Energy Levels Calculations of ^{32}Cl and ^{33}Cl Isotopes

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Abstract: In this article by using OXBASH shell model code the energy levels of Chlorine isotopes ^{32}Cl and ^{33}Cl are calculated. This code which is based on one of the most applicable nuclear models, deals with evaluating energy levels. Applying the program for each isotope using the defined codes, introduces several files which each file contains a set of data. Meanwhile, the ground state of excitation energy evaluated by OXBASH code together with energy levels and also probable places for nucleons placements in each energy level. Programs will be reliable only when results meet experimental procedures. A compilation of SD-shell energy levels calculated with the USD Hamiltonian and has been published around 1988. A comparison had been made between our results and the available experimental data to test theoretical shell model description of nuclear structure in Chlorine isotopes. The calculated energy spectrum is in good agreement with the available experimental data.

Keywords: Chlorine Isotopes, OXBASH Code, Shell Model Structure, USD Interaction
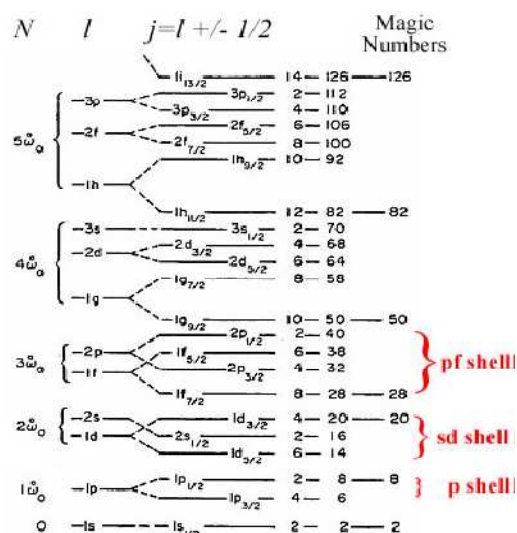
1. Introduction

Figure 1. p, sd and pf shell model spaces.

The nuclear shell model has been very successful in our understanding of nuclear structure: once a suitable effective interaction is found, the shell model can predict various observables accurately and systematically. For light nuclei, there are several "standard" effective interactions such as the Cohen-Kurath [1] and the USD [2] interactions for the *p* and *SD* shells, respectively. Analysis of neutron-rich SD nuclei has been of intense curiosity in recent years as they present new aspects of nuclear structure [3].Traditional shell-model studies have recently received a renewed interest through large scale shell-model computing in no-core calculations for light nuclei, the 1s0d shell, the 1p0f shell and the 3s2d1g$_{7/2}$ shell with the inclusion of the 0h$_{11/2}$ intruder state as well. It is now therefore fully possible to work to large-scale shell-model examinations and study the excitation levels for large systems. In these systems, inter core is assumed and space is determined by considering shell gaps. Figure 1 shows the shell model and some model spaces.

The crucial starting point in all such shell-model calculations is the derivation of an effective interaction, based on a microscopic theory starting from the free nucleon-nucleon (NN) interaction. Although the NN interaction is too short but finite range, with typical inter particle distances of the order of 1–2 fm, there are indications from both studies of few-body systems and infinite nuclear matter, both real and effective ones, may be of importance. Thus, with many valence nucleons present, such large-scale shell-model calculations may tell us how well an effective interaction which only includes two-body terms reproduces properties such as excitation spectra and binding energies. The problems of deriving such effective operators and

interactions are solved in a limited space, the so-called model space, which is a subspace of the full Hilbert space. Several formulations for such expansions of effective operators and interactions exist. For example, for nuclei with *4 < A < 16* p-shell is used of Cohen-Kurath interaction and USD interaction is suitable for *16 < A < 40* SD-shell [1, 2].

In order to calculate the nuclear structure properties of both ground and excited states based on the nuclear shell model one needs to have wave functions of those states. These wave functions are obtained by using the shell-model code OXBASH[4].The code OXBASH for Windows has been used to calculate the nuclear structure for Chlorine nucleus, by employing the SD (independent charges) and SDPN (depending charges) model space with three effective interactions[4]. The first interaction for the lower part of the SD-shell is Chung-Wildenthal particle interaction (CW), secondly, the Universal SD-shell Hamiltonian (USD interaction). In the third interaction the New Universal SD-shell Hamiltonian (USDAPN) is used [4]. Richter *et al*[5] used this shell model successfully in the p-shell, and fp-shell [6], [7] and Wildenthal [8] and Brown *et al*[9] in the SD-shell to describe the systematics observed in the spectra and transition strengths.In the present work, we focus our attention on the description of energy levels of SD shell of Chlorine isotopes ^{32}Cl and ^{33}Cl which have configurations *$0d_{5/2}$, $1s_{1/2}$* and *$0d_{3/2}$*.

