclei are calculated. In both cases, the student can compare the results with experiment and vary the parameters of the calculation to best fit the data. © 2000 American Association of Physics Teachers.

I. INTRODUCTION

One of the most important courses in an undergraduate physics student's education is quantum mechanics. Part of every quantum course is the development of the Schrödinger equation and an interpretation of its solution. Applications of the Schrödinger equation focus on the scattering and the bound state problem, both usually handled in coordinate space. For the bound state problem, potentials which can be solved analytically are given as examples in most textbooks. The one- and three-dimensional square well, the harmonic oscillator, and the Coulomb potential have analytic solutions and are used to illustrate the fundamentals of energy quantization in bound systems. The Coulomb potential is particularly important, since the solutions can be compared with experimental data.

In recent years, the personal computer has entered the classroom and given students and teachers the ability to obtain accurate numerical solutions to differential equations in a short time. Thus, in addition to using potentials which have analytic solutions, the student can insert any reasonably behaved potential into the Schrödinger equation and solve for the allowed energies of the system. With this new mathematical tool, one can supplement the analytic solutions with interesting potentials to be solved numerically.

In this article, we present two problems in atomic and nuclear physics for students in an undergraduate quantum or computational physics class. In both examples the students compare the calculations with experimental data. Many abstract ideas are introduced in an undergraduate quantum mechanics course, so calculations that can be compared with experiment are particularly valuable.¹ In the first example, the energy levels of the valence electron in the alkali elements are computed. The students vary one parameter to best fit the data. In the second example, the binding energy of valence nucleons for certain mirror nuclei are calculated. The potential has a size and strength parameter, which are varied to fit the data.

We first discuss the numerical method we used to calculate the energy levels, followed by the atomic and nuclear examples.

II. NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

Numerical solutions to differential equations are taught in numerical methods and computational physics courses,² and we apply these techniques to solve the Schrödinger equation. In this section we summarize the specific approach that our students used. We assume that the interaction between the

valence particle and the other particles in the atom or nucleus can be represented by a mean field potential, $V(r)$. For the two cases we consider, $V(r)$ is spherically symmetric.

The potential, $V(r)$, is inserted into the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi. \quad (1)$$

For bound state solutions, the wave function Ψ and the integral $\int\Psi^*\Psi dV$ over all space must be finite. Thus, as $r \rightarrow \infty$, Ψ must approach zero faster than $1/r$. Since the potential is spherically symmetric, the angular dependence can be separated from the radial. Writing $\Psi = R(r)Y_{lm}(\theta, \phi)$ as a product of a radial part times a spherical harmonic, the above equation reduces to

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{l(l+1)}{r^2}R(r)\right) + V(r)R(r) = ER(r). \quad (2)$$

A further simplification is obtained by writing $R(r) = u(r)/r$. The radial part of the Schrödinger equation finally becomes

$$-\frac{\hbar^2}{2m}\left(\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)\right) + V(r)u(r) = Eu(r). \quad (3)$$

For Ψ to be finite, $u(0)$ equals 0, and for bound states, $u(r)$ goes to zero as $r \rightarrow \infty$.

We solve Eq. (3) numerically by making the radial coordinate discrete with a step size Δ . The variable r and the functions $V(r)$ and $u(r)$ become arrays: $r \rightarrow r(i)$, $V(r) \rightarrow V(r(i)) \rightarrow V(i)$, and $u(r) \rightarrow u(r(i)) \rightarrow u(i)$. We use a finite difference method for the second derivative of $u(r)$:

$$\frac{d^2u(r)}{dr^2} \rightarrow \frac{u(i+1) + u(i-1) - 2u(i)}{\Delta^2}. \quad (4)$$

After substituting these expressions into Eq. (3), one obtains a discrete version of the Schrödinger equation:

$$u(i+1) = 2u(i) - u(i-1) + \Delta^2 \frac{l(l+1)}{r^2} u(i) + \frac{2m\Delta^2}{\hbar^2} (V(i) - E)u(i). \quad (5)$$

The boundary conditions $u(0) = 0$ and $u(i \rightarrow \infty) \rightarrow 0$ can only be satisfied for certain values of E , which correspond to the allowed "bound-state" energies of the particle.

