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CALCULATION OF THE COULOMB ENERGY OF THE ^{40}Ca NUCLEUS IN THE OSCILLATOR SHELL MODEL USING THE TALMI TECHNIQUE

by

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Abstract: *A calculation is performed for the Coulomb energy of the ^{40}Ca nucleus by adopting the harmonic oscillator shell model and using the Talmi Technique*[8,9,11]. *The result obtained by this method agrees exactly with that obtained by A.Dellafiore who used a Fourier transform technique*[2].

1. INTRODUCTION

One of the attractive features of the harmonic oscillator shell model is that one can perform analytically various calculations based on it. One of the interesting quantities which one might obtain is the Coulomb energy of closed shell light nuclei. Of course, the obtained results provide an estimate, which, however, may be compared to more accurate results.

The expressions for the Coulomb energy of the ^{4}He and ^{16}O nuclei in the oscillator shell model have been known for a long time. Very recently the relevant expression for ^{40}Ca has been derived[2] (using a Fourier transform technique).

The aim of this paper is to give some details of the calculation of the same quantity by the more standard method of the Talmi technique[5], which is more complicated, but it is useful in order to provide an independent check of Dellafiore's result.

In the following section we give an outline of the method and we use it for the calculation of the Coulomb energy of ^{16}O. This result is useful for the main calculation (section 3) in which the expression for the Coulomb energy of ^{40}Ca is derived in detail.

2. OUTLINE OF THE METHOD

a. Tensor Expansion of the interaction[9].

The evaluation of the matrix elements of an interaction $V(|\vec{r}_1 - \vec{r}_2|)$, that depends on the relative distance $|\vec{r}_1 - \vec{r}_2|$ of the two particles and not on their spins or isospins, in a given configuration $(l_1 l_2)$:

$$<l_1 l_2 LM \mid V(|\vec{r}_1 - \vec{r}_2|) \mid l_1 l_2 LM> = \int \psi^*(l_1 l_2 LM) V(|\vec{r}_1 - \vec{r}_2|) \psi(l_1 l_2 LM) d\tau$$

is complicated because V is a function of $|\vec{r}_1 - \vec{r}_2|$, whereas $\psi^*\psi$ is a product of a function of $\vec{r}_1$ and a function of $\vec{r}_2$. The method consists in expanding $V(|\vec{r}_1 - \vec{r}_2|)$ in a series of Legendre polynomials of $\cos\omega_{12} = \cos\Theta$, (ref. 9, p. 208)

$$V(|\vec{r}_1 - \vec{r}_2|) = \sum_{k=0}^{\infty} v_k(r_1, r_2) P_k(\cos\Theta)$$

where $v_k(r_1, r_2) = \frac{2k+1}{2} \int V(|\vec{r}_1 - \vec{r}_2|) P_k(\cos\Theta) d(\cos\Theta)$

The result is:

$$\Delta E = <l_1 l_2 LM \mid V(|\vec{r}_1 - \vec{r}_2|) \mid l_1 l_2 LM> = \sum_{k \text{ even}} f_k F^k ,$$

where the summation over k goes from $k = 0$ to $k = 2 \min(l_1, l_2)$, or, more generally, for antisymmetric states:

$$\Delta E_{SLJ} = <l_1 l_2 SLJM \mid V(|\vec{r}_1 - \vec{r}_2|) \mid l_1 l_2 SLJM> =$$

$$= \sum_k f_k F^k + (-1)^{l_1 + l_2 + L + S} \sum_k g_k G^k ,$$

where F^k, G^k are the Slater integrals:

$$F^k = F^k(n_1 l_1 n_2 l_2) = \iint R^2_{n_1 l_1}(r_1) R^2_{n_2 l_2}(r_2) v_k(r_1 r_2) dr_1 dr_2$$

$$G^k = G^k(n_1l_1n_2l_2) = \iint R_{n_1l_1}(r_1)R_{n_2l_2}(r_1)R_{n_1l_1}(r_2)R_{n_2l_2}(r_2)$$

$$\cdot\ \upsilon_k(r_1r_2)dr_1dr_2$$

which depend on the interaction under consideration, and f_k,g_k are geometrical factors, independent of the interaction, given by:

$$f_k = \langle l_1l_2LM \mid \frac{4\pi}{2k+1}\ (\mathbf{Y}_k(\Omega_1)\ .\ \mathbf{Y}_k(\Omega_2)) \mid l_1l_2LM\rangle =$$

$$= (-1)^{l_1+l_2+L}(l_1 \parallel \mathbf{C}^k \parallel l_1)(l_2 \parallel \mathbf{C}^k \parallel l_2) \begin{Bmatrix} l_1 & l_2 & L \\ l_2 & l_1 & k \end{Bmatrix}$$

$$g_k = (-1)^L(l_1 \parallel \mathbf{C}^k \parallel l_2)(l_2 \parallel \mathbf{C}^k \parallel l_1) \begin{Bmatrix} l_1 & l_2 & L \\ l_1 & l_2 & k \end{Bmatrix}$$

We have followed the notation of reference[9].