2. Theory

One of the approaches to study the structure of a nucleus and NN interactions, named Shell model structure that we deal with all degrees of freedom in this space and consider such all many-body configurations. In this model protons and neutrons move all active single particle orbits with three restrictions, Isospin, Angular momentum and Parity conservation [1, 2]. A *J* orbit has *(2J+1)* degeneracy for *J_z,* if we put N_π protons and N_ν neutrons on such orbits, then the numbers of possible configurations are $_{2J+1}C_{N_\pi} \times _{2J+1}C_{N_\nu}$. Of course numbers of basis increases in a combinatorial way and the irrelevant numbers must are taken into account.

As is well known, the interaction between two protons, two neutrons or a proton and a neutron is approximately the same, $\nu_{\pi\pi} = \nu_{\nu\nu} = \nu_{\pi\nu}$, so Isospin (T) was introduced as a new quantum number.

Single-particle wave functions of a neutron and a proton can be expressed with the t = 1/2 spinors .The nuclear states of a nucleus with *N* neutrons and *Z* protons *(A=N+Z)* can be characterized by definite values of T and M_T quantum numbers [1-3]

$$M_T = 1/2(N - Z), \quad 1/2(N - Z) \le T \le A/2$$

The configuration for a given nucleus partitioned into core part *(N_c, Z_c)* and an active valance part *($N-N_c$,$Z-Z_c$)*. For practical reasons the number of valance nucleons must be small, as the numerical computations increase dramatically in magnitude with this number. Valance nucleons move in a finite number of j-orbits and their Hamiltonian of the valance

nucleons is given by [2]

$$H = E_0 + \sum_i \varepsilon_i a_i^+ a_j + 1/2 \sum_{ijkl} \langle ij|V|kl\rangle a_i^+ a_j^+ a_l a_k$$

Where E_0 is the energy of the inert core, ε_i's are the single particle energies of the valance orbits and $\langle ij|V|kl\rangle$ are the two-body matrix elements (TBME) of residual interaction amongst the valance particles $\varepsilon_i's$ effectively take account of interaction between a valance particle and those in the inert core and V is taken from theoretical calculations or phenomenological models. The eigenvectors obtained from H-matrix in turn are used to obtain matrix elements of other physically interesting operators such as electric and magnetic moments, *EM* transition probabilities, β-decay matrix elements, one- and two-nucleon transfer probabilities, etc.

Finely, the shell-model calculations are confronted with all the available data. A commonly used procedure is to parameterized the effective interactions and even single particle energies of valance orbits and other such operators (M1, GT, E2 etc.) and then obtain the values of these parameters which give the best numerical fit to the observed set of data points. Computer programs to construct and diagnolize Hamiltonian matrices have been existence for almost 40 years now. An improved modern version ones is OXBASH [3, 10] that uses the angular momentum coupled (J) scheme. As the interaction between two valence neutrons, we have to know the set of two-body matrix elements (TBME's) $\langle ab; JT|V|cd; JT\rangle$ with $(JT) = (01)$

OXBASH code only works for $J_z=J$. By applying J^+ operator, it predicts a set of m-scheme vectors that if used for projection will produce a good *J*-basis. The treatment that follows cannot be generalized for both spin and Isospin to predict exactly a number of m-scheme vectors equal to the good *JT*-basis dimension. One disadvantage of an m-scheme basis is that it is much larger than the corresponding basis consisting of wave functions coupled to J and T. The n/p formalism enters naturally in the m-scheme formalism, since it only needs to skip those unwanted t_z values in each J-orbit in the corresponding SPS_le (Single Particle State _le)

In the second line of approach the two body matrix elements are treated as parameters, and their values are obtained from best fit to experimental data [11].

Brown and coworkers [12] have carried extensive studies of energy level and spectroscopic properties of SD-shell nuclei in terms of a unified Hamiltonian applied in full SD-shell model space. The universal Hamiltonian was obtained from a least square fit of 380 energy data with experimental errors of 0.2MeV or less from 66 nuclei. The USD Hamiltonian is defined by 63 SD-shell two body matrix element and their single particle energies. In more recent work Brown and co-workers have modified USD type Hamiltonian to USDA and USDB based on updated set of binding energy and energy levels of O, F, Ne, Na, Mg and P isotopes.

