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Hyperfine Structure of the 2^3P Level in He^3 †

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The hyperfine structure levels of the 2^3P state of He^3 (at zero magnetic field) are given by the eigenvalues of a matrix whose elements are expressed in terms of three integrals, which are calculated using Hylleraas-type wavefunctions.

Recent measurement[1] of the hfs of He^3 and of the g-factor of its nucleus[2] makes it possible to compare the results of calculations using accurate variational wave functions with experiment.

The hfs Hamiltonian is[3]

$$\mathcal{H}_{\text{hfs}} = -2\mu_0 \sum_{i=1}^{2} \left[-\frac{8\pi}{3} (\vec{s}_i \cdot \vec{\mu}) \delta(\vec{r}_i) - \frac{1}{r_i^3} \vec{l}_i \cdot \vec{\mu} + \frac{1}{r_i^3} \left(\vec{s}_i \cdot \vec{\mu} - 3 \frac{(\vec{s}_i \cdot \vec{r}_i)(\vec{\mu} \cdot \vec{r}_i)}{r_i^2} \right) \right], \tag{1}$$

where $\vec{\mu} = -g_I \mu_0 \vec{I}$ is the nuclear magnetic moment. In terms of spherical tensor operators, we may write

$$\mathcal{H}_{\text{hfs}} = T^{(1)}(I) \cdot \{ T^{(1)}(S) + T^{(1)}(L) + [T^{(1)}(S) T^{(2)}(L)]^{(1)} \}, \tag{2}$$

where S and L refer to the product spaces of the spins and the orbital angular momenta of the two electrons

We now give the matrix elements of $\mathcal{H}_{\text{hfs}}$ in the F-representation, where $\vec{F} = \vec{L} + \vec{S} + \vec{I}$ is the total angular momentum, using $\vec{J} = \vec{L} + \vec{S}$ as the intermediate angular momentum. $L = S = 1$, $I = \frac{1}{2}$. Using a well-known theorem[4] on spherical tensors we obtain

$$M(JJ'F) = \langle LS(J')I; F | \mathcal{H}_{\text{hfs}} | LS(J)I; F \rangle$$

$$= 3(-1)^{J' + F + \frac{3}{2}} \begin{Bmatrix} F & J' & \frac{1}{2} \\ 1 & \frac{1}{2} & J \end{Bmatrix} [(2J'+1)(2J+1)]^{1/2} \left[(-1)^{J'} \begin{Bmatrix} J & J' & 1 \\ 1 & 1 & 1 \end{Bmatrix} [C + (-1)^{J+J'} D] + 12 \begin{Bmatrix} 1 & 1 & 2 \\ 1 & 1 & 1 \\ J' & J & 1 \end{Bmatrix} E \right],$$

where C, D, and E are proportional to the reduced matrix elements of the three parts of the Hamiltonian (2), i.e., C is the contact term, D is the nuclear-spin-electron-orbit term, and E is the nuclear-spin-electron-spin term. We get

$$M(2, 2, \tfrac{5}{2}) = -\frac{2}{3} M(2, 2, \tfrac{3}{2}) = \frac{1}{2} (C + D + \tfrac{4}{5} E), \quad M(1, 2, \tfrac{3}{2}) = M(2. 1, \tfrac{3}{2}) = \frac{\sqrt{5}}{4} (-C + D + \tfrac{8}{5} E),$$

$$M(1, 1, \tfrac{3}{2}) = -\frac{1}{2} M(1, 1, \tfrac{1}{2}) = \frac{1}{4} (C + D - 4E), \quad M(0, 1, \tfrac{1}{2}) = M(1, 0, \tfrac{1}{2}) = \frac{1}{\sqrt{2}} (-C + D - 2E);$$

all other elements are zero.