For instance, for the simple ls configuration, i.e. $l_1 = 1$ (arbitrary) and $l_2 = 0$, there are two multiplets: ^1L, ^3L with $L = 1$. Thus we obtain:

$$\Delta E(^1L) = F_0 + G_1$$

$$\Delta E(^3L) = F_0 - G_1$$

here $F_0 = f_0F^0$, $G_1 = g_1G^1$.

For the case of the p^2 configuration, i.e. $n_1 = n_2 = n$, $l_1 = l_2 = 1$, it is evident that only the $k = 0$ and $k = 2$ terms will give nonvanishing contributions and there are only tbe direct integrals F^k:

$$\Delta E(p^2,{}^1S) = F^0 + \frac{10}{25}\ F^2$$

$$\Delta E(p^2,{}^3P) = F^0 - \frac{5}{25} F^2$$

$$\Delta E(p^2,{}^1D) = F^0 + \frac{1}{25} F^2$$

Expressions for other configurations can be derived in a similar way and have been tabulated (Energies in terms of Slater integrals for Wigner force in LS-coupling[9]).

The Slater integrals are expressible in terms of the very simple Talmi integrals[9,10].

b. Description of the method in the case of the ^{16}O nucleus.

For the ^{16}O nucleus, the nucleons configurations are: $(1s^2)_N(1p^6)_N(1s^2)_p(1p^6)_p$. The Coulomb energy is given by:

$$E_c(^{16}O) = E_c(Z = 8) = \sum_{i<j}^{\text{protons}} \int \Psi^* \frac{e^2}{r_{ij}} \Psi dq \ ,$$

where Ψ is the normalized to unity wave function of the system, which is taken to be a Slater determinant.

We assume for the radial dependence of the single nucleon wave functions the analytic form of a 3-dimensional harmonic oscillator wave function[11], namely:

$$R_{nl}(r) = N_{nl}(\nu) e^{-\frac{1}{2}\nu r^2} \quad r^{l+1} L^{l+1/2}_{n+l+1/2}(\nu r^2) \ ,$$

where the normalisation factor N_{nl} is given by:

$$N^2_{nl}(\nu) = \frac{2^{l-n+2}(2l + 2n + 1)!!\, \nu^{l+3/2}}{\pi^{1/2} n![(2l + 1)!!]^2}$$

and n,l are the radial and azimuthal quantum numbers respectively, L^{λ}_{μ} is the associated Laguerre polynomial and ν is the harmonic oscillator parameter: $\nu = m\omega/(h/2\pi)$.

The calculation of E_c may proceed in the following steps[11]:

1. We calculate the average energy of each «bond» in terms of Slater integrals, using statistical weights[5].
2. The energy E_c is subsequently expressed as a linear combination of Slater integrals.
3. The Slater integrals are expressed in terms of Talmi integrals[9,12].
4. The Talmi integrals are calculated analytically. The final result is a constant multiplied by $e^2\sqrt{\nu/2\pi}$.

Thus, in the case $E_c(Z = 8)$:

1) The average energies of the «bonds» in terms of Slater integrals are:

$$E(1s^2)_{AV} = F^0(0,0,0,0)$$

$$E(1p^2)_{AV} = \frac{1 \cdot \Delta E_{L=0} + 9 \cdot \Delta E_{L=1} + 5 \cdot \Delta E_{L=2}}{15} =$$

$$= F^0(0,1,0,1) + \frac{1}{15}\left(-\frac{6}{5}\right) F^2(0,1,0,1)$$

$$E(sp)_{AV} = \frac{3 \cdot \Delta E_{(singlet)} + 9 \cdot \Delta E_{(triplet)}}{12} =$$

$$= F^0(0,0,0,1) - \left(\frac{1}{12}\right) 2G^1(0,0,0,1)$$

2) The contribution of the 1s-s «bond» is:

$$S_c(s - s) = F^0(0,0,0,0)$$

of the 15 p—p «bonds» is:

$$S_c(p - p) = 15F^0(0,1,0,1) - \left(\frac{6}{5}\right) F^2(0,1,0,1)$$

and of the 12 s—p «bonds» is:

$$S_c(s - p) = 12F^0(0,0,0,1) - 2G^1(0,0,0,1)$$

The expression of the Coulomb energy is then:

$$E_c(Z = 8) = F^0(0,0,0,0) + 12F^0(0,0,0,1) - 2G^1(0,0,0,1) +$$
$$+ 15F^0(0,1,0,1) - \left(\frac{6}{5}\right)F^2(0,1,0,1)$$