We determine the bound-state energies using a bisection method. First, a trial energy E_t is chosen which lies below the ground state energy. In Eq. (5), $u(i+1)$ is determined from the values of $u(i)$ and $u(i-1)$. We assign $u(0)$ a value of 0, and $u(1)$ is assigned a nonzero value [e.g., $u(1)=1.0$]. Equation (5) can then be used to iterate $u(i)$ to a large value of $i=i$ max, well outside the core. We assign $u(i$ max) the value $u(i$ max) \equiv test0. Next, the trial energy is increased by an amount δE and the process is repeated. The function $u(i$ max) will have a different value, $u(i$ max) \equiv test1. If test0 and test1 have the same sign, then the trial energy is changed again by an amount δE , test1 \rightarrow test0, and the process is repeated. If test0 and test1 have opposite signs, then the wave function at $r=i$ max $\cdot \Delta$ has changed sign and the trial energy has passed over the ground state energy. The energy step is reversed and halved, $\delta E \rightarrow -\delta E/2$, test1 \rightarrow test0, and the process is repeated to the desired accuracy.

To determine the energy of the first excited state, one starts with a trial energy just above the ground state energy. The trial energy is stepped up in a similar manner until the energy converges. The next higher allowed energy is found in a similar manner.

The bisection method is a simple way to solve for the energy levels. Another method is to match $u(r)$ to the Coulomb wave functions at large values of r . In both our examples, the potential reduces to that of a point Coulomb potential when r is beyond a certain value. Beyond this value of r , the wave functions are the Coulomb wave functions due to a point charge. There are analytic forms for these Coulomb wave functions, so one often matches the solutions of Eq. (5) to these known functions. This method is quicker than the bisection approach, but involves a knowledge of the Coulomb wave functions which is usually not covered in an undergraduate quantum course. We have successfully used the bisection method in our undergraduate computational chemistry and computational physics courses. It is simple, and the students can visualize how the wave function goes to zero for large r as the energy is varied.

For the alkali problem, we used a step size for r of 0.01 Å, and iterated out to 20 Å. In the nuclear problem, a step size of 0.01 fm was used, and we iterated the wave function out to 12 fm. In both cases we were able to obtain a numerical accuracy of four significant figures for the ground states. The higher excited states required iteration to larger radial distance for comparable numerical accuracy. The accuracy was tested by computing the ground and excited states of the hydrogen atom and comparing the numerical answer to the analytic solution. One can also use commercial software to solve the Schrödinger equation (e.g., MATHEMATICA, MAPLE).³ Desktop computers are fast enough for quick convergence.

III. ENERGY LEVELS IN ALKALI ELEMENTS

For the atomic application, we focus on the alkali elements: Li, Na, K, Rb, and Cs. The alkalis are relatively simple atoms, since they have one valence electron orbiting about a core of electrons in closed shells.⁴ Thus a mean field approximation might be an accurate representation for the electrostatic potential that the valence electron experiences. We find that a simple model for the alkali atoms can yield interesting results.

Table I. Experimental and calculated values for the energy levels of the alkali elements. The parameter c is the radius of the “screening sphere” of uniform charge.

$l=0$	$l=1$	$l=2$
Calc Expt	Calc Expt	Calc Expt
	Lithium ($c=0.56$ Å)	
5.39 5.39	3.45 3.65	1.51 1.51
2.02 2.02	1.53 1.55	
	Sodium ($c=0.55$ Å)	
5.15 5.15	3.15 3.03	1.51 1.52
1.92 1.95	1.43 1.39	
1.02 1.02	0.78 0.80	
	Potassium ($c=0.66$ Å)	
4.34 4.34	2.93 2.72	1.50 1.67
1.76 1.73	1.35 1.28	0.83 0.94
0.94 0.94	0.73 0.74	
	Rubidium ($c=0.58$ Å)	
4.18 4.18	2.90 2.60	1.53 1.78
1.74 1.68		
	Cesium ($c=0.60$ Å)	
3.87 3.87	2.87 2.49	1.52 2.10
1.63 1.63		