Using the wave functions of Schwartz[5] for the "stretched" state, where $F = m_F = \frac{5}{2}$, we calculate C, D, and E by taking the expectation values of the three terms in (1). The wave function is

$$\psi = \alpha(I)\alpha(1)\alpha(2) \frac{1 - P_{12}}{4\pi\sqrt{2}} \frac{x_1 + iy_1}{-\sqrt{2}} \sum_{l,m,n=0}^{l+m+n \leqslant \omega} C_{lmn} r_1^{\,m} r_2^{\,n} r_{12}^{\,l} e^{-\kappa\sigma/2r_1} e^{-\kappa/2r_2}.$$

The results are given in Table I. The computations were done on a CDC 6400 computer in single precision, corresponding to about 14 decimals (48 bits). By iterating the procedure for finding ψ,[5] several slightly different wave functions and values of C, D, and E were obtained. From this it was concluded that about six decimals in the values of C and D and about four decimals in the values of E were free from round-off errors, for the three highest values of ω. The eigenvalues to which the wave functions correspond were accurate to ten decimals.

If one assumes that the 2^3P state can be described as a $1s2p$ configuration, then only the $2p$ orbital contributes to D and E, and one obtains[6]

$$\frac{D}{E} = -\frac{1}{4} \frac{\langle l_1 l_2; L \| r_2^{-3} \vec{l}_2 \| l_1 l_2; L \rangle \langle s_1 s_2; S \| 1 \| s_1 s_2; S \rangle}{-\sqrt{10} \langle l_1 l_2; L \| r_2^{-3} \vec{C}^{(2)}(2) \| l_1 l_2; L \rangle \langle s_1 s_2; S \| \vec{s}_2 \| s_1 s_2; S \rangle} = -\frac{1}{4},$$

TABLE I. C, D, and E in a.u.

ω	Number of terms in Ψ	$-C$	$-D$	E	$-D/E$
0	1	[illegible]	0.200 4189	0.050 105	4.000
1	4	20.806 09	0.136 2157	0.033 145	4.110
2	10	21.187 15	0.131 1251	0.032 934	3.981
3	20	21.080 99	0.134 7901	0.034 416	3.916
4	35	21.099 12	0.136 8811	0.034 876	3.925
5	56	21.090 52	0.137 8980	0.035 053	3.934
6	84	21.092 57	0.138 3408	0.035 138	3.937
7	120	21.092 05	0.138 5195	0.035 093	3.947
8	165	21.092 50	0.138 5934	0.035 071	3.957
Extrapolated		21.092 ± 0.001	0.1386 ± 0.0001	0.0351 ± 0.0001	3.95 ± 0.01

where $\vec{L}=\vec{l}_1+\vec{l}_2$, $\vec{S}=\vec{s}_1+\vec{s}_2$, $l_1=0$, $l_2=1$, $s_1=s_2=\frac{1}{2}$, and $\vec{C}^{(2)}$ is the angular momentum tensor of rank 2. The computed values of D/E are given in the last column of Table I. Johnson and Pichanick[1] assumed $D/E=-\frac{1}{4}$ in the analysis of their experimental data, thereby reducing the number of parameters to be fitted from three to two.

As ω increases C, D, and E do not behave smoothly enough to permit an accurate extrapolation to the limit when ω goes to infinity. We have merely guessed at the extrapolated results and their error limits. C has been calculated more accurately by Shiff *et al.*,[7] who obtain $C=21.092\,409\,6$ a.u. using a wave function with 560 terms, and the result $D=0.138\,636\,755$ a.u. was obtained by Schwartz[5] using a 439-term wave function. We believe the calculation E is new.

