CM-P00057840

Archives

Ref TH. 925

SHELL MODEL ANALYSIS OF THE MAGNETIC HYPERFINE SPLITTING
IN MUONIC THALLIUM

R. Engfer

Institut für Technische Kernphysik, Darmstadt

and

F. Scheck

CERN - Geneva

A B S T R A C T

The magnetic hyperfine splitting of the ground and first excited state in muonic ^{203}Tl and ^{205}Tl is calculated on the basis of the shell model with configuration mixing. Fair agreement with the recently measured ground state splitting is found.

1. INTRODUCTION

As is well known, the magnetic hyperfine structure of the $1s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ states in muonic atoms, with heavy nuclei, is rather sensitive to the spatial distribution of the nuclear magnetization density ^{1),2)}. The magnetic hf splitting for the nuclear ground state of ^{209}Bi , for instance, which has been measured and discussed by several groups ³⁾⁻⁶⁾ shows a deviation of about 33% from its value for a point-like nucleus. Johnson and Sorensen ²⁾ have discussed these data on the basis of various models for the nuclear magnetization density. Although the splitting is about 5 keV, it has, so far, only been determined from a small broadening of the muonic K and L X-ray transitions.

In contrast to this case, the magnetic hf structure of muonic ^{203}Tl and ^{205}Tl has recently been measured directly from nuclear γ rays ⁷⁾. Due to the near degeneracy of the muonic $2p_{\frac{1}{2}} - 2p_{\frac{3}{2}}$ splitting and the excitation energy of the first $\frac{3}{2}^+$ state of thallium, the nucleus can be excited during the cascade of the muon ^{8),9)}. It then decays while the muon is still in its $1s_{\frac{1}{2}}$ orbit. Both the nuclear ground state and the $\frac{3}{2}^+$ excited state are split by the magnetic interaction with the $1s_{\frac{1}{2}}$ muon, and four nuclear γ lines should appear. However, due to a fast $M1$ transition from the $F=2$ to the $F=1$ sublevel of the excited doublet (F being the total angular momentum of the nucleus and the muon), only the nuclear transitions from the $F=1$ excited state to the $F=1$ and $F=0$ ground state sublevels are observed. From these well-resolved lines the magnetic hf splitting of the ground state was found to be $(2.66 \pm 0.30)\text{keV}$ in ^{203}Tl and $(2.32 \pm 0.06)\text{keV}$ in ^{205}Tl ⁷⁾.

2.

2. CALCULATION OF THE hf SPLITTING

Bohr and Weisskopf ¹⁰⁾ have given the general expression for the magnetic hyperfine splitting for $1s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ electrons, taking into account the finite size of the nuclear magnetization density. Stroke et al. ¹¹⁾ and Le Bellac ¹⁾ have generalized their calculations by including mixing of the pure shell model configurations due to residual interactions, following the method of Arima et al. ¹²⁾ for the calculation of magnetic moments of odd A nuclei.

For the muonic 1s state and for any nuclear state ϕ_n^{IM} with angular momentum I, the orbital and the spin part of the magnetic interaction energy are given by

$$W_{L,S}(n, F) = \frac{F(F+1) - I(I+1) - 3/4}{I} A_{L,S}(n) \quad (1)$$

with

$$A_L(n) = \frac{4}{3} e \mu_0 \langle \phi_n^{II} | \sum_{N=1}^A g_N^L \ell_0^{(N)} \left\{ \int_0^{R_N} \left(\frac{r}{R_N} \right)^3 f(r) g(r) dr + \int_{R_N}^{\infty} f(r) g(r) dr \right\} | \phi_n^{II} \rangle \quad (2)$$

$$A_S(n) = \frac{4}{3} e \mu_0 \langle \phi_n^{II} | \sum_{N=1}^A g_N^S \left\{ -\frac{\sqrt{2\pi}}{2} [\gamma_2 \otimes \sigma^{(N)}]_0^{(1)} \times \int_0^{R_N} \left(\frac{r}{R_N} \right)^3 f(r) g(r) dr + \frac{1}{2} \sigma_0^{(N)} \int_{R_N}^{\infty} f(r) g(r) dr \right\} | \phi_n^{II} \rangle \quad (3)$$

Here $g_p^\ell = 1$ for a proton, $g_n^\ell = 0$ for a neutron, $g_p^s = 5.58$ and $g_n^s = -3.82$, f and g are the radial functions of the muonic $1s$ state normalized according to

$$\int_0^\infty (f^2 + g^2) r^2 dr = 1$$

n numbers the nuclear states. In the configuration mixing model the nuclear state ϕ_n^{IM} is of the form

$$\begin{aligned} \phi_n^{IM} = & |j_1^{m_1}(0) j_2^{m_2}(0) j^1; I=j, M\rangle + \\ & + \sum_\nu \alpha_\nu^{(n)} |(j_1^{m_1+1}(j_1) j_2^{m_2-1}(j_2))(J_{12}) j^1; I=j, M\rangle \end{aligned} \quad (4)$$

with $\nu \equiv j_1, j_2, J_{12}$ and further quantum numbers of the particle-hole state. j denotes the angular momentum of the odd particle.