The full potential energy for the valence electron consists of two pieces: the static Coulomb attraction due to the positive nucleus, and a repulsive mean field potential due to the “core” electrons. The Coulomb potential energy in Gaussian units due to the nucleus is given by $V_{\text{nucleus}} = -Ze^2/r$ for a nucleus with Z protons. Numerically, e^2 equals 14.4 eV Å or 1.44 MeV fm for the nuclear problem. We take the mean field potential due to the core electrons to be that of a uniformly charged sphere of charge $-(Z-1)e$. The size of the sphere, c , is a parameter which is varied to best fit the data. The complete potential energy, which we refer to as simply the potential, is given by

$$V(r) = -\frac{Ze^2}{r} + V_{\text{screening}}, \quad (6)$$

where

$$V_{\text{screening}} = + (Z-1)e^2 \frac{3c^2 - r^2}{2c^3} \quad \text{if } r \leq c$$

$$= + \frac{(Z-1)e^2}{r} \quad \text{if } r > c. \quad (7)$$

The potential $V(r)$ is substituted into Eq. (3) and the bound state energies of the valence electron are solved for $l=0$, $l=1$, and $l=2$. In Table I we list the results of this calculation along with data for selected energy levels.⁵ Although the model is very simple, it produces surprisingly good results.

The ground state $l=0$ energies are fitted for the different elements by adjusting the parameter c . It is interesting to note that the value of c does not vary much for the different atoms. This would suggest that the size of atoms does not increase substantially as the atomic number is increased. Once the ground state energy is fitted, one can examine how well the other energy levels match the data. Remarkably, the excited $l=0$ energy levels agree well with the data. The l

Table II. Values of the range parameter c which reproduces the correct experimental ground state energy and spin-orbit splitting for the $l=1$ level.

Element (Z)	c (Å)	c (Å)
	for ground state energy	for spin-orbit splitting
Na(11)	0.55	0.528
K(19)	0.66	0.657
Rb(37)	0.58	0.576
Cs(55)	0.60	0.589

$=1$ and $l=2$ energy levels of the lighter elements also fit the data fairly well. The model starts to break down with the $l=1$ and $l=2$ energy levels in Rb and Cs.

Wave functions for the different energy levels are also calculated in the code. These wave functions can be used to calculate spin-orbit splittings by numerically integrating⁶

$$E_{s-o} = \frac{\hbar^2(2l+1)}{4m^2c^2} \int_0^\infty \psi^*(r) \left(\frac{dV}{dr} \right) \psi(r) r dr. \quad (8)$$

We had our students calculate the $l=1$ spin-orbit splittings and compare to data. They varied the parameter c to best fit the experimental values of the spin-orbit splittings. Our results are listed in Table II along with the values of c which give the experimental ground state energy. The two values of c are quite close to each other.

This exercise has benefitted our students in a number of ways. They apply the Schrödinger equation to an atom other than hydrogen. They experience the validity and limitations of applying a phenomenological model to experimental data. The students also learned about energy level schemes and spin-orbit splitting in alkalis. The exercise turned out to be an interdisciplinary project. Chemistry and physics senior students wrote the code in C to solve for the energy levels. Computer science students translated the C code into a Java applet⁷ for use on the web. Other chemistry and physics students use the applet as a homework exercise to investigate energy levels in the alkalis.

IV. BINDING ENERGY IN MIRROR NUCLEI

The independent particle model, or shell model, of the nucleus has been successful in understanding many properties of nuclei. See Ref. 8 for a nice discussion of the historical development of the independent particle model. In this model, the nucleons are treated as independent particles that move in an average potential due to the other nucleons in the nucleus.^{9,10} A detailed shell model treatment over a wide range of nuclei is too specialized for an undergraduate class. However, the spin-orbit and pairing interactions make interesting topics. Here we describe a calculation that introduces the student to some of the ideas behind the nuclear shell model. We calculate the valence nucleon binding energy for a set of mirror nuclei. The approach we take is relatively simple, and appropriate for undergraduate students.