Using the results of Williams and Hughes[2] and values of other constants as quoted by Cohen and du Mond,[8] one gets a conversion factor from atomic units to Mc/sec of

$$\tfrac{1}{2}\alpha^2 R_\infty c\times 10^{-6}=202.9900 \text{ Mc/sec}.$$

We make a simple estimate of the relativistic, radiative, and finite nuclear size and mass corrections to C by multiplying it with the ratio of the accurately measured[9] hfs of the ground state of $(\mathrm{He}^3)^+$ to its calculated nonrelativistic value. The result is

$$C=-4283.8\pm 0.2)\text{Mc/sec}.$$

We multiply D by the reduced mass factor $r=M/(m+M)$, where M is the nuclear and m is the electronic mass. This gives

$$D=28.13\pm 0.02 \text{ Mc/sec}$$

Finally we multiply E by r^3 and by $1+\alpha/2\pi$, because of the electron's anomalous magnetic moment, which gives

$$E=7.13\pm 0.02 \text{ Mc/sec}.$$

The experimental results[1] are,

$$C=4282.72\pm 0.04 \text{ Mc/sec}, \quad\text{and}\quad D=-29.85\pm 0.14 \text{ Mc/sec}.$$

There are further corrections because of admixture with the ${}^1P_1$ and higher states, and because of corrections to the hfs Hamiltonian. These remain to be calculated.

Most of the tricks needed in the numerical work have been described by Schwartz.[5] When calculating E, use was made of the formula

$$\int\frac{d\Omega_1}{4\pi}\int\frac{d\Omega_2}{4\pi}(3\cos^2\theta_{12}-1)r_{12}{}^L=2\sum_{k=3,5,7,\ldots}^{k\leq L+4} r_>^{L+1-k}\, r_<^{k-1}\,\frac{(L+1)!(k-1)(k+1)(L-1+k)(L-3-k)}{(k+2)!\,(L+4-k)!},$$

where $r_>$ $(r_<)$ is the greater (smaller) of r_1 and r_2. The integrals

$$F_N(M)=\int_0^\infty dr\, r^{M-1}e^{-ar}\int_r^\infty ds\, e^{-bs}/s^N$$

for $N=1,2,3$, and 4 were required. The asymptotic expansion

$$F_1(M) = \sum_{k=0}^{n} \frac{k!(-1)^k}{b^{k+1}} \frac{(M-k-2)!}{(a+b)^{M-k-1}} + R_n, \quad \text{where } |R_n| < \frac{(n+1)!}{b^{n+2}} \frac{(M-n-3)!}{(a+b)^{M-n-2}}$$

was used for a fairly high value of M, together with a backwards recursion formula. The scheme can be checked by noticing that $F_1(1) = (1/a)\ln[(b+a)/b]$. Once $F_N(M)$ has been found for $N=1$, it is a simple matter to calculate the integrals for $N=2, 3$ and 4 by partial integration.

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Experimental Evidence for the Parratt X-Ray Excitation Theory*

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The intensity distribution of the Cr $K\alpha_1$ line in Cr metal and some of its (II) and (III) valence halides has been studied by means of a high-resolution x-ray spectrometer. It is found that while the $K\alpha_1$ line appears continuous in the metal, it splits up in the (II) and (III) valence compounds, the magnitude of splitting being 0.21 ± 0.03 eV and 0.29 ± 0.03 eV, respectively. The results obtained are interpreted by considering a new aspect about the formation of the energy levels. These levels could be taken as made up of ionization states split into sublevels owing to the exchange interaction between $2p$, $3d$ electrons and the excitation states. This provides evidence for the excitation states in solids as proposed by Parratt in his modified x-ray energy-level diagram.

INTRODUCTION

A new approach to the investigation of the x-ray excitation states in solids is presented. The fundamental excitation-level[1] aspects first used by Landshoff[2] and later by Cauchois and Mott[3] to explain the absorption edge structure have been incorporated into a more general theory by Parratt.[4] In his modified x-ray energy-level diagram Parratt proposes two types of excitation states. One type, the bound-ejected-electron excitation state (BEE), is characterized by the assumption that the ejected electron resides in one of the bound orbitals. The other type, the valence-electron-configuration excitation states (VEC), are those produced due to regrouping of valence electrons as a consequence of a change of wave functions of the electrons in the atom when an inner vacancy is created. In addition there are also present the states called ionization or unexcited states which refer to the limiting case when the ejected electron approaches infinity with zero kinetic energy.