The coefficients α_ν , which characterize the admixture of a particle-hole excitation from the orbit j_2 to the orbit j_1 are calculated in first order perturbation theory, thus the terms in α_ν^2 have to be neglected. Denoting the magnetic energy of the unperturbed configuration by A^0 and the contribution of the ν th particle-hole admixture by A^ν , the magnetic hf energy of the nuclear state ϕ_n^{IM} is then given by

$$\begin{aligned} W_{L,S}(n, F) = & \frac{F(F+1) - I(I+1) - 3/4}{I} \left\{ A_{L,S}^0(n) + \right. \\ & \left. + 2 \sum_\nu \alpha_\nu^{(n)} A_{L,S}^\nu(n) \right\} \end{aligned} \quad (5)$$

3. DISCUSSION OF THE hf STRUCTURE

For the sake of illustration and in order to demonstrate the finite size effect, we first discuss the "Schmidt values" of the splittings for a point-like nucleus (fourth line of Table 2) and for finite size (fifth line), for both the $\frac{1}{2}^+$ and the $\frac{3}{2}^+$ states, i.e., the magnetic splittings obtained if these states are described by the pure shell model wave functions $3s_{\frac{1}{2}}$ and $2d_{\frac{3}{2}}$, respectively. The modification due to the finite size of the nucleus is considerable, in particular for the excited state where the near compensation of the spin part and of the orbital part of the nuclear magnetization density is much less pronounced than for a point (-like) nucleus. The corresponding Schmidt values for the magnetic moments are $\mu_{3s_{\frac{1}{2}}} = 2.79$ n.m. and $\mu_{2d_{\frac{3}{2}}} = 0.124$ n.m., in rough agreement with the experimental value 0.16 for the excited state but in strong disagreement with the experimental values 1.61 and 1.63 (cf. Table 2) for the ground state. Clearly, any nuclear model used in predicting the muonic hf splitting should reproduce, as a boundary condition, the observed magnetic moments. As a first estimate one may assume an effective g_p^s factor for the $3s_{\frac{1}{2}}$ hole chosen such as to obtain the correct value for the magnetic moment, i.e., $g_{\text{eff}}^s \approx 3.2$. The hf splitting $\Delta E_{s.p.}$ is then reduced from 4.56 to 2.64 keV. The detailed calculation shows that also in the presence of configuration mixing, the magnetic interaction in the ground state is still due almost entirely to the spin part of the nuclear magnetization. This last number $\Delta E_{s.p.}(g_{\text{eff}}^s \approx 3.2) = 2.64$ keV thus represents a lower limit of what can be expected from a realistic calculation.

The value found with configuration mixing, Eq. (5), (third line of Table 2) lies indeed somewhat higher than this limit. The same model yields the correct magnetic moment for the ground state but too large a value (0.39 n.m.) for the magnetic moment of the excited state. The magnetic hf splitting of the excited state is however rather insensitive

to the configuration mixing (cf. Table 2): from its Schmidt value 1.11 keV it is increased to 1.34 keV only. We expect the correct value to lie between these limits, probably closer to 1.11 keV. The rough magnitude of this splitting is needed for the calculation of the conversion coefficients for the M1 transition in the excited doublet. If the splitting is smaller than 800 eV (N_I binding energy) only 0 conversion is possible which would reduce the interdoublet M1 transition [~ 20 ps, Ref. ⁷⁾] by a factor 4 resulting in a not completely negligible contribution of the transitions from the $F=2$ excited sublevel.

As can be seen from Table 2, the experimental hf splitting of the ground state seems to be somewhat different in the two isotopes, whereas the magnetic moments are rather close to each other. Also the shell model calculation with configuration mixing gives nearly the same hf splitting for both isotopes ^{*)}.