The set of nuclei we consider are mirror nuclei which have $|Z-N|$ equal to 1, where Z is the number of protons and N is the number of neutrons in the nucleus. In each case, the binding energy of the valence nucleon will be calculated and compared with experiment. For example, the binding energy of the valence neutron in ^{13}C and the binding energy of the valence proton in ^{13}N will be calculated and compared with the data. We treat the nucleus as a core plus the valence

nucleon, where the core contains an equal number of neutrons and protons. The allowed energies of the valence neutron or proton are calculated by assuming it moves in a mean field due to the core nucleus. The parameters of the mean field potential are varied to fit the binding energy data.

The mean field potential consists of a strong part, and a Coulomb repulsion for valence protons. Thus the proton's binding energy will be lower than that of a neutron interacting with the same core in the mirror nucleus. This can be seen in the data shown in Table III.¹¹ In columns 3 and 4 we list the experimental values for the binding energies of the valence neutron and proton about the core nucleus given in column 1. For example, the binding energy of the valence neutron in ^{13}C is 4.946 MeV, and the binding energy of the valence proton in ^{13}N is 1.943 MeV. The difference in these two numbers is due to the Coulomb interaction, and gives information about the size of the nucleus. The magnitude of the binding energies is determined by the strength of the mean field potential.

To represent the strong interaction between the valence nucleon and the core nucleus, we use a Woods-Saxon potential:¹²

$$V(r) = \frac{-V_0}{1 + e^{(r-c)/a}}. \quad (9)$$

This potential form has been successful in describing nuclear densities.¹³ There are three parameters: the potential strength V_0 , the diffusivity parameter a , and the size parameter $c = r_0 A^{1/3}$, where $A = Z + N$. The bound state energy levels are mainly determined by the strength and range of the potential. Since we want to minimize the number of parameters we vary, we keep the parameter a fixed at 0.5 fm, and vary r_0 and V_0 . A value of $a = 0.5$ fm is consistent with the values listed in Ref. 13.

Nuclei with an equal number of neutrons and protons often have spin and isospin zero. This is the case for all 15 nuclei listed in Table III whose cores contain an even number of neutrons (and protons). For these nuclei, it is reasonable to approximate the strong mean field potential as spherically symmetric, and to be the same for both valence neutron or proton in the corresponding mirror nucleus. Of the 15 nuclei in Table III whose core have an odd number of neutrons (and protons), only ^{34}Cl , ^{42}Sc , ^{46}V , ^{50}Mn , ^{54}Co , and ^{62}Ga are spin zero nuclei. In general, for odd-odd nuclei it is not clear if a spherically symmetric potential is an appropriate form to use. For completeness, we include all the nuclei in Table III in the analysis, bearing in mind that a simple model might not be appropriate for odd-odd nuclei.

The orbital angular momentum, l , of the valence nucleon can be determined from the total spin, j , and parity of the nucleus by the relation $l = j \pm 1/2$. The parity is positive for even l and negative for odd l . In the second column of Table III we list the total spin and the parity for the nuclei we examined. The values for j and parity correspond to the nuclei with the listed core plus one nucleon. For example, for the ^{12}C core, both ^{13}C and ^{13}N have a spin of $j = 1/2$ and a negative parity. The l value listed is the one we used in our calculation. The values of j and parity in Table III are obtained from Ref. 11.

In Table III we have grouped successive nuclei that have the same value of l . Evidence for a shell structure is seen in the grouping of the orbital angular momenta. However, nuclei are too complicated for the independent particle model

Table III. Experimental and calculated values for the valence nucleon. The binding energies are given in units of mega electron volts.

