ON THE 9/2$^-$ LEVEL EXCITATION ENERGY OF ODD Tl, Au AND Ir ISOTOPES

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Abstract

A semi-empirical method inspired by Blomqvist previous calculations of the excitation energy of the lowest 9/2$^-$ state of ^{201}Tl is applied to similar calculations in different Tl, Au and Ir isotopes. These semi-empirical estimates agree well with the experimental values of these excitation energies as well as with the energy differences deduced from the analysis of the total potential energy surfaces calculated microscopically with Nilsson's model. The same excitation energies are computed with a spherical HFBCS model which does not reproduce so well the available experimental data. An interpretation of these deviations is attempted.

1. Introduction

Recently several particle (or quasiparticle) - rotor descriptions were given [1-6] for the negative parity states of odd mass Tl, Au and Ir isotopes. In these descriptions the odd proton occupies an orbital belonging to $1h_{9/2}$ (or $1h_{11/2}$) subshell in the spherical limit ($\varepsilon_2 = 0$).

However the energy difference between these subshells was not considered in any of these calculations.

The only such estimate available was previously made for ^{201}Tl by Blomqvist [7]. In this work the lowest 9/2$^-$ state observed in the light thallium isotopes with odd mass number A was interpreted as a core excited state built upon a $^{A-1}$Hg core coupled to a pair of proton holes $(3s_{1/2})^{-2}$ and a $1h_{9/2}$ proton. According to this interpretation the excitation energy of this 9/2$^-$ state can be evalueted from the expression :

$$\Delta E(1h_{9/2} - 3s_{1/2}) = \Delta S_p - E_c - E_{int}$$

where ΔS_p , E_c and E_{int} have the following meaning :

$\Delta S_p = S_p(A,81) - S_p(A + 2, 83)$ is the difference between the proton separation energies of Tl and Bi,

$E_C \equiv E_C \ |(1h_{9/2}),(3s_{1/2})^{-1}|$ is the Coulomb proton-proton hole interaction energy,

$E_{int} \equiv E_{int} \ |\pi_1, \ \pi_2^{-2} + \pi_3^{-2} + \ldots (\nu,\nu')^{-2}|$

is the interaction between the proton $\pi_1 \equiv \pi\ (1h_{9/2})$ and the proton and neutron hole pairs $\pi_2 \equiv \pi(3s_{1/2})$, $\pi_3 \equiv \pi(2d_{3/2})$, $\nu,\nu' \equiv$ neutrons.

Applying the previous relation to the evaluation of the 9/2$^-$ state of ^{201}Tl Blomqvist estimated the Coulomb proton-proton hole energy to 430 keV and assigned the remaining energy difference between the experimental and calculated values to the interaction between the $1h_{9/2}$ proton and the other proton and neutron holes.

In principle the same method can be applied to other odd mass Tl isotopes as well as to Au and Ir isobars. However, according to Blomqvist [8] an estimate of the polarization interaction between the $1h_{9/2}$ single proton and four proton holes (core of the gold isotopes) will be rather inaccurate. Furthermore the exact evaluation of the different terms becomes more difficult as soon as the number of interacting particles (holes) increases. Consequently this method was not extended to other applications of this kind. However the possibility still remained of searching a semi-empirical method inspired by this type of calculation which could describe satisfactorily the available experimental data with only a few adjusted parameters.

Such attempt was recently made in the frame of a systematic investigation concerning the properties of odd mass Tl, Au, Ir negative parity levels [9]. In this work were included also preliminary results obtained with Nilsson microscopic model.

The present investigation has three main purposes :

- to give a full account of these preliminary results,
- to present results of new calculations made with a spherical Hartree-Fock-BCS model,
- to compare these semi-empirical or theoretical predictions to the available experimental data.

2. Calculations and results

The main steps of different types of calculations and parametrization used are briefly described (2.1) as well as the semi-empirical and theoretical results obtained with them (2.2), for the different nuclides considered.

2.1.Types of calculations and parametrization

For greater clearness the different types of calculations are described separately.