3) We express now the Slater integrals in terms of Talmi integrals:

$$F^0(0,0,0,0) = I_0$$

$$F^0(0,1,0,1) = \frac{1}{12}[5(I_0 + I_2) + 2I_1]$$

$$F^2(0,1,0,1) = \frac{25}{12}[(I_0 + I_2) - 2I_1]$$

$$F^0(0,0,0,1) = \frac{1}{2}[I_0 + I_1]$$

$$G^1(0,0,0,1) = \frac{3}{2}[I_0 - I_1]$$

4) The Talmi integrals are given by:

$$I_l(\nu) = e^2 N_l^2(\nu/2) \int e^{-\frac{1}{2}\nu r^2} r^{2l+1} dr ,$$

that is: $I_0 = 2C$, $I_1 = \frac{4}{3}C$, $I_2 = \frac{16}{15}C$,

where: $C = e^2\sqrt{\nu/2\pi}$.

The result is: $E_c(Z=8) = \frac{83}{2} C = \frac{83}{2} e^2 \sqrt{\frac{\nu}{2\pi}}$ (ref. 1)

3. Calculation of E_c for ^{40}Ca

For the ^{40}Ca nucleus, the nucleons configurations are: $(1s^2)_N (1p^6)_N (1d^{10})_N (2s^2)_N (1s^2)_p (1p^6)_p (1d^{10})_p (2s^2)_p$. The Coulomb energy is given by:

$$E_c(^{40}Ca) = E_c(Z=20) = \sum_{i<j}^{\text{protons}} \int \Psi^* \frac{e^2}{r_{ij}} \Psi \, dq \ .$$

The calculation is made following the steps described previously.

1) The protons configurations: $(1s^2)_p (1p^6)_p (1d^{10})_p (2s^2)_p$ contain: 1 s-s «bond», 15 p-p «bonds», 45 d-d «bonds», 1 2s-2s «bonds», 12 1s-1p «bonds», 20 1s-1d «bonds», 4 1s-2s «bonds», 60 1p-1d «bonds», 12 1p-2s «bonds», 20 1d-2s «bonds».

We calculate, as an example the average energy of a d-d «bond». The multiplicity $2L + 1$ of the orbital wave-function ($L = 0,1,2,3,4$) is multiplied by 1 when L is even and by 3 when L is odd, yielding the statistical weights 1,9,5,21,9 respectively and the average energy is then:

$$E(1d^2)_{AV} = \frac{1\cdot\Delta E_{L=0} + 9\cdot\Delta E_{L=1} + 5\cdot\Delta E_{L=2} + 21\cdot\Delta E_{L=3} + 9\cdot\Delta E_{L=4}}{45}$$

Substituting the ΔE_L in terms of Slater integrals, as before, we obtain:

$$E(1d^2)_{AV} = F^0(0,2,0,2) + \frac{1}{45}\left(-\frac{70}{49}\right)F^2(0,2,0,2) +$$

$$+ \frac{1}{45}\left(-\frac{630}{441}\right)F^4(0,2,0,2)$$

The contribution of the $\binom{10}{2} = 45$ d-d «bonds» to the Coulomb energy

is then:

$$S_c(1d^{10}) = 45E(1d^2)_{AV} =$$

$$= 45F^0(0,2,0,2) - \frac{70}{49} F^2(0,2,0,2) - \frac{630}{441} F^4(0,2,0,2)$$

In a similar manner, we find the contributions from the other «bonds». Thus, we obtain:

$$S_c(1s^2) = F^0(0,0,0,0)$$

$$S_c(1p^6) = 15F^0(0,1,0,1) - \frac{6}{5} F^2(0,1,0,1)$$

$$S_c(1d^{10}) = 45F^0(0,2,0,2) - \frac{70}{49} F^2(0,2,0,2) - \frac{630}{441} F^4(0,2,0,2)$$

$$S_c(2s^2) = F^0(1,0,1,0)$$

$$S_c(1s^2 - 1p^6) = 12F^0(0,0,0,1) - 2G^1(0,0,0,1)$$

$$S_c(1s^2 - 1d^{10}) = 20F^0(0,0,0,2) - 2G^1(0,0,0,2)$$

$$S_c(1s^2 - 2s^2) = 4F^0(0,0,1,0)$$

$$S_c(1p^6 - 1d^{10}) = 60F^0(0,1,0,2) - 4G^1(0,1,0,2) - \frac{630}{245} G^3(0,1,0,2)$$