Core nucleus	$l(jP)$	Binding energy of valence		r_0 (fm)	V_0 (MeV)
		neutron	proton		
He(4)
Li(6)	1(3/2-)	7.250	5.606	1.52	43.11
Be(8)	1(3/2-)	1.665
B(10)	1(3/2-)	11.454	8.689	1.34	47.41
C(12)	1(1/2-)	4.946	1.943	1.29	35.11
N(14)	1(1/2-)	10.833	7.297	1.33	40.11
O(16)	2(5/2+)	4.144	0.601	1.34	47.71
F(18)	2(1/2+)	10.432	6.412	1.36	52.64
Ne(20)	2(3/2+)	6.761	2.431	1.32	46.80
Na(22)	2(3/2+)	12.419	7.580	1.32	53.09
Mg(24)	2(5/2+)	7.331	2.271	1.29	44.91
Al(26)	2(5/2+)	13.058	7.463	1.28	51.81
Si(28)	0(1/2+)	8.473	2.748	1.28	46.54
P(30)	0(1/2+)	12.312	6.133	1.30	49.91
S(32)	2(3/2+)	8.641	2.276	1.27	41.42
Cl(34)	2(3/2+)	12.644	5.896	1.29	45.05
Ar(36)	2(3/2+)	8.789	1.857	1.27	39.29
K(38)	2(3/2+)	13.077	5.764	1.29	43.39
Ca(40)	3(7/2-)	8.363	1.085	1.29	51.62
Sc(42)	3(7/2-)	12.138	4.488	1.29	55.22
Ti(44)	3(7/2-)	9.520	1.614	1.28	51.49
V(46)	1(3/2-)	13.001	4.767	1.31	58.03
Cr(48)	3(5/2-)	10.582	2.085	1.27	51.14
Mn(50)	3(5/2-)	13.687	4.885	1.27	53.66
Fe(52)	3(7/2-)	10.683	1.599	1.25	50.11
Co(54)	3(7/2-)	14.090	4.614	1.25	53.82
Ni(56)	1(3/2-)	10.247	0.694	1.27	51.34
Cu(58)	1(3/2-)	12.763	2.887	1.28	53.16
Zn(60)	1(3/2-)	10.231	0.454	1.31	47.21
Ga(62)	1(?)	12.765	2.203	1.25	53.26

to be universally valid, and the l value for some nuclei do not match the group. For the ^{18}F core, both ^{19}F and ^{19}Ne have positive parity with $j=1/2$. This would imply that l equals zero. However, the core ^{18}F has a spin of $j=1$, so the valence nucleon could have $l=2$, $j=3/2$, and couple to the core, resulting in a total spin of $j=1/2$. We chose $l=2$, which is the same as the other nuclei in the shell. One other exception is with ^{47}V and ^{47}Cr for the ^{46}V core nucleus. Both these nuclei have negative parity and $j=3/2$. Since the ground state of ^{46}V has a spin of $j=0$, we use a value of $l=1$ for the valence nucleons in ^{47}V and ^{47}Cr .

For the Coulomb potential, which only the proton feels, we use the potential due to a uniformly charged sphere of radius $c=r_0A^{1/3}$ [see Eq. (7)]. The same Woods-Saxon potential represents the strong interaction for both the valence neutron and valence proton in mirror nuclei which have $|N-Z|=1$. Thus, the two binding energies, valence neutron and proton, for each pair of mirror nuclei in Table III can be used to determine the two Woods-Saxon parameters r_0 and V_0 . For example, for the ^{12}C core, one picks a value for r_0 and determines V_0 such that the $l=1$ binding energy of the valence neutron in ^{13}C is 4.946 MeV. Using these same values for r_0 and V_0 , the Coulomb potential is added to the strong potential and one calculates again the $l=1$ binding

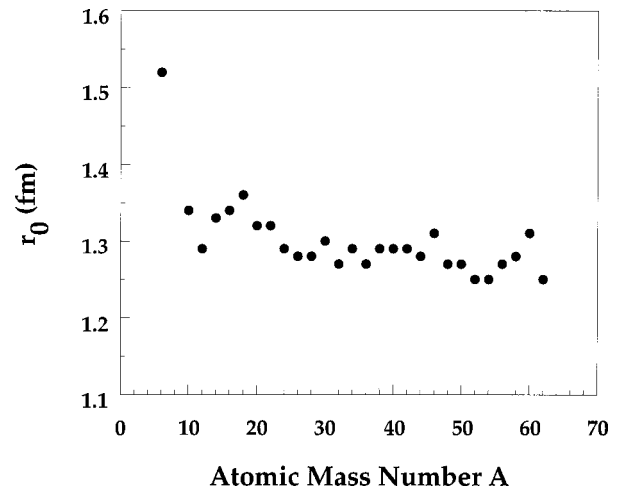


Fig. 1. A graph of the size parameter r_0 , from Table III, as a function of atomic mass number A . r_0 is defined in the text.