2.1.1. Semi-empirical estimates

The simplest semi-empirical estimate of the 9/2$^-$ level excitation energy is given by the relation :

$$\Delta E_1(A,Z) = S_p(A,Z) - S_p(A,83)$$

where A is the mass number, Z = 77, 79 or 81 and $S_p(A,Z)$ are the proton separation energies of the nuclides considered. These

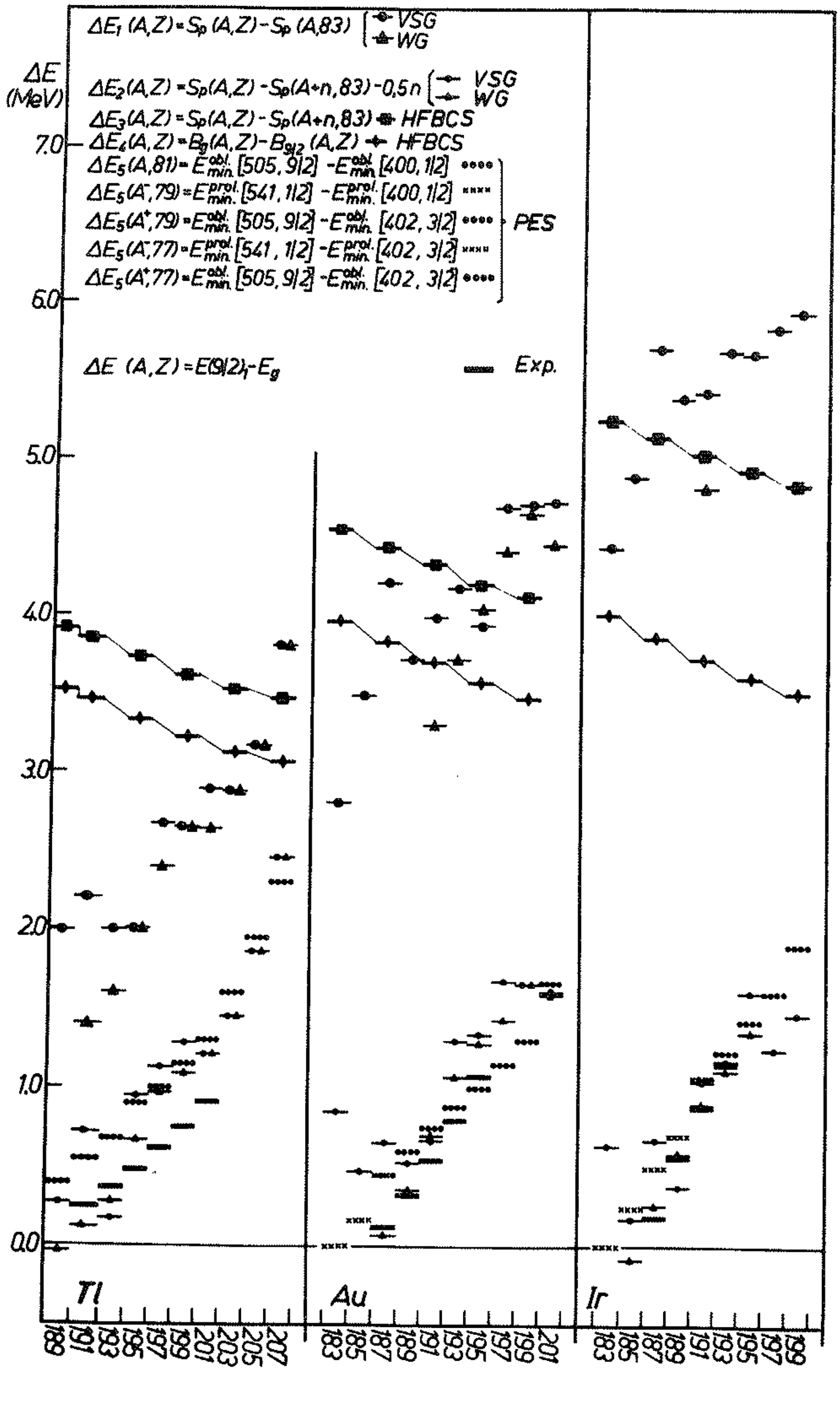

Fig. 1 - The (9/2-) level excitation energy of odd mass Tl, Au and Ir isotopes

The ΔE_1 -●-, -▲- and ΔE_2 -•-, -▴- energy differences are semi-empirical estimates derived from mass tables (VSG : Viola, Swant, Graber ; WG : Wapstra, Gove). The ΔE_3 -▪- and ΔE_4 -+- energy differences are theoretical estimates obtained by Hartree-Fock BCS calculations (see § 2.1.3. in the text). The ΔE_5(•••• or ××××) energy differences are theoretical estimates deduced from the Nilsson's potential energy surfaces (see § 2.1.2. in the text). Experimental data are represented by full, thick lines (▬)

separation energies are taken from the mass tables [10-11].