3. OXBASH Code

The calculations have been carried out using the code

OXBASH for Windows [4]. The code uses an m-scheme Slater determinant basis and works in the occupation number representation, where the occupancy (vacancy) of a bit in any given position of the computer word symbolizes the presence (absence) of a particle in a specific single particle state (i.e. in a given $|n, l, j, m_j, t_z >$ state). Using a projection technique, wave functions with good angular momentum J and Isospin T are constructed. The SDPN and SD model spaces consist of ($0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$) above the $Z = 8$ and $N=8$ closed shells for protons and neutrons. CW is an effective interaction that has been used with the SD model space, where the single-particle energies are 0.877, -4.15 and -3.28 MeV for subshells $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively. Also the USD effective interaction has been used with the SD model space, where the single-particle energies are 1.647, -3.948 and -3.164 MeV for subshells $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively. Meanwhile USDAPN is the effective interaction that has been used, where the single-particle energies for protons and neutrons are 1.980, -3.061 and -3.944 for $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$, respectively [13].

The OXBASH code uses both m-scheme and jj-coupling. It utilizes a basis of the Slater determinants that are anti-summarized product wave functions. Each of these *m*-scheme basis states has definite total angular momentum projection quantum number $J_z = M$ and total Isospin projection quantum number T_z. An appropriate expression of the shell-model Hamiltonian is given as the sum of one- and two-body operators [14]

$$H = \sum_a \varepsilon_a \vec{n}_a + \sum_{a \leq b, c \leq d} \sum_{JT} V_{JT}(ab; cd) \hat{T}_{JT}(ab; cd),$$

Where ε_a are the single-particle energies, $\vec{n}_a$ is the number operator for the spherical orbit *a* with quantum number (n_a, l_a, j_a), $V_{JT}(ab \, cd)$; is a two-body matrix element, and

$$\hat{T}_{JT}(ab; cd) = \sum_{MT_z} A^+_{JMTT_z}(ab) A_{JMTT_z}(cd),$$

is the scalar two-body transition density for nucleon pairs (*a, b*) and (*c, d*), each pair coupled to spin quantum numbers *JM*.[15]

4. Results

The isotopes of Chlorine ³²Cl and ³³Cl provide a unique laboratory for examining the foundation of SD shell model calculations. The nucleons of the core (¹⁶O) are 8 protons and 8 neutrons which are inert in the $(1s_{1/2}, 0p_{3/2}, 0p_{1/2})J=0, T=0$ configuration and the remaining nucleons are distributed over all possible combinations of the $0d_{5/2}, 1s_{1/2}$ and $0d_{3/2}$ orbits according to Pauli Exclusion Principle. The package of program called "SHELL" was used to generate the One Body Density Matrix Element (OBDME), and the package of program called "LPE" is used to calculate the wave functions and energy levels.

We present here some results concerning Ground and excitation energies properties of the Cl isotopes for which recent data has been reported in the literature. Table 1 and

figure 2 shows data for ³²Cl isotope and table 2 and figure 3 shows data for ³³Cl isotope. E (OXBASH) are data calculated in this work (blue squares) and E (exp) are experimental data (red squares).

Table 1. *Data for ³²Cl. All energies are in keV.*

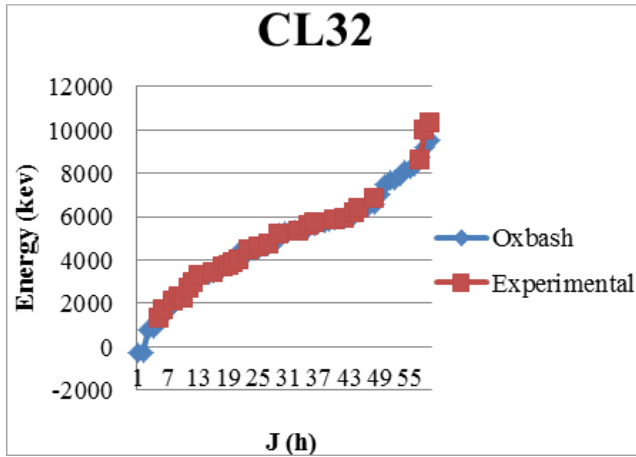| E(exp)	E(OXBASH)	J/CL32
	-255	1→J=1
	-260	2→J=2
	788	3→J=1
	875	4→J=2
1326	1268	5→J=3
1719	1705	6→J=1
	1776	7→J=2
2122	1964	8→J=3
2270	2342	9→J=2
2194	2462	10→J=1
2665	2656	11→J=3
2941	2908	12→J=4
3290	3258	13→J=2
	3327	14→J=2
	3332	15→J=3
3437	3437	16→J=1
	3467	17→J=4
3692	3649	18→J=3
3767	3716	19→J=1
3883	3957	20→J=3
4002	4373	21→J=2
	4415	22→J=3
4432	4429	23→J=1
	4470	24→J=3
4590	4504	25→J=0
	4669	26→J=4
4757	4717	27→J=5
	4789	28→J=2
5166	5249	29→J=4
	5304	30→J=3
	5319	31→J=2
	5354	32→J=5
5340	5355	33→J=1
	5514	34→J=2
5578	5544	35→J=4
5698	5555	36→J=1
	5679	37→J=3
	5738	38→J=0
	5746	39→J=5
5813	5853	40→J=4
	5885	41→J=1
5905	5897	42→J=4
	6058	43→J=4
6178	6093	44→J=5
6360	6280	45→J=0
	6453	46→J=4
	6485	47→J=5
6820	6554	48→J=4
	7011	49→J=5
	7475	50→J=5
	7671	51→J=0
	7673	52→J=5
	7877	53→J=0
	8149	54→J=5
	8224	55→J=5
	8375	56→J=0
8600	8730	57→J=0
10000	9186	58→J=0
10300	9560	59→J=0