energy. If this binding energy is not equal to 1.943 MeV, then the value of r_0 is changed and the procedure is repeated until both binding energies are correct. For each nucleus we could only find one set of values of r_0 and V_0 that gave correct binding energies for both mirror nuclei. We used a computer program to carry out the two-parameter search.

We list our results in Table III. The values of r_0 and V_0 given in the last two columns produce the experimental proton and neutron binding energies in columns 3 and 4. We applied the model to all the nuclei that had experimentally measured binding energies. We were unable to calculate values for ^4He and ^8Be since neither ^5Li nor ^9B is sufficiently stable. The width of ^5Li is 1.5 MeV and that of ^9B is 0.5 keV. The heaviest nuclear core we fit is ^{62}Ga . Heavier nuclei which have an equal number of neutrons and protons are not stable enough for this analysis. The results listed in Table III are graphed in Figs. 1–4.

Having calculated r_0 and V_0 , the student can search for trends in these values for the different nuclei. Some qualitative patterns are noticeable, and we discuss below some properties of the shell model that the student can investigate.

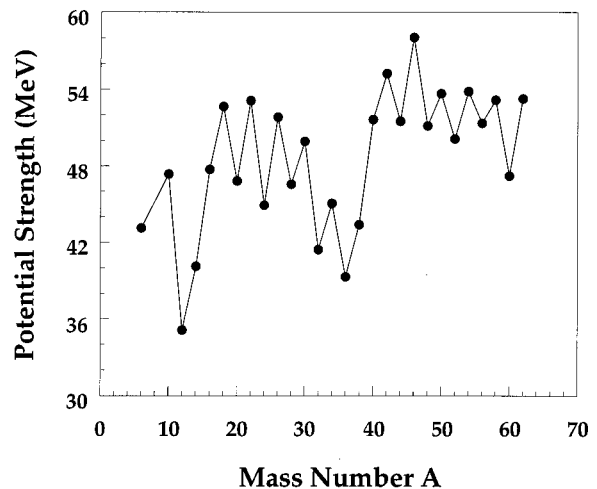


Fig. 2. A graph of the Woods-Saxon potential strength V_0 , from Table III, as a function of atomic mass number A .

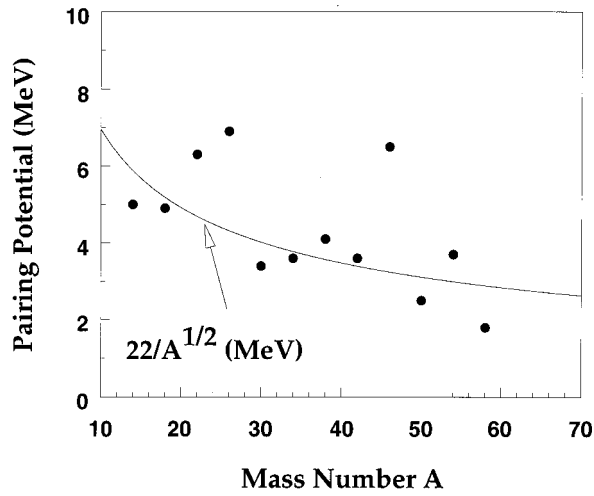


Fig. 3. The difference in V_0 , from Table III, for successive nuclei for values of A from 12 to 58. The curve is $22/\sqrt{A}$ MeV, which is our best $1/\sqrt{A}$ function fit to the data.