A similar relation is given by the first term, ΔS_p, of a Blomqvist type formula. A better approach of such formula is obtained by introducing a single correcting term, E_{corr}, into $\Delta E_1(A,Z)$.

In the first attempts to describe the odd mass Tl experimental energies we adopted $E_{corr} = 2E_c = 880$ keV (for ^{201}Tl). Later the same relation was extended to Au and Ir similar calculations. For that purpose it was necessary to choose the Z dependence of the correcting term, E_{corr}. The simplest assumption is to consider a linear variation with the number n = 82-(Z-1) of proton holes coupled to the lead core ;

$$E_{corr} = k\ n$$

With such expression the semi-empirical relation becomes :

$$\Delta E_2(A,Z) = S_p(A,Z) - S_p(A+n,83) - k\ n$$

The constant k is adapted to fit the experimental data. In the present case k=0,5 MeV. This value should be compared with $E_c = 0.43$ MeV obtained by Blomqvist for thallium 201.

2.1.2. The total potential energy

Recently, numerous calculations of Tl, Au, Ir and Re total potential energies were made [12] with an extended version of the programme previously applied to the neighbouring even-even nuclei [13]. The main improvement relatively to the old programme [13] is the possibility to block the proton in any given orbit.

From the analysis of the experimental and theoretical data concerning the static and dynamical properties of such nuclei the 9/2⁻ level arises either from the oblate 9/2|505| or from the prolate 1/2|541| orbital. Similarly, the 3/2+ or 1/2+ ground states are identified to 3/2|402| or 1/2 |400|. Finally, these assignments lead to the following energetic relations between the minimum total potential energy values corresponding to such orbitals :

$$\Delta E_5 = E^{obl}_{min}\ 9/2|505| - \begin{cases} E^{obl}_{min}\ 1/2|400|^{a)} \\ E^{obl}_{min}\ 3/2|402|^{b)} \end{cases}$$

$$\Delta E_5 = E^{prol}_{min}\ 1/2|541| - \begin{cases} E^{prol}_{min}\ 1/2|400|^{c)} \\ E^{prol}_{min}\ 3/2|402|^{d)} \end{cases}$$

where the items a), b), c) and d) indicate the validity of each relation :

a) all Tl isotopes
b) Au and Ir for A $\gtrsim$ 193
c) light Au
d) light Ir

2.1.3. Hartree-Fock BCS calculations

Two types of Hartree-Fock BCS calculations are made for the odd mass Tl, Au and Ir isotopes :

(i) Constraint spherical calculations without blocking (similar to those of even nuclei).

(ii) Constraint spherical calculations with blocking (where an odd particle occupies a given orbital).

The computing programme and parametrization are the same as previously used in extensive calculations of bulk nuclear properties [14-15].

The former approach (i) gives more reliable estimates of the total ground state binding energies except for odd mass nuclei which have low spin or which are adjacent to magic nuclei. In the last cases, the latter approach (ii) gives more accurate estimates.

The excitation energy of the 9/2⁻ states in odd Tl, Au and Ir isotopes was taken as the difference between the total self consistent HF-BCS binding energies of the ground state and the lowest 9/2⁻ state:

$$\Delta E_4(A,Z) = B_g(A,Z) - B_{9/2}(A,Z)$$

On the other hand, the difference between the ground state proton separation energies of Tl (Au or Ir) and Bi isotopes

$$\Delta E_3(A,Z) = S_p(A,Z) - S_p(A+n,83)$$

was also calculated. Finally, ΔE_3 and ΔE_4 are connected, in the present approach, by the following relation:

$$\Delta E_4(A,Z) = \Delta E_3(A,Z) - \{S_p^{9/2}(A,Z) - S_p^{9/2}(A+n,83)\}$$

where $S_p^{9/2}(A,Z)$ represents the proton separation energy of the $9/2^-_1$ state in nuclei (A,Z). The bracket on the right hand side is proportional to n=83-Z, assuming a linear variation of $S_p^{9/2}$ with Z.