This question clearly deserves further investigation, both theoretically and, in view of the relatively large experimental error on the hf splitting in ^{203}Tl , also experimentally. Furthermore, the theoretical value $\Delta E_{\text{conf.mix.}}$ is slightly too high by 0.2 to 0.5 keV. As discussed above it is very unlikely to find a value lower than 2.64 keV (Schmidt value with $g_{\text{eff.}}^s \approx 3.2$) from the configuration mixing model. Although the polarizability of the nucleus by the muon may well affect the distance of the ground state and the excited state doublets, it is certainly the same within each doublet and cannot explain this small remaining energy shift. Nevertheless, the agreement of the calculated hf splitting with the experimental value is fair. Furthermore, as turns out from the detailed calculation, the theoretical hf splitting is fairly independent of the precise choice of the residual interaction in the configuration mixing model, provided the model yields the correct magnetic moment.

^{*)} The program fills the neutron shells in the order $1i_{13/2}$, $3p_{3/2}$, $2f_{5/2}$, $3p_{1/2}$. The $1i_{13/2}$ and $3p_{3/2}$ shells are thus filled completely in both isotopes. Our results change a little if the $3p_{3/2}$ and the $2f_{5/2}$ levels are inverted. However, as long as the magnetic moments are nearly the same, no drastic changes can be expected.

4. COMMENTS ON THE ISOMER SHIFT IN THALLIUM

The experimental energies for ^{203}Tl ⁷⁾ result in an isomer shift of the centre of gravity of the two doublets of $\Delta E_{\text{isom.}} = -(0.3 \pm 0.5) \text{ keV}$. Although there might well be an important core contribution to the isomer shift [in the core excitation model ^{13), 14)}, for instance, the whole shift would come from the core], it is interesting to consider the isomer shift due to the odd particle. For harmonic oscillator wave functions it is zero; for the Saxon-Woods potential with the parameters of Ref. ¹⁸⁾, one finds a negative shift of -2.71 keV ^{*)}. However, this single particle contribution turns out to be very sensitive to the choice of the parameters for the shell model potential: a few percent variation of the parameters, chosen such as to keep the $3s_{\frac{1}{2}}$ and $2d_{\frac{5}{2}}$ single proton energies nearly unchanged, changes the isomer shift by about 20%, whereas the magnetic splittings change by less than 1%.

If it is possible to determine the core contribution to the isomer shift (e.g., by measuring the isomer shift in neighbouring even-even nuclei, in particular Hg), a more accurate experimental value in Tl will strongly restrict the possible choice of the parameters of the shell model potential, while still leaving the ground state hf splitting essentially unchanged.

The authors acknowledge fruitful discussions with Professors P. Brix, T. Ericson and E. Kankeleit. This work was supported by the Bundesministerium für wissenschaftliche Forschung.

*) Obviously, the admixed particle hole configurations do not contribute, to first order, to the isomer shift.

state		$1+\frac{1}{2}$			$\frac{3}{2}+$		
Configuration		A_L^i	A_S^i	α_γ	A_L^i	A_S^i	α_γ
odd particle state							
$(1h\ 11/2)^{-1}$	(1h 9/2) p excitation	0	1,14	-	0.87	-0.45	-
$(3p\ 3/2)^{-1}$	(3p 1/2) n excitation	-0.32	1,37	-0.055	-0.43	1.83	0.015
$(1i\ 13/2)^{-1}$	(1i 11/2) n excitation	0	-0.59	0.233	0	-0.80	-0.021
		0	-0.91	0.016	0	-1.22	-0.004

TABLE 1 :

Hyperfine constants $A_{L,S}^i$ in keV, as defined in Eqs. (1) and (5) for the unperturbed shell model states and the admixed configurations for the ground and first excited state of Tl (muon in $1s_{\frac{1}{2}}$ orbit), ($i=0$ or γ). The contributions in the last three lines still have to be multiplied by the coefficients α_γ as calculated according to the model of Arima et al.¹².

state	$\frac{1}{2}^+$		$\frac{3}{2}^+$	
	μ [n.m.]	Δ [keV]	μ [n.m.]	Δ [keV]
Experiment ^{203}Tl	1.61169 20)	2.66 ± 0.3 7)	0.16 20)	
^{205}Tl	1.62754 20)	2.32 ± 0.06 7)		
Configuration mixing	1.61	2.87	0.39	1.34
single particle <u>point</u> nucl.	2.79	8.05	0.124	0.24
single particle <u>extended</u> nucl.	2.79	4.56	0.124	1.11

TABLE 2 :

Muonic hf splitting ΔE in the Tl isotopes.

μ : magnetic moments. The calculated values are practically the same for both isotopes (see text).

$$g_p^s = 5.58, \quad g_n^s = -3.82, \quad g_p^l = 1, \quad g_n^l = 0.$$

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