The first feature is seen in Fig. 1. The value of r_0 is fairly constant, and is approximately 1.3 fm. This indicates that the volume of the nucleus is proportional to mass number A . In the shell model, the mean field potential is broken up into three parts:

$$V(r) = V_{\text{central}}(r) + V_{\text{spin-orbit}}(r)\mathbf{L} \cdot \mathbf{S} + V_{\text{pairing}}. \quad (10)$$

The central potential, V_{central} , is the strongest of the three, and does not depend on the nucleon's l or j value. The spin-orbit potential is often taken to be proportional to $(1/r)dV_{\text{central}}/dr$. The pairing interaction is present in odd-odd nuclei, where the valence nucleon can pair up with an odd nucleon in the core. Motivated by the shell model, we express the potential strength V_0 in Eq. (9) in a similar manner:

$$V_0 = V_c + V_{\text{so}}\mathbf{L} \cdot \mathbf{S} + V_{\text{pairing}}. \quad (11)$$

This is equivalent to having the same Woods-Saxon function for all three terms in Eq. (10). Next we examine how

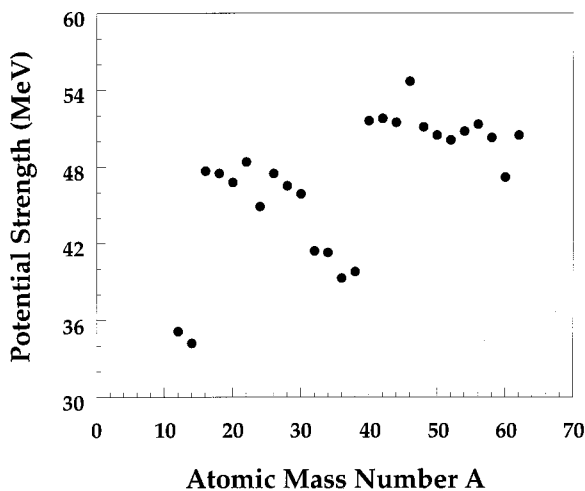


Fig. 4. A graph of the Woods-Saxon potential strength, V_0 , minus the pairing potential, $22/\sqrt{A}$ MeV, vs atomic mass number A .

Table IV. Average central and spin-orbit potentials.

First nucleus in shell	$l(jP)$	$V_0 - V_{\text{pairing}}$ average (MeV)	$3.2\mathbf{L} \cdot \mathbf{S}$ (MeV)	V_c (MeV)
He(4)	1(3/2-)	40.4	+1.6	38.8
C(12)	1(1/2-)	34.6	-3.2	37.8
O(16)	2(5/2+)	47.1	+3.2	43.9
Si(28)	0(1/2+)	46.2	0	46.2
S(32)	2(3/2+)	40.4	-4.8	45.2
Ca(40)	3(7/2-)	51.5	+4.8	46.7
Ni(56)	1(3/2-)	49.8	+1.6	48.2

well the variations of V_0 follow the pattern described by Eq. (11).

In Fig. 2 we plot the value of V_0 versus atomic mass number A . The see-saw variation of potential strength with mass number is clearly seen. Nuclei whose core have an odd number of neutrons, or protons, have a value for V_0 that is greater than that for nuclei with an even number of neutrons, or protons, in the core. We plot this difference, which is due to the pairing interaction, in Fig. 3 for values of A up to 58. One can see that the trend of the pairing potential is to decrease with mass number A . Some estimates of the pairing strength have a $1/\sqrt{A}$ dependence.⁹ For comparison, we also plot $22/\sqrt{A}$ MeV, which is our best $1/\sqrt{A}$ function fit to the data.

If one subtracts the pairing interaction from nuclei with an odd number of core protons (or neutrons), the l and j dependence of V_0 can be seen. In Fig. 4 we plot V_0 minus the pairing interaction, $22/\sqrt{A}$ MeV, as a function of mass number. The first two nuclei plotted are for the ^{12}C and ^{14}N core, which have $l=1$ and $j=1/2$. The potential increases for the next six nuclei, which have $l=2$ and $j=5/2$. The next two $l=0$, $j=1/2$ nuclei have approximately the same potential. The potential drops for the next four $l=2$, $j=3/2$ nuclei. There is a large increase for the next eight nuclei ($l=3$), and a slight decrease in V_0 for the last four $l=1$ nuclei in the list.