$$S_c(1p^6 - 2s^2) = 12F^0(1,0,0,1) - 2G^1(1,0,0,1)$$

$$S_c(1d^{10} - 2s^2) = 20F^0(1,0,0,2) - 2G^2(1,0,0,2)$$

2) The addition of the Sc's yields:

$$E_c(Z=20) = F^0(0,0,0,0) + 15F^0(0,1,0,1) - \frac{6}{5} F^2(0,1,0,1) +$$

$$+ 45F^0(0,2,0,2) - \frac{70}{49} F^2(0,2,0,2) - \frac{630}{441} F^4(0,2,0,2) + F^0(1,0,1,0) +$$

$$+ 12F^0(0,0,0,1) - 2G^1(0,0,0,1) + 20F^0(0,0,0,2) - 2G^2(0,0,0,2) +$$

$$+ 4F^0(1,0,0,0) + 60F^0(0,1,0,2) - 4G^1(0,1,0,2) - \frac{630}{245} G^3(0,1,0,2) +$$

$$+ 12F^0(1,0,0,1) - 2G^1(1,0,0,1) + 20F^0(1,0,0,2) - 2G^2(1,0,0,2) \ .$$

3) The Slater integrals are expressed in terms of Talmi integrals (following references 9 and 12).

4) The Talmi integrals are evaluated using the formula

$$\int_0^\infty x^m e^{-ax^2} dx = \frac{\Gamma[(m+1)/2]}{2a^{\frac{m+1}{2}}}$$

The first five integrals are:

$$I_0 = 2C, \ I_1 = \frac{4}{3} C, \ I_2 = \frac{16}{15} C \ ,$$

$$I_3 = \frac{32}{35} C, \ I_4 = \frac{256}{315} C$$

The final result is:

$$E_c(Z = 20) = \frac{7905}{32} e^2 \sqrt{\frac{\nu}{2\pi}}$$

in agreement with the result of calculations made by A. Dellafiore[2].

The model parameter ν should be determined by obtaining a best fit to the experimental data of electron scattering[4]. Using harmonic oscillator wave functions, one finds that the proton density distribution of ^{40}Ca is[7]:

$$\rho_{SM}(r) = \frac{1}{4} \left(\frac{\nu}{\pi} \right)^{3/2} \left[1 + \frac{4}{5} (\nu r^2)^2 \right] e^{-\nu r^2}$$

and $$\langle r^2 \rangle = \frac{3}{\nu}$$

Using the experimental value of $<r^2>_c^{1/2} = 3.49$ fm, we obtain:

$$\frac{3}{\nu} = (3.49)^2 \ , \ \frac{1}{\sqrt{\nu}} = 2.015 \text{ fm} \ , \ e^2\sqrt{\frac{\nu}{2\pi}} = 0.2851 \text{ MeV}.$$

Thus, the formula that we derived yields:

$$E_c(^{40}\text{Ca}) = E_c(Z = 20) = 70.43 \text{ MeV}$$

Note added in proof: If the finite proton size and the centre of mass motion are taken into account in determining ν,[7] then: $E_c(Z = 20) = 71.83$ MeV. It should also be noted that the values of the Coulomb energy of ^{40}Ca are close to the value of 71.74, which one obtains from the Coulomb term of the Myers and Swiatecki semiempirical mass formula[6], while the Fermi gas model[3] leads to a larger value (82.36 MeV).

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ΠΕΡΙΛΗΨΗ

ΥΠΟΛΟΓΙΣΜΟΣ ΤΗΣ ΕΝΕΡΓΕΙΑΣ COULOMB ΤΟΥ ΠΥΡΗΝΑ ΤΟΥ ^{40}Ca ΣΤΟ ΠΡΟΤΥΠΟ ΑΡΜΟΝΙΚΟΥ ΤΑΛΑΝΤΩΤΗ ΜΕ ΤΗΝ ΤΕΧΝΙΚΗ TALMI

ὑπὸ

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Πραγματοποιεῖται ἕνας ὑπολογισμὸς τῆς ἐνέργειας Coulomb τοῦ πυρήνα τοῦ ^{40}Ca μὲ τὸ πρότυπο φλοιῶν ἁρμονικοῦ ταλαντωτῆ καὶ τὴν τεχνικὴ Talmi. Τὸ ἀποτέλεσμα ποὺ παίρνουμε μὲ τὴ μέθοδο αὐτὴ συμφωνεῖ ἀκριβῶς μὲ τὸ ἀποτέλεσμα τοῦ A. Dellafiore, ὁ ὁποῖος χρησιμοποίησε μιὰ τεχνικὴ μὲ μετασχηματισμοὺς Fourier.