Figure 2. Comparison Calculated data with Experimental data for ^{32}Cl.
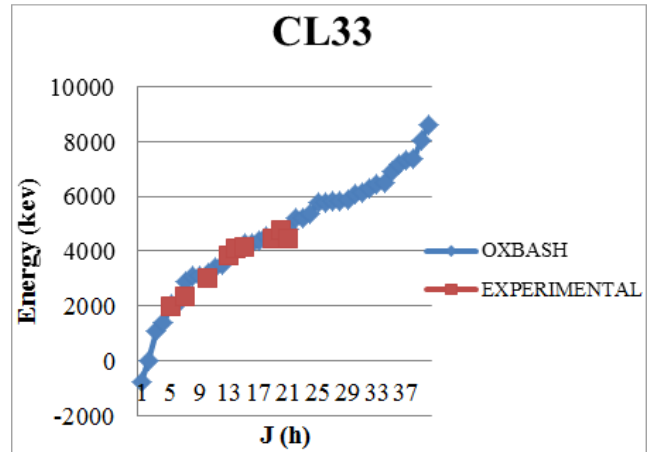

Figure 3. Comparison Calculated data with Experimental data for ^{33}Cl.

Table 2. Data for ^{33}Cl. All energies are in keV.

E(exp)	E(OXBASH)	J/CL33
	-779	1→J=3/2
	0000	2→J=1/2
	1116	3→J=5/2
	1395	4→J=3/2
1986	2060	5→J=5/2
	2112	6→J=7/2
2351	2888	7→J=3/2
	3084	8→J=1/2
	3119	9→J=5/2
2975	3194	10→J=7/2
	3407	11→J=3/2
	3507	12→J=1/2
3816	3918	13→J=5/2
4099	4028	14→J=3/2
4112	4297	15→J=3/2
	4305	16→J=7/2
	4366	17→J=5/2
	4527	18→J=7/2
4463	4530	19→J=3/2
4746	4743	20→J=5/2
4438	4782	21→J=1/2
	5207	22→J=5/2
	5224	23→J=1/2
	5366	24→J=7/2
	5774	25→J=3/2
	5782	26→J=7/2
	5840	27→J=5/2
	5851	28→J=3/2
	5900	29→J=7/2
	6071	30→J=5/2
	6139	31→J=7/2
	6312	32→J=3/2
	6442	33→J=5/2
	6494	34→J=1/2
	6908	35→J=7/2
	7169	36→J=1/2
	7316	37→J=7/2
	7376	38→J=1/2
	8036	39→J=1/2
	8598	40→J=1/2

5. Conclusions

As seen from all figures, very good agreement is obtained for most of energy levels of Chlorine isotopes, and the ordering of levels is correctly reproduced. Unfortunately, enough experimental data were not available for ^{33}Cl, but regarding to USD data we can judge almost all calculation meet with reasonable success in reproducing the observed level structure.

In general the best and most complete results are found with the largest model space while calculations in an infinite space are not possible and the computation time increases exponentially with model space size so some truncation is required. Also the interaction used must be appropriate for the model space. The empirical interactions are (usually) better determined for smaller model spaces. The model space in OXBASH is defined by the active valance nucleon orbits and our calculated results are reasonably consistent with experimental data, although the structure of odd-even nuclei is much more complicated than their odd-odd neighbours.

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