A key observation in Fig. 4 is that nuclei whose total angular momentum j is equal to $l+1/2$ have a higher mean field potential than nuclei with $j=l-1/2$. This is indicative of an $\mathbf{L} \cdot \mathbf{S}$ interaction. In the case of $s=1/2$, $\mathbf{L} \cdot \mathbf{S} = +l/2$ if $j=l+1/2$, and $\mathbf{L} \cdot \mathbf{S} = -(l+1)/2$ if $j=l-1/2$. Thus, if V_{so} in Eq. (11) is positive, then V_0 is greater for $j=l+1/2$ than for $j=l-1/2$. This feature is seen in Fig. 4.

Obtaining a value for V_c and V_{so} is complicated by the fact that certain nuclei satisfy the shell model better than others. Nonetheless, one can obtain an estimate for V_c and V_{so} from the data by averaging the values of V_0 in each shell. In Table IV we list the average potential for each shell. The spin-orbit potential strength V_{so} can be estimated from the splitting between the $l=1$ shells of ^4He and ^{12}C and the $l=2$ shells of ^{16}O and ^{32}S . The difference of $\mathbf{L} \cdot \mathbf{S}$ for $j=l+1/2$ and $j=l-1/2$ is $(2l+1)/2$. Applying this formula to the lowest $l=1$ nuclei gives $40.4 - 34.6 = 1.5V_{\text{so}}$, or $V_{\text{so}} = 3.8$ MeV. For $l=2$ we have $47.1 - 40.4 = 2.5V_{\text{so}}$, or $V_{\text{so}} = 2.6$ MeV. So on average, $V_{\text{so}} \approx 3.2$ MeV. In the fourth column of Table IV, we list the value of $3.2\mathbf{L} \cdot \mathbf{S}$ for each of the shells. The last column lists $V_c = V_0 - 3.2\mathbf{L} \cdot \mathbf{S}$. For nuclei with $A > 16$ the values of V_c are approximately the same, 46.1 ± 2.2 MeV.

Thus the potential form of Eq. (11) fits the data fairly well, particularly for nuclei with $A > 16$. Using only five potential parameters, one obtains a close fit for the valence nucleon binding energies for these 46 nuclei: $r_0 = 1.3$ fm, $a = 0.5$ fm, $V_c = 46.1 \pm 2.2$ MeV, $V_{s-o} = 3.2$ MeV, and $V_{\text{pairing}} = 22/\sqrt{A}$ MeV. The lighter nuclei have a somewhat lower value for V_c of around 38.5 MeV.

This simple mean field approach yields results close enough to the experimental data for students to apply the shell model to the set of mirror nuclei listed in Table III. We should point out that the theoretical analysis of nuclear energy levels is a complicated problem. In particular, some of the odd-odd nuclei examined here are not well described by the shell model. The student should realize that the conclusions and parameter values determined here have meaning only within the context of the model used. Recognizing these limitations is in itself a good lesson for physicists.

V. SUMMARY

We have presented two examples which use a mean field approximation to calculate energy levels. The examples are appropriate for an undergraduate class in quantum mechanics, computational physics, or modern physics. The mean field calculations are interesting, since the students are able to compare with experimental data. These problems complement “standard” textbook problems in quantum mechanics, and let the student experience the successes and failures of a model calculation.

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⁶Richard L. Liboff, *Introductory Quantum Mechanics* (Addison-Wesley, Reading, MA, 1992). See equation 12.6. Our potential $V(r)$ equals $e\Phi$. The difference between $j=l+1/2$ and $j=l-1/2$ for the $\mathbf{L}\cdot\mathbf{S}$ term is $(2l+1)/2$.

⁷A java applet which solves for the energy levels is available at <http://www.csupomona.edu/~pbsiegel>

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REAL LEARNING

After all, what’s a computer program except a construct of someone else’s mind? If you’re satisfied with that, well, go right ahead. But to me, real learning means inventing my own ways of solving problems...ways that might not fit into prearranged software.

Clifford Stoll, *Silicon Snake Oil* (Doubleday, New York, 1995), pp. 121–122.