2.2. Semi-empirical and theoretical results

In the figure 1 are represented the semi-empirical excitation energies ot the lowest 9/2⁻ level calculated with the formulae previously given for $\Delta E_1(A,Z)$ and $\Delta E_2(A,Z)$ (see sect. 2.1.1). With the adopted value of the constant k (= 0.5 MeV) appearing in the correcting term, E_{corr}, of the semi-empirical relation $\Delta E_2(A,Z)$ one has (in MeV) :

$$E_{corr} = \begin{cases} 1.0\ (Tl) \\ 2.0\ (Au) \\ 3.0\ (Ir) \end{cases} \text{corresponding to } n=83-Z= \begin{cases} 2 \\ 4 \\ 6 \end{cases}$$

protons holes in the lead core. Consequently the difference, $\Delta E_6(A,Z)$, between the proton separation energies of Tl (Au, or Ir) and Bi isotones is easily derived from the relation $\Delta E_2(A,Z)$:

$$\Delta E_6(A,Z) = \Delta E_2(A,Z) - E_{corr}(Z) = S_p(A,Z) - S_p(A+n,83)$$

Indeed, it suffices a translation of the $\Delta E_2(A,Z)$ curve parallel to the energy axis, E, amounting to the correcting term, E_{corr} = 1.0 (2.0 or 3.0) MeV for Tl (Au or Ir). For that reason the curves $\Delta E_6(A,Z)$ are not represented in fig.1 to avoid overcharging it. The semi-empirical values $\Delta E_2(A,Z)$ agree remarkably well with the theoretical values, $\Delta E_5(A,Z)$, deduced from the total potential energy results. This agreement is particularly remarkable because no free parameters were used in the potential energy calculations to fit the 9/2⁻ excitation energies.

The results of the Hartree-Fock BCS

calculations obtained with the relations $\Delta E_3(A,Z)$ and $\Delta E_4(A,Z)$ should be compared to the semi-empirical results deduced from the relations ΔE_6 and ΔE_2 respectively. This comparison shows a very good agreement between $\Delta E_3(A,Z)$ and $\Delta E_6(A,Z)$ for ^{207}Tl. For the other Thallium isotopes the HFBCS calculations give the order of magnitude of the 9/2- excitation energies but do not reproduce exactly its dependence with the neutron number. However the difference between ΔE_3 and ΔE_4 is constant for each set of isotopes (see fig.1) and varies approximately linearly with the number of proton holes, $n = 82-(Z-1)$ of the lower even nucleus (Z-1) relatively to the lead core. So this numerical result is in agreement with the last remark concerning the HFBCS calculations (section 2.1.3) and the assumption made for the correcting term E_{corr} of the ΔE_2 semi-empirical relation (section 2.1.2).

3. Comparison between calculated and experimental values.

The experimental data included in fig.1 are taken from the latest compilations |6|. From the comparison between the results of the present calculations and the experimental values several regularities are observed :

(i) The semi-empirical calculated values $\Delta E_2(A,Z)$ are close to the experimental energies of gold and iridium but deviate slightly from those of thallium.

(ii) The potential energy differences calculated with the extended Nilsson computing programme are in good agreement with the experimental data for gold and iridium isotopes. For the tallium isotopes they are somewhat larger than the observed ones.

(iii) The spherical constrained Hartree-Fock BCS calculations deviate considerably from the experimental data except for the heavy Tl isotopes. For the light iridium isotopes the observed discrepancies can be considerable. This increasing deviation with the distance from the double closed shell may be interpreted as a regular departure from the validity of the spherical constrained assumption.

4. Conclusions

The general trend of the excitation energies of the lowest 9/2- levels in Tl, Au and Ir is well described both by a semi-empirical relation inspired from Blomqvist core-excited desciption of these levels and the differences between total potential energies. The spherical constrained HFBCS results reproduces the order of magnitude of these energies but predict a different dependence of these energies on the neutron number.

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